

JEHT 112114 1

QUARTLY STATUS REPORT

REPORTING PERIOD: JUNE 27, 1997-SEPTEMBER 26, 1997

DARPA CONTRACT #: DABT63-97-C-008

CONTRACT TITLE: "ULTRA SENSITIVITY SENSORS HIGH EXPLOSIVES:  
NEW RECEPTORS AMPLIFICATION MECHANISMS,  
AND DEVICE CONCEPTS"

PI: TIMOTHY M. SWAGER

LOCATION: MIT, DEPT. OF CHEMISTRY, CAMBRIDGE, MA 02139

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OVERALL PROJECT OBJECTIVE:

This contract is directed at the development of ultra-sensitive detection schemes for TNT, RDX, and PETN. The principle technologies are based on conducting polymers. The collective transport properties of these materials are used to amplify binding events of analytes. This effort is comprehensive and involves the development and optimization of sensory polymers, specific receptors, and sensory devices.

ACCOMPLISHMENTS:

In the second quarter of Swager's contract significant expansions of synthesis of sensory materials has been made as well as critical key demonstrations of the detection of dinitrotoluene (DNT). An efficient procedure for the synthesis of triptycene scaffolds has been developed which allows for a diverse family of materials to be synthesized from common intermediates. These materials have shown themselves to be extremely durable, exhibiting reproducible fluorescence intensity in solid films after multiple solvent treatments and thermal cycling. Additionally these materials have been demonstrated to sequester (bind) DNT into cavities formed as a result of the rigid three-dimensional structure of the polymer. The response to DNT is rapid and fluorescence attenuations greater than 30% have been demonstrated in less than 10 seconds of exposure to vapors ( $10^{-4}$  mm) this chemical. The response to DNT was found to be dependent upon polymers the chemical structure with more electron rich polymeric structures creating higher responses. This later point suggests a presence of charge transfer interactions and additional efforts are underway to synthesize systems which should display yet stronger interactions with polynitro-aromatics. Amino functionalized cyclophanes have been synthesized. An efficient general procedure has been developed which can allow for the synthesis of peptide elaborated cyclophanes, as well as incorporation of additional functional groups to augment binding of nitro-organic compounds. The synthesis of a thiol containing rigid scaffold to create porous monolayers, which should bind nitro aromatics, has been developed. This later aspect will be explored in collaboration with Professor Steinfeld (MIT) to demonstrate the use of monolayers as pre-concentrating elements for SERS detection schemes for TNT. Photophysical studies of the aligned rigid-rod polymers reported in the last quarterly report have revealed the presence of highly efficient energy migration processes. The processes are fundamental to all amplification procedures under development and critical polarization measurements have revealed a wavelength dependence on the energy migration. Also designed in this last period was a field-effect transistor capable of being modified with polymeric coatings which are amenable to Langmuir-Blodgett or spin coating techniques. This last device will for the basis of a highly sensitive sensory device.

PLANS FOR THE NEXT 12 MONTHS:

**DTIC QUALITY INSPECTED 2**

During the next 12 months of this program Swager intends to conduct extensive photoconductivity experiments directed at the detection of TNT. The high degree of success in fluorescence quenching with DNT as mentioned above has prompted us to expand on this approach and design

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a variety of porous polymers which will exhibit greater charge transfer interactions with nitro aromatics. We are also designing materials which are conducive to the Langmuir-Blodgett techniques developed for the alignment of rigid-rod polymers. Collaborative studies will be conducted with Professor Steinfeld to determine the effectiveness of monolayers in SERS detection schemes. Solid phase peptide synthesis for the elaboration of amino substituted cyclophane receptors will begin. Field effect transistor devices utilizing polymers which are photochemically doped in the presence of TNT will be developed to create high sensitivity sensory devices.

EXPENDITURES (Total costs)

June 28, 1997-September 26, 1997

Salary support

3.5 Postdoctoral Associate/Fellow  
1.5 Research Assistants  
.50 Administrative  
100% summ. sal. PI

\$67,413

Materials and Supplies

Chemicals, software,  
instrumentation costs, glassware

\$45,332

Overhead @ 63.5%

\$71,593

Equipment

HPLC System and Detector  
(Electrochemical System)

\$56,755


HPLC Accessories

\$ 1,690

Total

\$184,338

\*Note: The listed expenditures were temporarily low as a result of pending invoices and the phase in of this contract.

 11/21/97

Timothy M. Swager

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18. Congressional Rep.: Joseph Kennedy  
Party: Democrate  
District: 8th
19. DARPA Line #:
20. ARPA Order #: HJ1500-7040-0254
21. Contract # DABT63-97-C-0008
22. Contract Title: "Ultra High Sensitivity Sensors or High  
Explosives: New Receptors Amplification  
Mechanisms, and Device Concepts"
23. Contract Start Date: 3/27/97
24. Contract End Date: 9/26/97
25. Contract Value: \$1,895,909
26. Most Recent  
Contract Increment: \$459,666
27. Date of Most  
Recent Contract Increment 3/27/97
28. Mod. No.: none

- 29. Total Contract Funds  
Received as of 5/31/97 \$459,666
- 30. Total Expenditures  
through 9/26/97 \$351,110 (This number is low due to initial phase in)
- 31. Total funds Remaining  
as of 9/26/97 \$108,555
- 32. Average Monthly Spending  
Rate as of 5/31/97 \$63,500 (This number is low due to initial phase in)
- 33. Your Estimate of When  
Current Contract Funds will  
be Expended (explain anticipated 9/26/99 major purchases) New equipment purchases  
as budgeted, added  
coworkers resulting in increased materials  
and supplies costs.
- 34. Estimated Funds Remaining  
as of 11/30/97: None
- 35. Funding Required to  
11/30/98: \$841,015