Supporting Information for:

**Solvent Dependence of ^{14}N Nuclear Magnetic
Resonance Chemical Shielding Constants as a Test
of the Accuracy of the Computed Polarization
of Solute Electron Densities by the Solvent**

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Date of preparation: May 12, 2009.

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Table S1. Nitrogen shielding constants for acetonitrile in 2,2,2-trifluoroethanol and water relative to CCl_4, calculated using bare solutes in implicit solvent with the M06-L density functional

	SM8	SMD	SM8AD	PCM-UA0	PCM-UAKS	PCM-1.2B	Experiment
CCl_4 – Water	8.1	11.8	5.9	9.6	12.8	10.7	18.2
CCl_4 – TFE	7.5	11.0	5.5	9.0	NA[a]	9.9	21.6

[a]NA denotes not applicable because the method is not defined for this solvent.

Table S2. Nitrogen shielding constants for acetonitrile in 2,2,2-trifluoroethanol and water relative to CCl_4, calculated using bare solutes in implicit solvent with the B3LYP and PBE0 density functionals

	B3LYP		PBE0		Experiment
	PCM-UA0	SM8AD	PCM-UAKS	SM8AD	
CCl_4 – Water	10.6	6.7	14.3	6.7	18.2
CCl_4 – TFE	9.8	6.2	NA[a]	6.3	21.6

[a]NA denotes not applicable because the method is not defined for this solvent.

Figure S1. Nitrogen shielding in acetonitrile as a function of solvent dielectric constant. In part a, all models have their intrinsic Coulomb radii scaled by 0.8, and in part b the radii are scaled by a factor of 1.2. Diamonds represent experimental results, the red line represents eq 11 fitted to SMD results, the blue line represents eq 11 fitted to SM8 results, and the green line represents eq 11 fitted to SM8AD results.
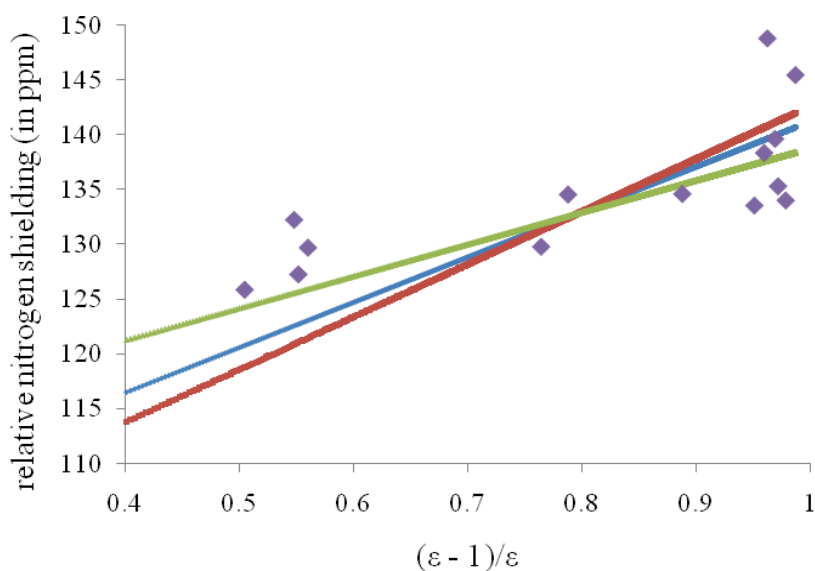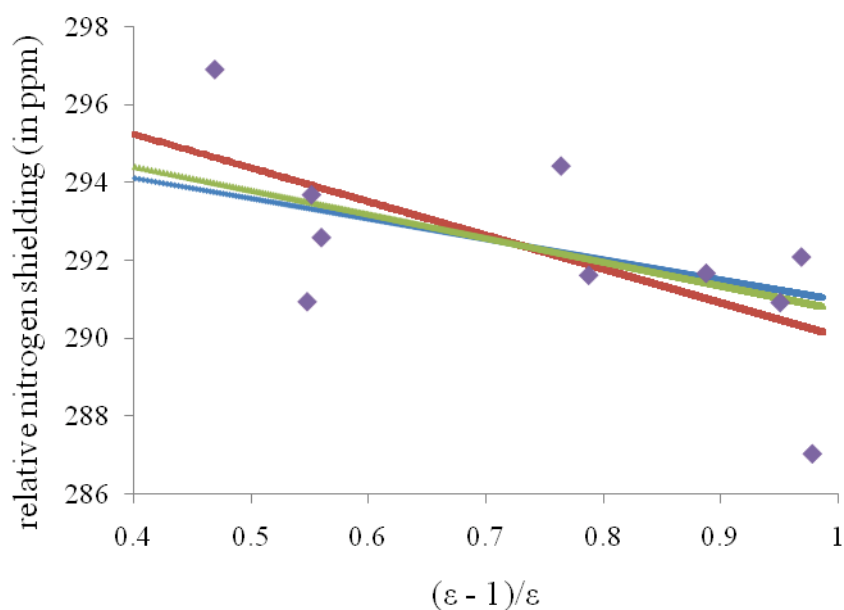
S1a)
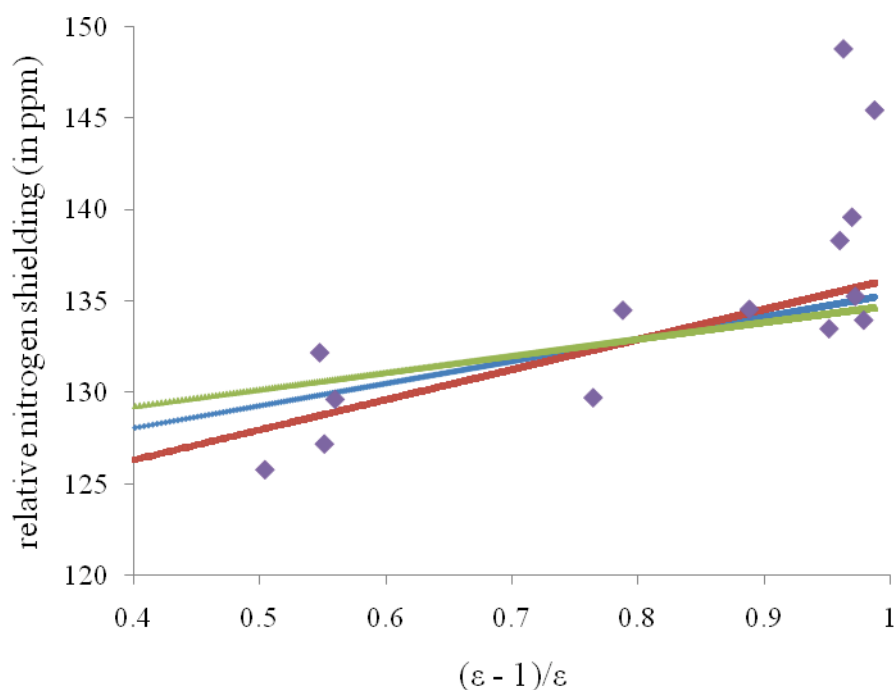
S1b)

Figure S2. Nitrogen shielding in methyl isothiocyanate as a function of solvent dielectric
constant. In part a, all models have their intrinsic Coulomb radii scaled by 0.8, and in
part b the radii are scaled by a factor of 1.2. Diamonds represent experimental
results, the red line represents eq 11 fitted to SMD results, the blue line represents eq
11 fitted to SM8 results, and the green line represents eq 11 fitted to SM8AD results.
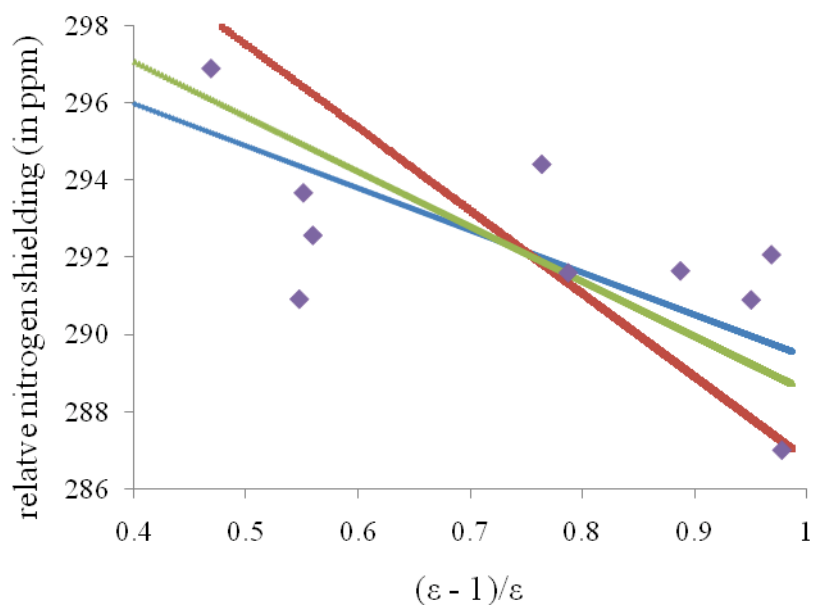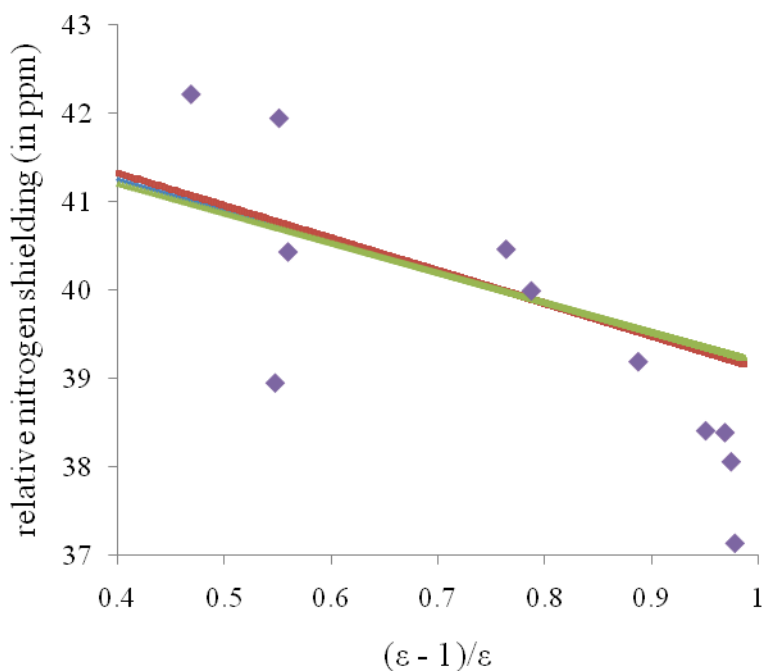
S2a)

S2b)

Figure S3. Nitrogen shielding in methyl nitrate as a function of solvent dielectric constant. In part a, all models have their intrinsic Coulomb radii scaled by 0.8, and in part b the radii are scaled by a factor of 1.2. Diamonds represent experimental results, the red line represents eq 11 fitted to SMD results, the blue line represents eq 11 fitted to SM8 results, and the green line represents eq 11 fitted to SM8AD results.
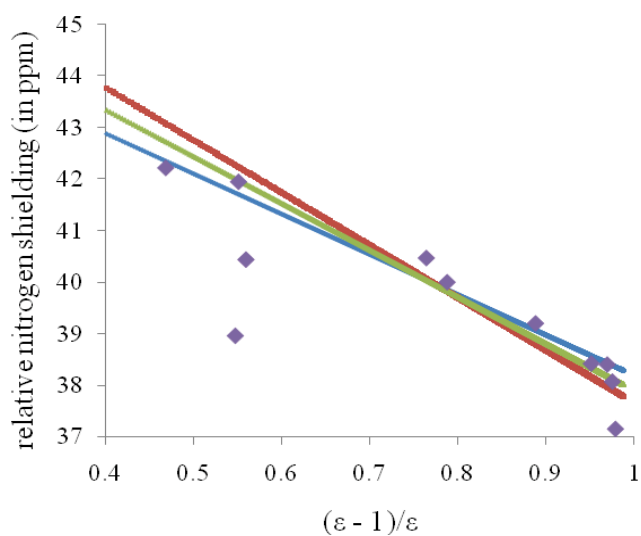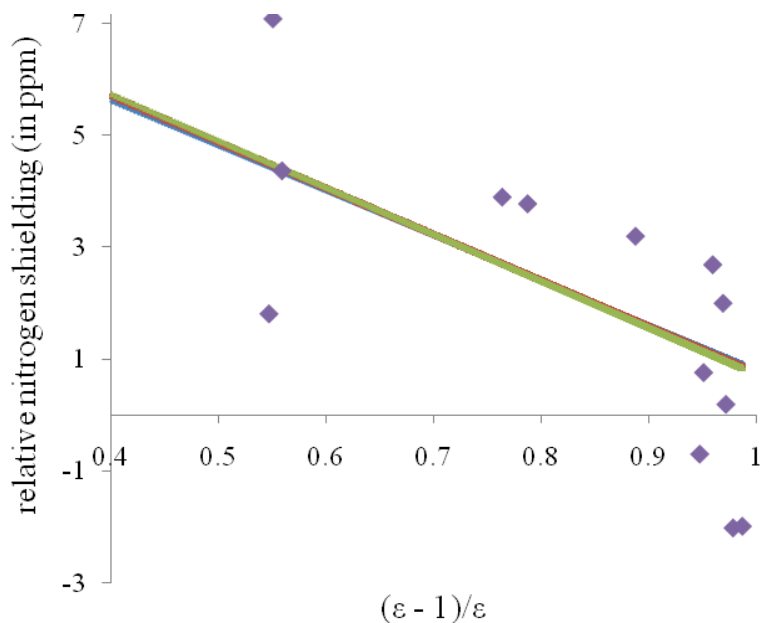
S3a)

S3b)

Figure S4. Nitrogen shielding in nitromethane as a function of solvent dielectric constant. In part a, all models have their intrinsic Coulomb radii scaled by 0.8, and in part b the radii are scaled by a factor of 1.2. Diamonds represent experimental results, the red, blue, and green lines represent eq 11 fitted to SMD, SM8, and SM8AD results, respectively. In part a, the blue and red lines are almost covered by the SM8AD line, and in part b the blue line is behind the green one.

S4a)

S4b)