**CONFIDENTIAL**

**6/30/08**

# REPORT OF THE INVESTIGATION COMMITTEE ALLEGATIONS OF POSSIBLE MISCONDUCT IN RESEARCH

This Investigation Committee was formed upon recommendation of the prior Inquiry Committee according to NC State University's administrative regulation for responding to allegations of possible research misconduct (Appendix A) and was charged by the Research Integrity Officer to determine whether research misconduct had occurred. This Investigation Committee held its initial meeting in October, 2007 and met on numerous subsequent occasions to (i) review the allegations, responses from each Respondent and additional evidence related to the allegation and (ii) determine if any of the allegations brought forth by the Complainant or identified by the Committee during its course of investigation could rightfully be considered research misconduct.

Prior to this investigation, an Inquiry Committee composed of the three Committee members from NC State University recommended an investigation due to concern regarding potentially misleading claims made by the Respondents in their publications. Prior to the Inquiry Committee, the Research Integrity Officer concluded that the allegations not only fall under the purview of NC State University's administrative regulations, but, because National Science Foundation (NSF) funding is involved, the allegations also fall under the purview of the NSF regulations on research misconduct and are subject to oversight by the Office of Inspector General, representatives of which met with the Committee to discuss their charge and answer procedural questions on January 29, 2007.

This report and recommendation are prepared for transmittal to the Vice Chancellor for Research and Graduate Studies.

**Table of Committee Members:**

| Name | Rank | Degree | Discipline | Department | Conflict Free? | Competent in Field Represented in the Allegations |
|---|---|---|---|---|---|---|
| Dr. Rich Spontak | Professor | Ph.D. | Nanostructured soft materials and transmission electron microscopy | Chemical and Biomolecular Engineering | Yes | Yes |
| Dr. Nadia El-Masry | Professor | Ph.D. | Nanostructured inorganic materials and transmission electron | Materials Science and Engineering | Yes | Yes |

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|---|---|---|---|---|---|---|
| | | | microscopy | | | |
| Dr. Carol Hall | Camille Dreyfus Distinguished University Professor | Ph.D. | Thermodynamics, simulations and phase behavior of complex systems | Chemical and Biomolecular Engineering | Yes | Yes |
| Dr. Stephen Craig | Fuchsberg-Levine Family Associate Professor | Ph.D. | Structure, dynamics and function in self-assembled materials | Chemistry (Duke Univ.) | Yes | Yes |
| Dr. Thom LaBean | Associate Research Professor | Ph.D. | Molecular engineering, self-assembly, bionano-science & technology | Computer Science and Chemistry (Duke Univ.) | Yes | Yes |

**Identification of Respondents, Whistleblowers and Witnesses Referenced Herein:**

| **Name** | **Role** | **Relationship to other in this case** |
|---|---|---|
| Dr. Stefan Franzen | Complainant | Co-Investigator on several grants with Dr. Feldheim and a past collaborator with Dr. Eaton. |
| Dr. Dan Feldheim | Respondent | Co-Investigator on several grants with the Complainant, Graduate Committee co-advisor to Dr. Gugliotti and collaborator with Dr. Eaton. |
| Dr. Lina Gugliotti | Respondent | Graduate of the NC State University Chemistry Department under Drs. Eaton and Feldheim. |
| Dr. Bruce Eaton | Respondent | Former member of the NC State University Chemistry faculty and now a University of Colorado at Boulder faculty member. Major Advisor of Dr. Gugliotti. Collaborator of Drs. Feldheim and Franzen. |
| Dr. Marta Cerruti | Witness | Former PostDoc for Feldheim and Franzen at NC State University. Second author on Franzen's JACS paper entitled "The Role of Selection…" |
| Dr. Donovan Leonard | Witness | Graduate of the NC State University Materials Science and Engineering Department under the partial oversight of Dr. Franzen who worked with Dr. Gugliotti regarding the acquisition of data from electron microscopy and subsequent interpretation of the data. |
| Dr. Gerd Duscher | Witness | Co-advisor to Dr. Donovan Leonard and collaborator of Dr. Stefan Franzen. Instructor to Dr. Gugliotti on the subject of transmission electron microscopy in the NC State University Materials Science and Engineering Department. |

**The Allegations:**

The allegation is described in the Complainant's "Statement for the Investigating Committee" (Appendix B) that states in part:

> "(1) There is no evidence for RNA-mediated particle formation as claimed in Gugliotti et al., Science, v.304, pp. 850-852 (2004)
>
> (2) It is not possible to perform the reactions in aqueous solution as claimed in Gugliotti et al., Science, v.304, pp. 850-852 (2004)
>
> (3) Structural and chemical experimental data acquired by Gugliotti et al. were unable to prove the hexagonal particles (documented with sizes ranging from microns to nanometers) in the Science paper to be crystalline Pd metal nanoparticles as claimed in Gugliotti et al., Science v. 304, pp. 850-852 (2004)"

The Complainant's "Statement for the Investigating Committee" and accompanying materials identified the same or substantially similar concerns with regard to findings presented in the following scholarly documents:

> "RNA-Mediated Control of Metal Nanoparticle Shape", Lina A. Gugliotti, Daniel L. Feldheim, and Bruce E. Eaton, J. Am. Chem. Soc. v. 127, pp. 17814-17818 (2005)
>
> "RNA-Mediated Synthesis of Palladium Nanoparticles on Au Surfaces", Dage Liu, Lina A. Gugliotti, Tong Wu, Magda Dolsak, Alexander G. Tkachenko, Mathew K. Shipton, Bruce E. Eaton, and Daniel L. Feldheim, Langmuir v.22, pp. 5862-5866 (2006)
>
> "RNA-Mediated Metal-Metal Bond Formation in the Synthesis of Hexagonal Palladium Nanoparticles", Lina A. Gugliotti, Daniel L. Feldheim, Bruce E. Eaton, Science, v. 304, pp. 850-852 (2004)
>
> NSF Proposal 0414527 entitled "RNA Mediated Evolution of Nanomaterials", Bruce E. Eaton, Daniel L. Feldheim.
>
> NSF Proposal 0553951 entitled "Summer Program on the Structural Role of Metal Ions in Modified RNA Enzymes", Stefan Franzen, Bruce E. Eaton, and Daniel L. Feldheim
>
> W. M. Keck Foundation Proposal entitled "Synthesis and Assembly of Nanoscale Materials Using RNA-Mediated Evolutionary Chemistry", Daniel L. Feldheim, Bruce E. Eaton and Stefan Franzen
>
> Doctoral Dissertation entitled "RNA-Mediated Synthesis of Particles from Organometallic Palladium and Platinum Precursors (Under the direction of Professor Bruce E. Eaton)", Gugliotti, Lina Ann

**Key Evidence Reviewed**

*Materials provided by Dr. Franzen*

1. Dr. Franzen's "Statement for the Investigating Committee"
2. Relevant Journal Articles appearing in Science (2a), JACS (2b) and Langmuir (2c)
3. Dr. Franzen's letter to Drs. Feldheim and Eaton dated June 16, 2006
4. Dr. Franzen's document entitled "On the nature of hexagonal aggregates of $Pd_2(dba)_3$"
5. Powerpoint presentations provided from Dr. Franzen entitled "When were hexagonal particles observed in the samples prepared by Marta Cerruti in the past months," and "Concerning Hexagons of Gugliotti, et.al., Science, 304 (2004)"
6. Materials received from Dr. Franzen in support of allegations:
    i. Document entitled "Pd NPs prepared with and without RNA" received as physical copy on 11/15/2006
    ii. Document entitled "HRTEM/EELS Analysis: Formation of Pd Nanoparticles" received electronically as DATA1.pdf on 11/15/2006
    iii. Untitled document received electronically as DATA2A1-5.pdf on 11/17/2006
    iv. Untitled document received electronically as DATA3.pdf on 11/15/2006
    v. Untitled document received electronically as DATA4.pdf on 11/15/2006

*Materials provided by Dr. Feldheim and Dr. Gugliotti*

7. Data CD containing electron microscopy images from Dr. Gugliotti
8. Publishing decision and reviews of Dr. Franzen's submission to Science, "Comment on RNA Mediated Metal-Metal Bond Formation in the Synthesis of Hexagonal Palladium Nanoparticles"
9. Reserved

*College of Physical and Mathematical Sciences Internal Review Documents*

10. Internal Memorandum for the record: (as 11/03/06-AM) Prepared by R. E. Fornes
11. Dr. Franzen's Report given to Dr. Fornes on 10/10/06 entitled "RNA-Mediated Materials Synthesis in the Keck Center"
12. Dr. Franzen's Draft Paper to Science entitled "The Importance of Selection Pressure for RNA-mediated Evolutionary Materials Synthesis", Franzen, S., Leonard, D., Duscher, G.
13. Dr. Franzen's Keck Foundation Grant Resignation Letter to Drs. Feldheim and Eaton dated 10/07/2006
14. Dr. Franzen's letter to the Keck Foundation dated 10/10/2006
15. Drs. Feldheim's and Franzen's e-mail exchanges regarding Dr. Franzen's Resignation letter dated beginning 10/08/2006
16. Drs. Feldheim's and Franzen's e-mail exchanges regarding Data

*Respondents' Responses to the Allegations*

17. Dr. Feldheim's Undated Response to the Allegations
18. Dr. Eaton's Undated Response to the Allegations
19. Dr. Gugliotti's Undated Response to the Allegations
20. Dr. Feldheim's supplemental response, received 12/13/06

*Grants and Contract Proposals and Dr. Gugliotti's Dissertation*

21. NSF Grant "RNA Mediated Evolution of Nanomaterials", Eaton, B.E., Feldheim, D.L.
22. NSF Grant "International: Summer Program on the Structural Role of Metal Ions in Modified RNA Enzymes", Franzen, S., Eaton, B.E., Feldheim, D.L.
23. Draft Final Technical Report related to the NSF grant entitled "International: Summer Program on the Structural Role of Metal Ions in Modified RNA Enzymes"
24. DOE Grant "Hydrogen Fuel Cell Catalyst Discovery Using RNA-Mediated Materials Synthesis", Feldheim, D. L., Eaton, B.E.
25. Keck Grant "Synthesis and Assembly of Nanoscale Materials Using RNA0Mediated Evolutionary Chemistry", Feldheim, D.L., Eaton, B.E, Franzen, S.
26. Lina Gugliotti's Dissertation

*Supplemental Timeline Information*

27. Timeline of Events from Dr. Franzen
28. Timeline of Events from Dr. Feldheim
29. Dr. Gugliotti Response to Dr. Franzen's Timeline of Events and Dr. Franzen's Presentation Materials presented to the Inquiry Committee
30. Document from Dr. Feldheim entitled "Response to Dr. Franzen's Timeline and Presentation to the Inquiry Panel."

*Interview Presentation Materials*

31. Dr. Franzen's Interview Presentation Materials
32. Dr. Feldheim's Interview Presentation Materials
33. Data CD provided by Dr. Leonard at his Inquiry Interview (including manuscripts that have been recently submitted by Dr. Franzen et al. and other materials).

*Supplemental Information from Dr. Feldheim and Dr. Gugliotti*

34. Electron Diffraction Pattern captured on Film and Analysis Report received from Mr. Keadey on 11/16/2006
35. Supplemental Information including Diffraction Pattern received from Dr. Feldheim on 02/12/2007
36. Original films from Dr. Gugliotti received from Mr. Keadey

*Supplemental Information from Dr. Eaton*

37. Reserved
38. Draft of "Scanning Probe-based Fabrication of 3D Nanostructures via Affinity Templates, Functional RNA, and Meniscus-mediated Surface Remodeling." Chung, S.W., Presley, A.D., Elhadj, S., Hok, S., Hah, S.S., Chernov, A.A., Francis M.B., Eaton B.E., Feldheim D.L., Deyoreo J.J. Scanning, 2008, 30, pp.159-171

*Information presented by Member of the Investigating Committee*

39. The research group of a member of the Investigation Committee was able to successfully, albeit informally reproduce the $Pd_2(DBA)_3$ solution in 5% THF/water by using fresh organometallic complex, THF solvent opened inside an oxygen-free, water-free glovebox, and adding freshly prepared THF-solvate of $Pd_2(DBA)_3$ to water.

*Lab Notebooks and other materials*

40. Lina Gugliotti's lab notebooks
41. Carly Carter's lab notebooks
42. Donovan Leonard's lab notebooks
43. Dage Liu's lab notebooks
44. Marta Cerruti's lab notebooks
45. Flash drive from Donovan Leonard containing image files
46. Powerpoint Presentation from Dr. Leonard's Ph.D. Defense entitled "Bio-Related Noble Metal Nanoparticle Structure Property Relationships dated 02/12/2007.
47. Copy provided by Dr. Franzen of "The Role of Selection Pressure in RNA-Mediated Evolutionary Materials Synthesis," Franzen, S., Cerruti, M., Leonard, D., Duscher, G., JACS 2007 129, 15340-15346
48. Written statements from TEM center personnel
49. Written testimony dated January 22, 2008 from Dr. Feldheim in lieu of interview
50. Email from Dr. DeYoreo to Dr. Franzen, dated May 2, 2008

**Deliberations and Interviews:**

The Committee met and received its charge from the NC State University Research Integrity Officer in October, 2007. The Committee developed a schedule of interviews. The Committee interviewed Drs. Franzen, Leonard, Cerruti and Duscher on campus. Drs. Eaton and Gugliotti were interviewed by teleconference. Ms. Carly Carter, a graduate student working for Dr. Feldheim both at NC State University and now at the University of Colorado (who apparently observed and/or was involved in the execution of relevant experiments), was asked to participate in an interview but declined. Dr. Feldheim was asked to participate in an interview but also declined. Dr. Feldheim, however, agreed to and did answer written questions via e-mail. The interviews consisted of targeted questions developed by the Committee to obtain specific details with regard to existing evidence. The Committee also explored whether or not accepted research practices were followed in the Respondents' laboratories. The Committee also contacted Mr. Alex Kvit, formerly of NC State University during Dr. Gugliotti's tenure at the University, and Dr. Mark Walters of Duke University because they had interacted with Dr. Gugliotti when she collected data using instrumentation (specifically, transmission electron microscopes) they maintained at their respective institutions.

The Committee reviewed the evidence that had been collected by the Research Integrity Officer and provided to the Committee; reviewed relevant journal articles; received testimony from the Complainant, the Respondents, and certain witnesses involved in collaboration with the principal individuals involved in this investigation. The Committee's deliberations and findings are described below.

***Allegation #1: There is no evidence for RNA-mediated particle formation as claimed in Gugliotti et al., Science, v.304, pp. 850-852 (2004)***

The Committee interpreted this allegation to question the role of RNA in particle formation. Therefore, the allegation is that the Respondents falsified their claim that RNA "mediates" particle formation. In evaluating this allegation, the Committee found that the following evidence supported the claims made by the Respondents that RNA mediated particle formation:

1. The RNA pool evolves in the presence of $Pd_2(DBA)_3$ (Science paper; JACS paper; evidence item # 26). In order for the $Pd_2(DBA)_3$ to influence the evolution of the RNA pool, it must interact with the RNA. Therefore, it is reasonable to conclude that there are interactions between some RNA sequences and $Pd_2(DBA)_3$. Unless the RNA sequences interact with all stages of the growing particles to exactly the same extent, they must at least somewhat mediate particle formation.
2. Different distributions of particle shapes are observed with different RNA sequences. Qualitatively, there is a difference between particles observed with different RNA sequences. This indicates that RNA in some way influences particle formation (e.g., particle size and/or geometry).
3. Similar, well-defined particles are not observed to the same extent in the absence of RNA (evidence item , Ntbk 8 p74 TEM Pd017-1 PD017-2 February 2005.pdf), although these experiments were performed after publication in the Science paper.
4. While Dr. Franzen is able to generate particles in the absence of RNA, those particles are not identical to at least some of the particles created by the Respondents because Dr. Franzen's particles are much thicker (evidence item #26, Figure 1.5; Leonard interview, May 29, 2007, p. 32, line 23 et seq.) This is evidence that the presence of RNA affects the size and thickness of the particles, although the Committee notes that Dr. Franzen's results had not been obtained at the time the original work was published, and that there are concerns regarding the relevance of his experiments due to solubility issues (see "Allegation #2" et seq.).

The Committee also recognized that some evidence does not support Drs. Eaton's, Feldheim's and Gugliotti's claims:

1. Particles precipitate without RNA for the Complainant (Evidence item #31 and #47), although the Committee notes that the Complainant's results had not been obtained at the time the original work was published, and that there are concerns regarding the relevance of his experiments (see "Allegation #2" et seq.).
2. Dr. Feldheim cites numerous controls and categorically states that they never see hexagons (evidence item #32 where Dr. Feldheim states, "Note from the timeline provided, that Ms. Carly Carter prepared solutions at least 19 times in the past 2 years … Every time she incubated a solution of $[Pt_2(DBA)_3]$ with RNA, she was asked to do a "No RNA control" for analysis by TEM. No hexagons or cubes were observed in the No RNA controls. No material with any well-defined shapes were observed in the

no-RNA controls".) However, many of the control experiments cited by Dr. Feldheim do show regular hexagons. For example, the laboratory notebooks of Ms. Carly Carter (evidence item #41, notebook 3A, page 73 – 74 plus inserts immediately following). The Committee also notes that, despite Dr. Feldheim's assertion that "for the purposes of this experiment, Pd and Pt are essentially interchangeable" (evidence item #17, Page 7), $Pt_2(DBA)_3$ is not a suitable control for experiments that involve $Pd_2(DBA)_3$. They also took place well after the work in question was published. These experiments, therefore, have limited relevance to the scientific claims in question, and the Committee considers them only insofar as they bear on Dr. Feldheim's assessment and interpretation of experimental data.

3. While the Respondents cite control experiments using poly(vinylpyridine) (PVP) instead of RNA, the value of these control experiments is not clear for two reasons. First, they occur under slightly different solvent conditions with respect to the RNA experiments (Gugliotti interview, June 5, 2007, p. 73, lines 5-16), and Dr. Feldheim notes that "synthetic conditions…may play a role in determining the observed structure" (evidence item #49). The Committee notes that the quantities of methylene chloride employed appear to have been very small, and the realization that small deviations in synthetic conditions might have a non-negligible effect on particle formation came well after the original work was published. Second, PVP has a limited solubility in water, and the Respondents appear to have not characterized whether or not the PVP is actually soluble under the conditions they employ (Eaton interview, December 21, 2007, p. 56, line 24 et seq.; evidence item #49).

The Committee also considered the Complainant's assertion that because particles form from a simple mixture of THF and $Pd_2(DBA)_3$, the Respondents' claim that RNA mediates particle formation is false. The Committee affirms the Respondents' observation that just because conditions can be found under which $Pd_2(DBA)_3$ in a THF and water solution will produce particles in the absence of RNA, this in no way disproves RNA-mediation of particle formation under other conditions. In fact, the Complainant himself points out that the two outcomes are not necessarily mutually exclusive (Franzen interview, November 19, 2007, p. 59, lines 8 - 13).

Nevertheless, it is clear that particle formation is more complicated than the Respondents realized at the time that the papers in question were published (evidence item #49, "The specific Pd structure may be either face-centered cubic (fcc) Pd, oxygen-doped Pd, or PdO, although I believe now further investigation to the structure is warranted as synthetic conditions, sequence, analysis method may play a role in determining the observed structure. These investigations are the subject of ongoing work.") This raises concerns as to whether or not the particle formation observed in the presence of RNA could be due in no small part to factors other than the presence of RNA. Dr. Feldheim apparently shares these concerns. These concerns, however, are a matter of scientific conclusion and not research misconduct. The Committee notes that the scientific debate

is properly conducted through the normal channels of laboratory research and peer-reviewed publications. Without taking a position on the claim in question, the Committee finds that evidence to support such a conclusion was certainly present at the time the papers in question were written, and that the evidence considered by the Respondents was faithfully reported in their publications. Indeed, the Complainant testifies that his group has concluded that RNA is capable of acting as a surfactant and altering the solubility and thus the crystallization or aggregation behavior of whatever solutes are present (Franzen interview, November 19, 2007, p. 69 - 71). The Committee recognizes this interaction between RNA and other chemical species to be a form of mediation.

Regarding the potential problems with Dr. Gugliotti's PVP control experiments, the Committee finds that even though those experiments may be flawed by the limited solubility of PVP, the presence of methylene chloride in the control experiment when none is present in the actual RNA experiment, and/or the limited miscibility of methylene chloride, the failure of the Respondents to carefully consider these factors is relevant only to criticisms of their scientific methods. The potential flaws in experimental design are not germane to misconduct regarding the allegation in question.

Based on a preponderance of the evidence, the Committee finds that enough evidence existed at the time of the Science paper to support the claim that RNA mediates particle formation, and that this evidence was reported faithfully in the 2004 Science publication. As with all scientific conclusions, it is subject to revision in light of subsequent data and discoveries, but even if the conclusion of RNA mediation should be overturned, there is no evidence that, at the time the Science paper was published, the Respondents intentionally withheld and/or failed to consider existing evidence that contradicted their claim. Therefore, this claim is not representative of a falsification or fabrication.

***Allegation #2: It is not possible to perform the reactions in aqueous solution as claimed in Gugliotti et al., Science, v.304, pp. 850-852 (2004)***

The allegations regarding the Respondents' solutions were determined to be unfounded by the Inquiry Committee but were reconsidered by the Investigation Committee in light of the added technical expertise of the Investigation Committee and additional evidence. The Committee considered the following information in addition to information discussed in the inquiry report:

1) Prior to the allegations, the research group of a member of the Investigation Committee (evidence item #39) was able to successfully reproduce the $Pd_2(DBA)_3$ solution in 5% THF/water by combining fresh organometallic complex with THF solvent from a container opened inside an oxygen-free, water-free glovebox, and then adding the freshly prepared THF-solution of $Pd_2(DBA)_3$ to water. This supports the Respondents' contention that the ease with which these solutions can be prepared varies significantly with respect to who is doing the experiment and the specific way in which the chemicals are prepared and handled.

2) The Respondents provided a digital image of what they claim is a solution of $Pd_2(DBA)_3$ in a 10% THF/water co-solvent that has stood for more than two hours without showing signs of precipitation. The image is consistent with the recollection of the committee member regarding his experience with the solutions. This is in stark contrast to the Complainant's published statement that "Turbid suspensions and precipitates were observed to form rapidly in any solution with a volume percentage of less than 50% THF." (evidence item #47).
3) Testimony from the Complainant that the research group of Dr. Nocera at MIT "stand by what was written in the [Complainant's] JACS paper." (Franzen interview, November 19, 2007, p. 74, lines 13-24)
4) Dr. Eaton's testimony that the Complainant "didn't ever contact me by e-mail, by phone, or in any other way to let me know that he was having difficulty with these experiments." (Eaton interview, December 21, 2007, p. 6, lines 3-6)
5) Dr. De Yoreo's email to the Complainant stating that his lab was eventually able to make stable solutions of $Pd_2(DBA)_3$ in THF/water solvents with THF content below 20% (evidence item #50) This too is in contrast to the Complainant's published statement that "Turbid suspensions and precipitates were observed to form rapidly in any solution with a volume percentage of less than 50% THF" (evidence item #47) and further supports the Respondents' contention that the ease with which these solutions can be prepared varies significantly with respect to who is doing the experiment and the specific way in which the chemicals are prepared and handled.

The phrase "aqueous solution" as it originally appeared in the 2004 Science paper is typically used in the field to describe a solution in which water is the solvent. The authors used the term to describe a solution that they purport to actually be 95% water and 5% THF. Such mixed aqueous/organic solvents are common in chemistry, but they are not typically referred to as "aqueous" without further clarification as to the presence and quantity of the co-solvent. In the context of the Science paper, the term "aqueous" was used inappropriately to describe this solvent mixture, but while its use was a falsification, the Committee finds that it was not intentional or knowing. In reaching this conclusion, the Committee notes that similar solvent mixtures have been used in many biochemistry labs (Biochemistry, **1980**, *19*, 3080-3087; PNAS **1995**, *92*, 1262-1266; J. Histochem. & Cytochem. **2003**, *51*, 797-808), including by the Eaton lab (Nature **1997**, *389*, 54-57) in previous work, so that there was no reason to hide the use of mixed solvents in this work. In addition, the Respondents acknowledged the error and provided a correction to the scientific record, entirely of their own accord, in their next paper (Evidence item #2 - JACS **2005**). While there remains an inconsistency between the Respondent and Complainant in terms of the solubility of $Pd_2(DBA)_3$ in aqueous solutions containing various concentrations of THF, the Committee feels that this is a matter of scientific dispute to be settled in the literature by continued research and accurate reporting of such research. Thus, the Investigation Committee reaffirms the finding of the Inquiry Committee that the Respondents are not guilty of misconduct with regard to this allegation.

***Allegation #3: Structural and chemical experimental data acquired by Gugliotti et al. were unable to prove the hexagonal particles (documented with sizes ranging from microns to nanometers) in the Science paper to be crystalline Pd metal nanoparticles as claimed in Gugliotti et al., Science v. 304, pp. 850-852 (2004)***

The allegation, as worded, criticizes a statement in the Respondents' 2004 Science paper, "A combination of scanning electron microscopy and electron diffraction showed that the hexagonal particles were crystalline Pd" (p. 851 of the Science paper). The statement refers to two independent experiments upon which the Respondents base their conclusion of metal-metal bond formation and crystalline Pd: EDS (Energy Dispersive Spectroscopy) and SAED (Selective-Area Electron Diffraction). The Respondents independently take the EDS data as confirmation that the particles were composed of Pd and the SAED data to indicate that the particles were crystalline (evidence item #17, p. 8). The problem with this statement is that it misleads a knowledgeable reader into believing that the authors had more data than they actually did at the time of publication. Accepted, standard practice in material science characterization would invoke this statement in circumstances in which the diffraction pattern was appropriately indexed and was quantitatively matched to the known lattice spacing for Pd metal. The Respondents' SAED data was not indexed at the time of the Science paper (Gugliotti interview, June 5, 2007, p. 107, line 6-13), therefore, the statement in question is a falsification as defined by National Science Foundation regulation §689.1(a)(2), "…changing or omitting data or results such that the research is not accurately represented in the research record."

The Committee notes that whether or not the particles actually are/were Pd is not determinative to the misconduct investigation. Conclusions can be wrong in the absence of misconduct, and it is possible for misconduct to occur in support of conclusions that ultimately turn out to be correct, by failure to accurately present the factual basis or lack thereof for conclusions reported in the scientific literature. Scientific interpretation is always subjective, and that subjectivity strengthens the field, but the faithful reporting of scientific data, observations, and procedures is the real foundation of the discipline, and that foundation is reflected in the NSF standard for appropriate scientific conduct. It is incumbent upon the Respondents to accurately and unambiguously present the factual basis (or lack thereof) for their conclusions.

In determining whether or not the Respondents' mischaracterization meets the definition of "falsification," the Committee considered the following information:

1. $Pd_2(DBA)_3$ is a known precursor of Pd. It is not uncommon in handling this compound under reactive conditions for Pd to form. The Committee understands that the Respondents chose $Pd_2(DBA)_3$ for this reason.
2. The EDS data show the presence of elemental Pd, but one cannot discern the form of Pd present from these data alone.
3. The EDS data, in particular the 1:1 Pd:O atomic ratio, are not consistent with $Pd_2(DBA)_3$, which has a Pd:O ratio of 2:3. These data, however, are consistent with other Pd-containing particles, for example, PdO or partially decomposed $Pd_2(DBA)_3$. There could, in fact, be metallic Pd in the particle, but the evidence

available at the time of publication is not conclusive, as implied by the statement in question.

4. A diffraction pattern was obtained prior to the Science paper and that pattern does indicate a crystalline structure (evidence item #32, p. 8).
5. The Committee did not have access to the specific details of the microscope conditions under which the diffraction pattern that is referenced in the Science paper was obtained. However, the Committee was able to analyze the details of other diffraction experiments carried out by the Respondents on similar samples, with similar objectives. The Committee finds that, in at least some of these cases, diffraction patterns were obtained under conditions where electron beam damage to the particles could easily have occurred resulting in the alteration of the materials being analyzed (e.g., session at Duke, from evidence item #7, Ntbk 12 p86 ED Pd034 May 2006.pdf, Sample pd034 DP#1 - DP #13). Sequential data files collected during the Duke TEM session and provided to the Committee by Dr. Gugliotti showed the following:
   i. At the beginning of the session, diffraction patterns (i.e. # 1 – 6 taken between 1:44PM and 2:07PM) indicate that the sample was amorphous. Dr. Gugliotti indicated in her first interview that her SAED patterns were typically taken from several hexagons on the sample (Gugliotti interview, June 5, 2007, p. 124).
   ii. After 23 minutes into the session; the diffraction patterns (taken from 2:12PM to 2:19PM) started to show some spots, indicating the formation and evolution of crystalline regions in the sample during image collection.
   iii. After 39 minutes on the microscope, from 2:23PM to 2:25PM, clear spotty rings form after the sample was exposed to the electron beam.

   Microscopy experts on the Committee conclude that the evolution of SAED patterns as the session proceeds is an unequivocal indication of electron beam damage that causes the hexagons in the sample to crystallize under the electron beam. Dr. Gugliotti indicated in her PhD thesis (on page 52) that the samples undergo gross (i.e., visible) beam damage and a 200kV electron beam is capable of burning holes in the samples. The Committee recognizes, however, that this awareness came after the Science, JACS, and Langmuir papers were published. The same electron beam could have caused atomic migration within the hexagons, thus resulting in formation of nanoscale crystalline domains within predominantly non-crystalline (amorphous) particles. This calls into question the origin of the crystallinity referenced in item number 4 above.
6. The Committee recognized other deficiencies in the practices applied by the Respondents when they attempted to characterize their particles by SAED, as evidenced by a series of SAED data (evidence item #17, figure S4; evidence items 34, 35, 36). These electron diffraction experiments were conducted by the Respondents after the papers in question were published, and the Committee considered them only in the context of judging the validity of the procedures that the Respondents employed, and whether those procedures were consistent with the claim made in the Science paper. The SAED patterns supplied by the Respondents reveal a mixture of different types of crystals. Some of the single-crystal patterns include extremely well defined spots that an expert recognizes

cannot be representative of nano-crystals as claimed by the Respondents. It is, however, possible to generate such diffraction patterns from the underlying copper grid. Without lattice imaging and/or proper indexing, the possibility that the diffraction pattern originates from the copper grid rather than from the hexagonal particles cannot be excluded. In the majority of cases, the supplied SAED data are not supported either by proper indexing using a standard or by a high-resolution lattice image of the particle. Without these additional data, the diffraction patterns cannot be conclusively attributed to the particle(s) in question and one cannot determine whether or not the diffraction patterns correspond to crystalline Pd. See JACS **2005**, *127*, 17118-17127 for a representative example of accepted materials characterization practices.

Based on a preponderance of the evidence, the Committee finds that the statement, "A combination of scanning electron microscopy and electron diffraction showed that the hexagonal particles were crystalline Pd" in the Respondents' Science (2004) paper is false. The statement is false not because we know that the particles are not crystalline Pd (they might be), but because the data in hand at the time did not "show that the particles are crystalline Pd" as claimed. This strong assertion of crystalline Pd distorts the research record.

However, in order to make a finding of research misconduct under the National Science Foundation regulations, the Committee must also find the falsification to be: 1) "a significant departure from accepted practices of the relevant research community" and 2) "…committed intentionally, or knowingly, or recklessly."

In determining if the actions of the Respondents were a significant departure from accepted practices of the relevant research community, the Committee recognized that the Respondents are not members of a research community in which EDS (Energy Dispersive x-ray Spectra) and SAED (Selective -Area Electron Diffraction) data are routinely used. Nonetheless, by using these techniques and working on this problem, the Respondents assume responsibility for proper practices and should have secured adequate advice from an outside expert. Specifically, the Committee considered the following:

1. A reasonable, knowledgeable reader would believe from the Science paper that the diffraction data collected by the Respondents had been properly indexed. Scientifically it is not the practice to conclude from the diffraction pattern that it is an X- or Y-crystal without a standard, a picture of an image from where the SAED pattern was taken, and proper indexing of the lattice spacing. The sample was on a Cu grid, which also possesses an fcc lattice and would have the exact look and indexing as Pd; proper quantitative indexing is necessary to distinguish whether the pattern is a consequence of the support grid and not the particles.
2. Consideration #1, above, is further supported by Dr. Leonard's reaction upon seeing the diffraction data for the first time (Leonard interview, May 29, 2007, p. 44, line 16, et seq.):

"…my jaw hit the floor at this point. These were unindexed diffraction data which you don't know anything from the negatives unless you do some indexing, unless you know what the camera length is, you know what the accelerating voltage is. There are just certain protocols, as a microscopist that … you have to follow to get some good data out of all this."

3. A reasonable, knowledgeable reader would believe from the Science paper that the elemental composition of the particles, as obtained from EDS, would show at least a strong majority presence of Pd relative to other elements. In fact, an atomic Pd:O ratio of 1:1 is observed (evidence item #26, figure 1.4, p. 13), and there is a very large carbon signal that cannot be attributed exclusively to either the carbon-coated copper grid or the particles.
4. A reasonable, knowledgeable reader would believe from the Science paper that the data were obtained under conditions that do not suggest the possibility of electron beam damage to the original sample.
5. The Respondents invoke a "chemical logic" (e.g. Eaton interview, December 21, 2007, p. 15, line 22) rationalization of their conclusion. This "chemical logic" refers to the expectation that pyridine would displace dba, thereby leaving behind Pd metal.

The Committee finds that the Respondents' errors in interpreting and reporting the TEM data represent a significant deviation from accepted practices of the relevant research community. The EDS and SAED results do not justify the conclusion of crystalline Pd as stated by the Respondents in the Science and JACS papers. Other compounds, for example $Pd_2(DBA)_3$ and PdO, could show the presence of Pd and apparent crystalline order without possessing metal-metal bonds. In fact, as cited in #3, above, in Dr. Gugliotti's dissertation figure 1.4, page 13, the EDS data show a strong oxygen ($K_\alpha$-line) peak that is ~1.5 times more intense than the Pd $L_\alpha$-line. A member of the Committee determined that the relative intensities of these peaks (evidence item #26, fig 1.4, p. 13) suggest an atomic Pd:O ratio very close to 1:1. This indicates that Pd may be partially in the form of an oxide.

The same member determined that SAED data used in support of the claim in the Science paper includes one reflection that can be indexed as (111) PdO (with the cubic NaCl crystal structure, fcc with a lattice constant of 0.565 nm, space group Fm3m). Therefore, the data are insufficient to support the conclusion that the particles are crystalline Pd.

The particles observed by the Respondents and disclosed in their publications resemble Pd nanoparticles synthesized by other means (JACS **2005**, *127*, 17118-17127), although morphological resemblances are not conclusive. Further, the Committee acknowledges that the "chemical logic" argument invoked by the Respondents (e.g. Eaton interview, December 21, 2007, p. 19, line 2, et seq.), namely that the nucleophilic amines are likely to displace the weakly coordinated DBA ligands, supports the hypothesis that the particles are Pd (the effect would be similar to that recently reported in Langmuir **2008**,

*24(5)*, 2090-2101). In his testimony, Dr. Eaton also cited two publications that made similar claims of Pd nanoparticles based on chemical reasoning (Organic Letters **2007,** *9*, 2409; Organometallics **2007**, *26*, 3306; Eaton interview, December 21, 2007, p. 49). The Committee notes that these papers actually reinforce the contention that the Respondents did not meet expected scientific standards for reporting their results in their 2004 Science paper. For example, the authors of the Organic Letters **2007** paper provide their own, independent characterization by EDS, even though they are repeating the synthesis of Pd particles that have been characterized previously (J. Org. Chem. **2006**, *71*, 4339). The EDS data are made available to the community, and importantly they do not show the large oxygen peak that is present in the data that supports the statement made by the Respondents in the Science paper. The Organometallics **2007** paper uses a combination of cyclic voltammetry and the subsequent catalytic activity (PdO is not expected to be catalytically active) of the nanoparticles to establish their chemical composition. Even though these papers cite chemical reasoning, they use several characterization methods to support their claims. Most importantly, they communicate the actual characterization clearly and unambiguously.

The Committee determined that the Respondents' use of the statement "A combination of scanning electron microscopy and electron diffraction showed that the hexagonal particles were crystalline Pd" (pg 851 of the Science paper) is a falsification, because it misrepresents the data on which that conclusion is based, and therefore prevents the knowledgeable reader from reaching his or her own conclusions or reinterpreting the claims of the Science paper in light of additional evidence. By definitively claiming metal-metal bonds and crystalline palladium without disclosing primary data, the knowledgeable reader would assume that these claims were beyond scientific dispute at the time the Science paper was submitted. They very much were not. The Respondents' "chemical logic", while appropriate in the context of the work, does not mitigate the falsification, and the "chemical logic" is not even described by the Respondents in their Science (2004) paper.

In considering Allegation #3, the Committee notes that Dr. Eaton was not involved in either the collection or interpretation of the microscopy data, and relied on Drs. Feldheim and Gugliotti (Eaton interview, December 21, 2007, p. 21, line 5 and p. 38, line 4, et seq.). Therefore, the Committee considers Dr. Eaton to be responsible only for his part in the failure to disclose the "chemical logic" argument behind the conclusion in the manuscript, and not for the presence of the statement, "A combination of scanning electron microscopy and electron diffraction showed that the hexagonal particles were crystalline Pd" (pg 851 of the Science paper).

In determining if the falsification was committed knowingly or intentionally the Committee considered the following:

1. When the EDS data in question were eventually presented in the public record (evidence item #26, Figure 1.4), they were faithful and accurate representations of the actual data, an apparent gesture of openness and confidence in their science. The Committee is aware of no attempt either to falsify those data or to withhold

them from Dr. Gugliotti's dissertation or dissertation committee. Notably, the dissertation was written and defended prior to the charges of misconduct.

2. When two of the Respondents, Drs. Feldheim and Gugliotti, presented their data to their collaborators on Dec. 6, 2005, they presented the authentic data, an apparent gesture of openness and confidence in their science. The presentation occurred prior to the charges of misconduct.
3. The Respondents make no explicit claims in their publications that the patterns were ever indexed.
4. Several witnesses observed that Dr Gugliotti was unschooled in the field of TEM analysis at the time the Science paper was written, and that she did eventually seek training. (Gugliotti interview, June 2, 2007, p. 42, line 14; p. 45, line 5; Duscher interview, December 12, 2007, p. 12, line 17; p. 20, line 18; p. 36, line 23)
5. The Respondents provided samples to collaborators, an apparent gesture of openness and confidence in their science (Eaton interview, December 21, 2007, p. 26, line 8; evidence item 38).
6. The Respondents invited the Complainant, Dr. Franzen, to join the team, another apparent gesture of openness and confidence in their science (Evidence item #28; Franzen interview, November 19, 2007, p. 7, lines 19 - 21). This invitation preceded the allegations of misconduct.
7. Drs. Eaton and Feldheim apparently assumed that the TEM facilities that provided access to necessary instrumentation provided more comprehensive assessment or analytical services than was actually the case, or that Dr. Gugliotti was sufficiently versed in executing all reasonable protocols in making the claimed determinations. (Eaton interview, December 21, 2007 p. 38, line 8; p. 74, line 21).
8. The errors made by Dr. Gugliotti were consistent with novice-level knowledge and "easy to make" (Duscher interview, December 12, 2007, p. 44, line 10).
9. Written testimony from relevant TEM-facility personnel indicated that their involvement when granting, on a fee-for-service basis, access to TEM facilities does not include sample assessment and data analysis or purport to draw specific scientific conclusions (evidence item 48).
10. Dr. Gugliotti's testimony that TEM-facility personnel told her she had found Pd metal (Gugliotti interview, June 5, 2007, pg. 112, line 4; Gugliotti interview December 21, 2007, p. 32, line 3).

While Dr. Gugliotti was inexperienced in the specific analyses under question, her major advisors of record were both responsible for ensuring that the relied-upon scientific data (the EDS spectra and SAED patterns in this specific regard) were complete and accurate, and that the proper SAED indexing was performed and included prior to asserting scientific findings. The Committee, however, recognizes that Drs. Eaton and Feldheim believed that Dr. Gugliotti had accurately conducted the TEM analyses, and furthermore, they believed that the TEM-facility personnel had definitively verified that Dr. Gugliotti had found crystalline Pd. While the TEM–facilities employed by Dr. Gugliotti report that their personnel generally refrain from interpreting results for clients (evidence item #48), it is understandable that a novice user of TEM facilities and data could misinterpret a general comment from a TEM-facility operator as formal validation of the results,

especially when those results are consistent with expectations. However, Dr. Feldheim should have been more diligent in his assessment, and as a senior scientist he was responsible for oversight of Dr. Gugliotti's experiments and interpretations.

Prior to the Science paper, Dr. Gugliotti was not competent in TEM analyses and lacked appropriate training; she did not understand the importance of proper diffraction indexing (Gugliotti interview, December 21, 2007, p. 64, line 20, et seq.), nor did she recognize the possibility of beam-induced changes in the sample and associated implications (Gugliotti interview, December 21, 2007, p. 50, line 8, et seq.). Dr. Feldheim should have been aware of the importance of proper indexing, but a preponderance of the evidence indicates that he was not.

In determining whether the falsification of the Respondents was executed knowingly or intentionally, the Committee finds that this original statement, while a falsification and representative of a significant departure from accepted practices, was not an intentional or knowing act. Rather, based upon a preponderance of the evidence, the Committee finds that the misleading statement appeared largely as a result of inexperience with this type of materials characterization in combination with the authors' honest conviction at the time that the particles were in fact Pd metal.

The Committee next considered whether the Respondents, and in particular Drs. Feldheim and Gugliotti, acted recklessly in a manner that led to the falsification of the research record. The specific concern is that they relied on their own interpretation of the microscopy data and did not secure an expert collaborator to validate their conclusions. The Committee is convinced that such collaboration would have prevented the false statement from appearing in the submitted Science paper.

In determining whether the actions of the Respondents were executed recklessly, the Committee considered the following:

1. The particles, at a minimum, do in fact contain Pd, as verified by the EDS data.
2. The Respondents point to their very limited SAED and EDS data to justify their claim of metal-metal bonds, and they invoke a "chemical logic" (Eaton interview, December 21, 2007, p. 15, line 22) rationalization of their conclusion. "Chemical logic" refers to the expectation that pyridine displaces dba, thereby leaving behind Pd metal. The Committee finds that this logic was reasonable at the time of the experiments.
3. Dr. Gugliotti explained in her Investigation Committee interview (Gugliotti interview, December 21, 2007, p. 17, line 8 - 11) that she did not believe indexing was necessary.
4. Following publication of the Science paper, Dr. Gugliotti enrolled in a course offered by the NC State University Materials Science & Engineering Department on the subject of transmission electron microscopy and was instructed by Dr. Duscher. During that course, Dr. Gugliotti endeavored to learn more about her research through a course project. These actions indicate an awareness that her training and competence level were not sufficient.

5. Prior to the Science paper, the Respondents attempted to index the electron diffraction patterns that Dr. Gugliotti obtained, but without success (Gugliotti interview, June 5, 2007, p. 96, line 19, et seq.), and so Drs. Gugliotti and Feldheim realized that they were not technically able to interpret all their data (Gugliotti interview, December 21, 2007, p. 13, line 4, et seq.).
6. With regard to her conclusion of crystalline Pd nanoparticles from a combination of non-indexed SAED and EDS data, Dr. Duscher indicated that it was an easy mistake to make by a novice graduate student (Duscher interview, December 12, 2007, p.44, line 16).
7. Drs. Gugliotti and Feldheim confirmed their continuing conviction that the nanoparticles are metallic Pd in their testimony (Gugliotti interview December 21, 2007, p. 64, line 12; and evidence item #49, respectively).
8. Dr. Gugliotti's testimony that the various TEM-facility personnel told her she had found Pd metal (Gugliotti interview, June 5, 2007, p. 112, line 4; Gugliotti interview, December 21, 2007, p. 32, line 3).
9. Dr. Gugliotti was a novice in TEM analysis (Gugliotti interview, June 5, 2007, p. 12, line 2, and p. 42, line 14), and Drs. Eaton and Feldheim assumed that the TEM facilities that provided access to necessary instrumentation provided comprehensive assessment or additional analytical services, or that Dr. Gugliotti was sufficiently versed in executing all reasonable protocols in making the claimed determinations. (Eaton interview, December 21, 2007, p. 38, line 8; p. 74, line 21).
10. References cited by Dr. Eaton in which Pd nanoparticles are claimed under similar circumstances (Organic Letters **2007,** *9,* 2409; Organometallics **2007**, *26*, 3306; Eaton interview, December 21, 2007, p. 49). The Committee also considered the differences in characterization described in those papers vs. the characterization carried out by the Respondents.
11. The particles observed by the Respondents and disclosed in their publications have morphologies that resemble those of other Pd nanoparticles formed by an entirely different reaction (JACS, **2005**, *127*, 17118-17127).
12. Dr. Gugliotti's testimony that at the time of the microscopy experiments, she (mistakenly) believed that beam damage would be recognizable as visual changes in the particle morphology (Gugliotti interview, December 21, 2007, p. 50, line 23 et seq. and p. 52, lines 15-17).

The evidence supports a consistent picture of the data available to Drs. Feldheim and Gugliotti at the time the Science paper was written, including the statement in question. They had chosen a Pd precursor that is known to form Pd metal readily. The particles that formed contained Pd, and according to the EDS data did not have enough oxygen or phosphorous to be $Pd_2(DBA)_3$ or to contain significant amounts of RNA (although there was enough oxygen that the particles could be PdO). The particles appeared to diffract (although the Committee has concerns regarding the possibility of beam damage; that possibility was not considered at the time by Dr. Gugliotti). While Drs. Feldheim and Gugliotti were aware both that their analysis was not complete (specifically, that indexing had not been properly performed) and that they were not experts in the techniques at hand, they believed that their expectations had been informally confirmed by the

technical staff that assisted Dr. Gugliotti with the measurements, although Dr. Kvit has denied any technical analyses concerning the data in question (evidence item # 48).

The Committee believes that the brunt of the responsibility here falls on Dr. Feldheim, and that he was negligent in his failure to consult more thoroughly with an expert on microscopy and relevant data interpretation. The Committee is split, however, on whether or not his actions rise to the level of recklessness: namely, would a reasonable individual in the same situation have been aware that proceeding without consulting an expert and indexing the diffraction pattern would be likely to open the door to an erroneous conclusion and distort the research record?

Four of the five Committee members believe that the preponderance of the evidence supports the conclusion that Dr. Feldheim's actions do not rise to the level of recklessness. This portion of the Committee was swayed especially by the reasonable expectation that Pd metal would form from the $Pd_2(dba)_3$ precursor and the fact that the expectation was reinforced by comments (potentially misinterpreted or the result of poor communication with Dr. Gugliotti) by the technical staff that assisted in data collection. The Committee also considered that this incident was atypical of Dr. Feldheim's conduct. The Complainant in an email referred to Dr. Feldheim as typically being "careful and always question experiments. You asked for more characterization and control experiments than anyone." (evidence item #10, p.6) and Dr. Cerruti states that research meetings were conducted professionally and carefully (Cerruti interview, December 10, 2007, p. 59, line 17 et seq.).

One of the five Committee members, however, found that the preponderance of the evidence supports a conclusion of recklessness on the part of Dr. Feldheim. In reaching this conclusion, this portion of the Committee was swayed by the fact that Drs. Feldheim and Gugliotti were aware of their limited competence in microscopy but did not secure adequate expert advice from any of the numerous sources available on campus. In the minds of this Committee member, Dr. Feldheim, given his experience, should have recognized that such a course of action would create a likelihood of falsely representing the research record, and, given his senior role in the project, he should have consulted appropriate experts before publishing the Science paper.

Therefore, the Committee unanimously finds that Drs. Eaton and Gugliotti are not guilty of research misconduct. By a final vote of 4 to 1, the Committee finds that Dr. Feldheim is not guilty of research misconduct. The dissenting member of the Committee finds that Dr. Feldheim is guilty of reckless falsification with regard to Allegation #3 and therefore research misconduct.

**Conclusion:**

Despite the majority conclusion that scientific misconduct did not occur in this case, the Committee is concerned about the integrity of the scientific record. The 2004 Science paper is frequently cited as proof of formation of pure metal nanoparticles or palladium crystals via an RNA-mediated mechanism. The Committee concludes that neither at the

time of the original publications nor presently, have the Respondents produced or published sufficient data to unambiguously justify this conclusion. The language that the Respondent's have used thus far includes misleading terms such as "Pd crystals" and "crystalline Pd" that lead a knowledgeable reader to understand that the particles have been proven to be crystals of pure Pd metal. Until such time as they are able to publish convincing data regarding the elemental composition (i.e., pure Pd metal) and the atomic structure (i.e., crystallinity), the Respondents are obliged to use more judicious descriptions of their findings. For example, given the current scientific record reviewed by the Committee, the particles would be more appropriately described with terms such as "Pd-containing." The Committee further urges the Respondents to either publish new conclusive data or to publish a clarification/reexamination of their previously reported data.

**Supplemental Information Regarding Allegation #2**

During their deliberations, the Investigation Committee received additional information from the Complainant regarding this allegation. The Complainant submitted additional information in the form of a new allegation, claiming, "*I must conclude that the polyvinylpyridine control experiment reported in the Science paper is a fabrication. By this I mean that there are no primary data to support the claim that this experiment was done. I base this allegation on the following facts: 1. There are no corroborating data or even mention of this control experiment in any of the other publications nor in the thesis of Dr. Gugliotti. 2. The experiment is not described in any detail. There are two isomers or polypyridine. Neither the concentration nor the molecular weight of the polymer used is specified. 3. The experiment as described is not possible. Polyvinylpyridine is not soluble in water. In the Science paper the only solvent claimed is water. We have corroborated this with our own experiments as well as the scientific literature.*"

The Investigation Committee determined that the Complainant is in fact resurrecting the original Allegation #2, because the Science paper states that the PVP experiment was done "under identical incubation and isolation conditions" to the RNA experiments. The Respondents agree that the details of the RNA experiments, and in particular the solvent conditions, are not accurately provided in the Science paper. The only solvent claimed by the authors in the Science paper is water, when in fact the substrate was dissolved in THF and this solution was then added to water. This failure to mention the presence of a co-solvent is the same as in the original allegation #2, and will not be considered further here.

The Investigation Committee also noted the following regarding the Complainant's claims:

1. "There are no corroborating data or even mention of this control experiment in any of the other publications nor in the thesis of Dr. Gugliotti."

This statement by the Complainant is wrong. Dr. Gugliotti's dissertation pg. 12 mentions PVP controls. This and other related control experiments are described in Carly Carter's lab notebooks (evidence item #42, notebook 3A, p. 73, et seq.). Ms. Carter's experiments occurred after the publications in question were submitted, and the Committee considers them only insofar as they demonstrate that it is standard practice for such control experiments to be done in association with the project.

2. "The experiment is not described in any detail. There are two isomers of poly(vinylpyridine). Neither the concentration nor the molecular weight of the polymer used is specified."

This statement by the Complainant is correct, and this shows that the Respondents were sloppy, but the Committee has already determined that a failure to provide details of an experiment does not rise to the level of falsification/fabrication as defined by NSF.

The Committee has identified a further consideration with respect to this allegation. The Science paper and Dr. Gugliotti's dissertation claim that the PVP experiment was carried out "under identical incubation and isolation conditions" to the RNA experiments (evidence item #26, p. 12), but in her testimony (Gugliotti interview, June 5, 2007, p. 73, line 5 - 16), Dr. Gugliotti notes that she used methylene chloride as a solvent for PVP. Methylene chloride is not present in the RNA experiments. The Committee notes that the presence of methylene chloride may be more significant than was realized at the time of the Science paper, because there is now an understanding that "synthetic conditions…may play a role in determining the observed structure" (evidence item #49). In contrast to the omission of the presence of 5% THF, as described in Allegation #2, the conditions of the PVP experiment are not corrected either in the subsequent JACS paper or in Dr. Gugliotti's dissertation. Following reasoning similar to that employed in evaluating original Allegation #2, the Committee concludes that this falsification is another careless error on the part of the Respondents but when carefully considered in concert with the deliberations detailed above, does not change the Committee's findings or conclusions insofar as it has already been considered above.

The Committee also noted that the concerns associated with the PVP control experiment have limited bearing on the major conclusions of the Science paper. If the PVP produced identical particles to one of the RNA sequences (it obviously could not match the particles produced from both Pd034 and Pd017), the other RNA sequence would still be unique relative to PVP, and it would be possible that both PVP and one RNA sequence mediate the formation of particles that appear to be nearly identical. However, this notation is only a scientific comment and has no bearing on the Committee's deliberations and as such does not change its findings or conclusions.