Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for:

Interplay of Molecular Dynamics and Radiative Decay of a TADF Emitter in a Glass-Forming Liquid

John R. Swartzfager,[1] Gary Chen,[1] Tommaso Francese,[2] Giulia Galli,[2,3,4] and John B. Asbury[1*]

1. Department of Chemistry, The Pennsylvania State University, University Park, PA 16802, USA.

2. Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL 60637, USA.

3. Materials Science Division and Center for Molecular Engineering, Argonne National Laboratory, Lemont, IL 60439, USA

4. Department of Chemistry, University of Chicago, Chicago, IL 60637, USA

Table of Contents:

Section S1. Evaluation of the influence of N_2 sparging on NAI-DMAC emission properties in mTHF solutions at room temperature

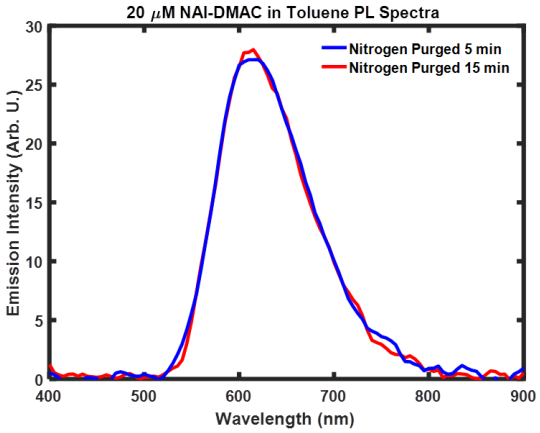

Figure S1. Comparison of the time-integrated photoluminescence spectra after 355 nm excitation of 20 μM solutions of NAI-DMAC in toluene sparged with N_2 for five versus fifteen minutes, respectively. The spectra are indistinguishable within experimental precision, indicating that O_2 was removed sufficiently after five minutes to eliminate the influence of O_2 on the triplet state population in solution.

Section S2. Comparison of PL spectra of NAI-DMAC in toluene and mTHF at 900 μM and 9.3 μM concentrations

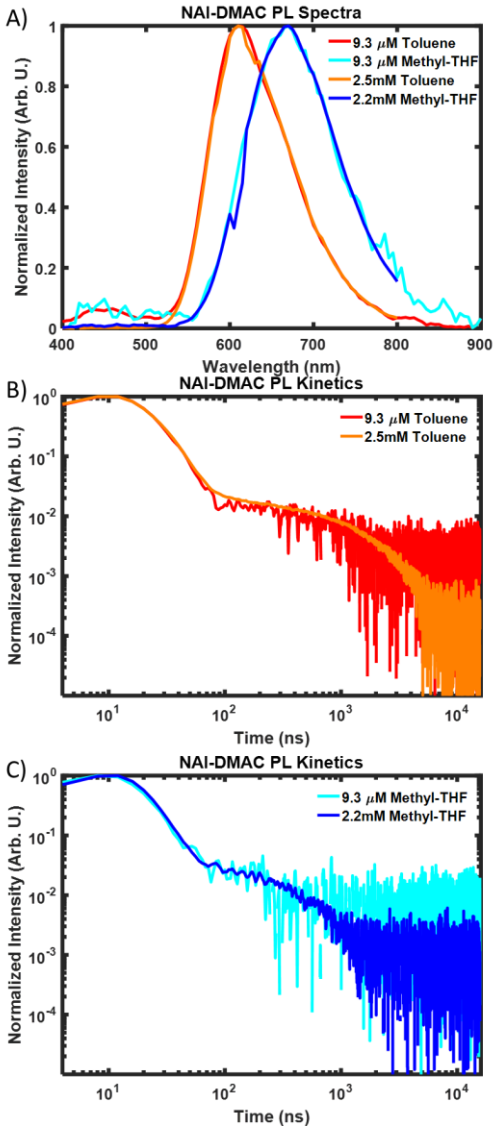

Figure S2. **A)** Normalized time-integrated photoluminescence spectra of NAI-DMAC measured following 355 nm excitation of 900 and 9.3 μM solutions in toluene and mTHF. These data show the same emission features regardless of concentration. Normalized time-resolved photoluminescence decay kinetics for **B)** toluene and **C)** mTHF at 900 and 9.3 μM concentrations. The higher concentration solutions were measured in the 1 mm pathlength cuvettes used in the experiments reported in the main body of the manuscript. The lower concentration samples were measured in 1 cm pathlength cuvettes. The comparison demonstrates that the spectra of the low concentration samples are identical to the higher concentration samples, indicating that the spectra and kinetics reported in Figure 2 and Figure 3 of the main body of the manuscript accurately reflect the emission properties of NAI-DMAC without self-absorption effects. The comparison also demonstrates that the PL measurements reflect the emission of isolated molecules in solution rather than from aggregates or exciplexes and are not influenced by energy transfer.