Supporting Information

Influence of solvent on electronic structure and the photochemistry of nitrophenols

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Photochemical Irradiation Source

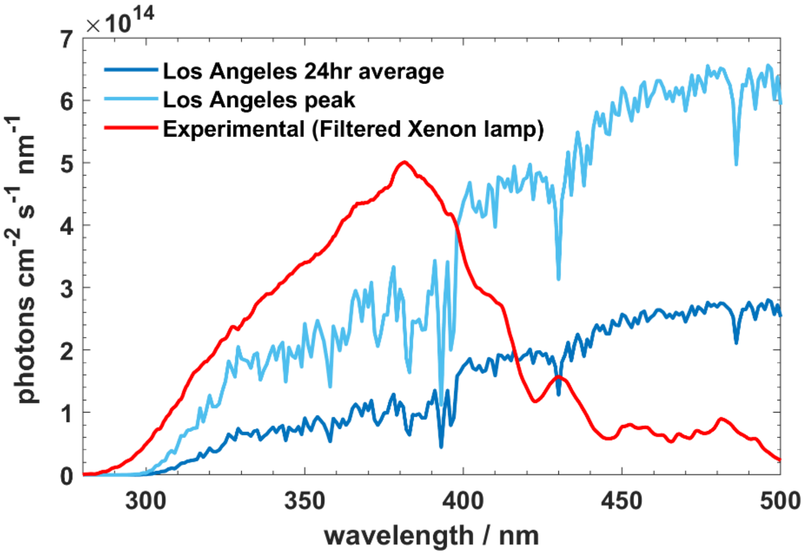

Figure S1. Spectral flux density of the irradiation source used to initiate photochemistry in these experiments is displayed in red. The dark blue trace shows the 24-h averaged flux for Los Angeles (1 July 2022) simulated with the National Center for Atmospheric Research (NCAR) Tropospheric Ultraviolet and Visible (TUV) calculator, used to estimate atmospheric lifetimes. The pale blue trace shows the maximum flux within the 24 h window. We used the 24-h average flux for the results reported in this paper, which is appropriate for molecules that have lifetimes exceeding 1 day. We note that for molecules with lifetimes <1 day, their actual ambient lifetime will be shorter during the peak of the solar irradiation.

Determination of Quantum Yields

Photochemical quantum yields were calculated from the absorption-based rate constant and averaged over a 100 nm window, the approximate width of the main absorption bands. The absorption of each nitrophenol was monitored via UV/Vis for 3-5 h, depending on the reactivity of the nitrophenol. To account for the effect of light-absorbing products, rate constants were determined at the minimum of the normalized absorbance, which would be at 235 nm in the 24DNP example shown in Figure 3. This rate, k (s^{-1}), can then be used in Equation S1 to determine the average quantum yield, $\langle \phi \rangle$.

$$\langle \phi \rangle = k \,/\, \int_{\lambda 1}^{\lambda 2} F(\lambda)\, \sigma(\lambda)\, d\lambda \qquad \textbf{Equation S1}$$

In this equation, $F(\lambda)$ is the irradiation source shown in Figure S1, and $\sigma(\lambda)$ is the absorption cross-section of the molecule. The bounds of the integration, λ_2 and λ_1, correspond to the wavelengths +50 nm and -50 nm from the point of greatest decay. For example, for 4NP the most decay in normalized absorbance occurred at 319 nm, so the integration window was λ_1 = 269 nm and λ_2 = 369 nm. The only exception to this was 24DNP, which showed the most change at 235 nm, and the integration center-point was set to 290 nm, the approximate location of the main absorption peak.

To determine estimated atmospheric lifetimes, this equation was flipped to solve for the rate constant resulting from using the 24-h average Los Angeles flux as F(λ), and then taking the inverse of the rate constant to be the lifetime.

Absorption Spectra from Photolysis in Acidic Organic Solutions

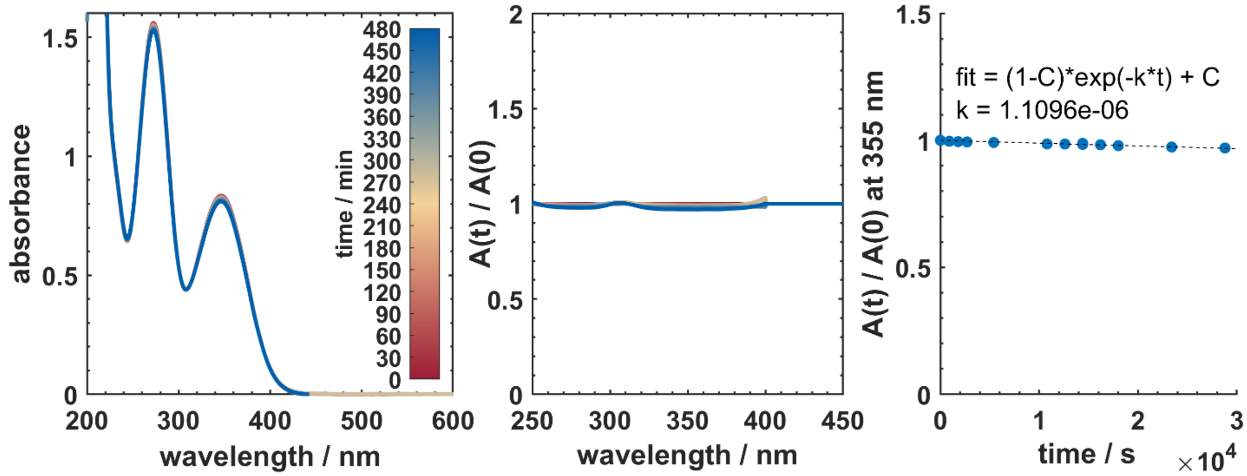

Figure S2. (a) The absorption spectrum of 2NP collected over 3 h of exposure to photochemical radiation, (b) the absorption spectrum of 2NP normalized to the absorption spectrum obtained before photolysis began, and (c) the decrease in the normalized absorbance at 355 nm, indicating loss of 2NP, fit to an exponential decay. For this experiment, the sample was irradiated without use of the light guide, exposing the sample to ~5× larger irradiance than the other samples.

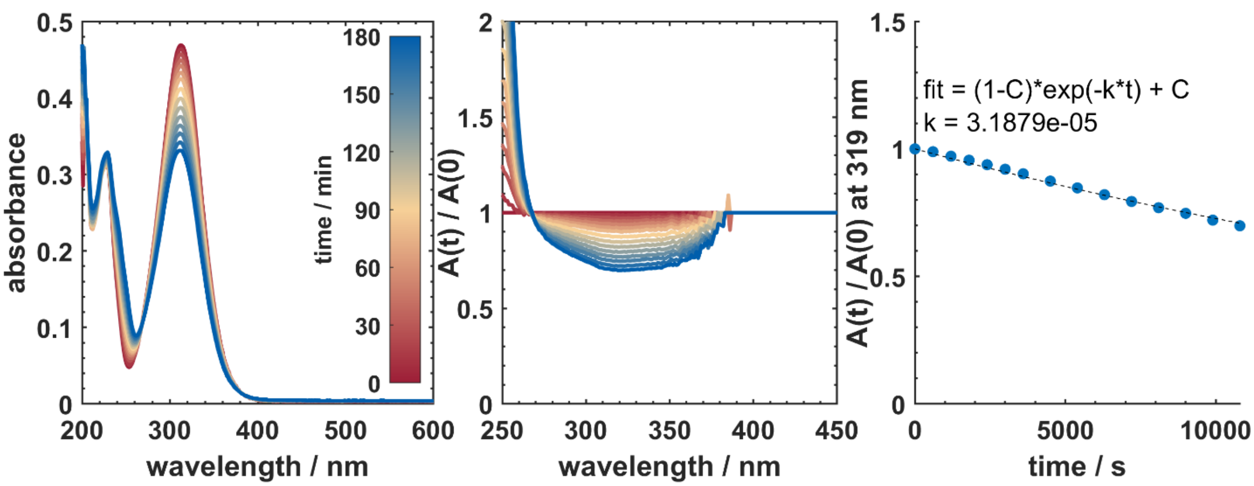

Figure S3. (a) The absorption spectrum of 4NP collected over 3 h of exposure to photochemical radiation, (b) the absorption spectrum of 4NP normalized to the absorption spectrum obtained before photolysis began, and (c) the decrease in the normalized absorbance at 319 nm, indicating loss of 4NP, fit to an exponential decay.

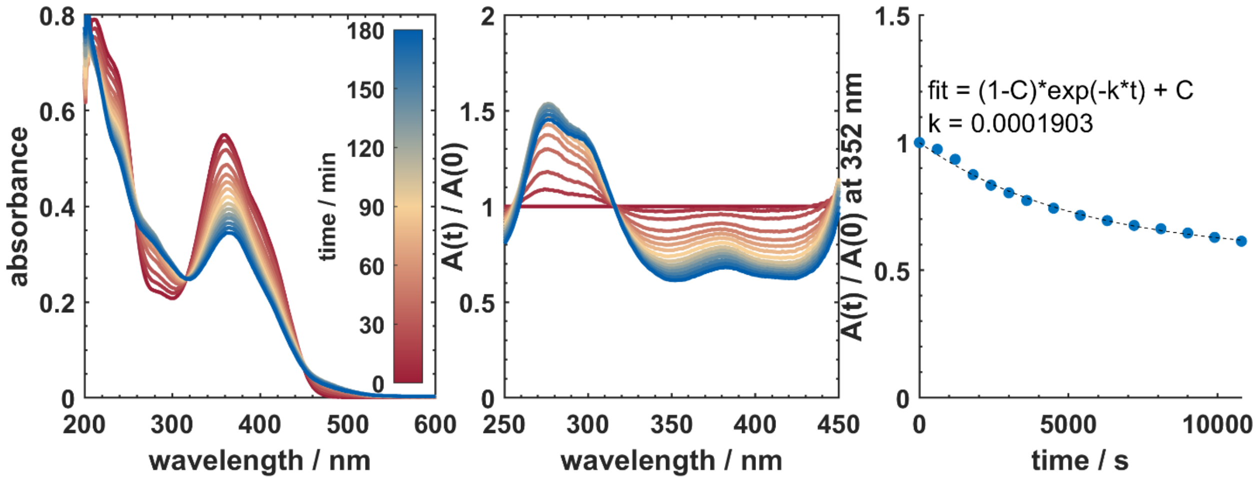

Figure S4. (a) The absorption spectrum of 246TNP collected over 3 h of exposure to photochemical radiation, (b) the absorption spectrum of 246TNP normalized to the absorption spectrum obtained before photolysis began, and (c) the decrease in the normalized absorbance at 352 nm, indicating loss of 246TNP, fit to an exponential decay.

Absorption Spectra from Photolysis in Basic Organic Solutions

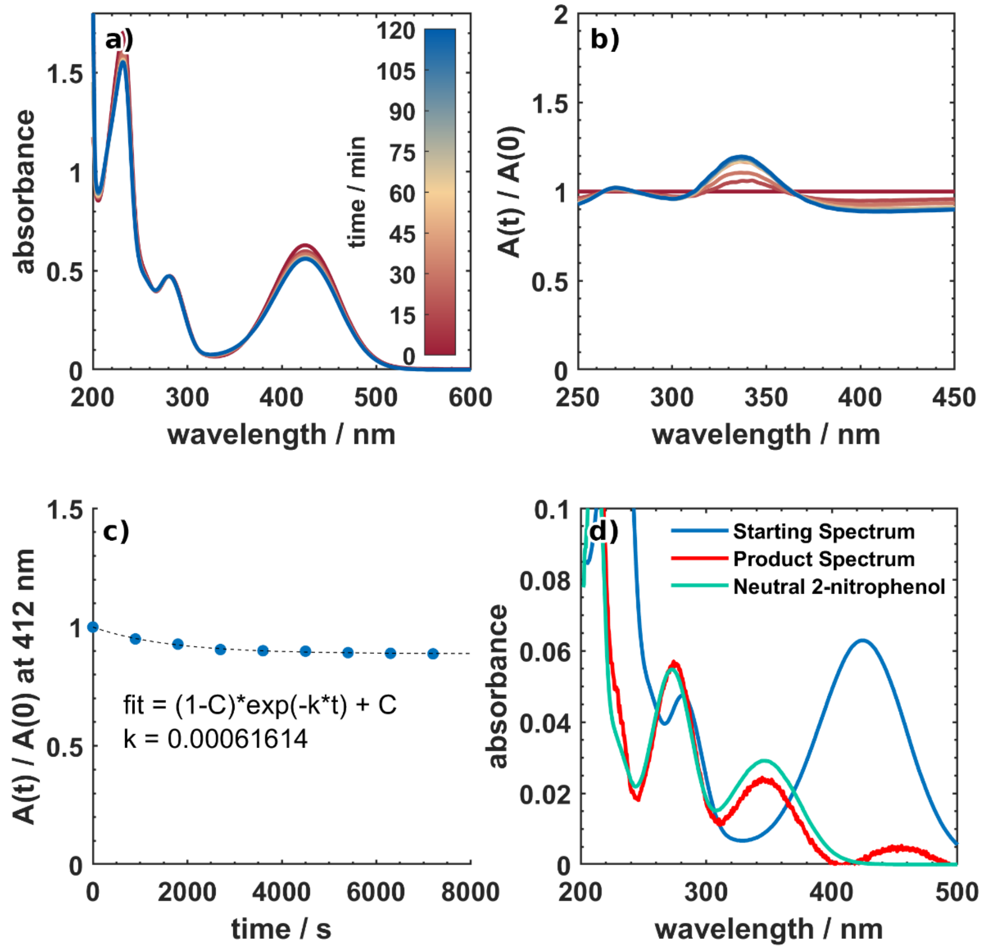

Figure S5. (a) The absorption spectrum of 2NP collected over 3 h of exposure to photochemical radiation, (b) the absorption spectrum of 2NP normalized to the absorption spectrum obtained before photolysis began, and (c) the decrease in the normalized absorbance at 412 nm, indicating loss of 2NP, fit to an exponential decay. Panel (d) illustrates the approximate "product" spectrum at the end of 120 minutes of photolysis, generated using the value of C from the original fit (0.89) to subtract out the contribution of the spectrum of the starting material: $A_{products} = A_{120min} - [C \times A_{0min}]$. This plot is shown to illustrate that this period of small change may be caused by a small portion of the sample returning to the neutral form.

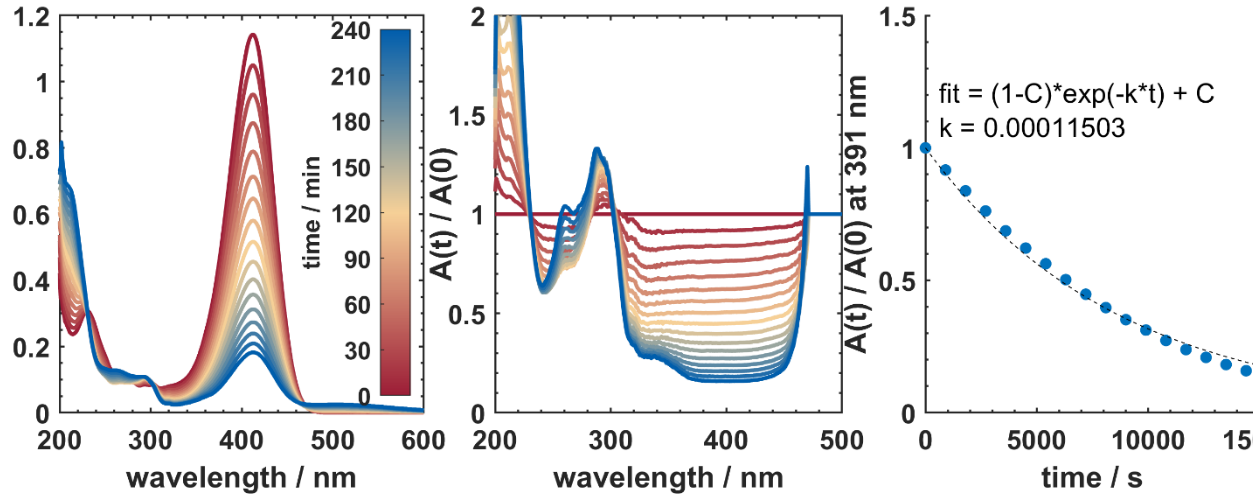

Figure S6. (a) The absorption spectrum of 4NP collected over 3 h of exposure to photochemical radiation, (b) the absorption spectrum of 4NP normalized to the absorption spectrum obtained before photolysis began, and (c) the decrease in the normalized absorbance at 391 nm, indicating loss of 4NP, fit to an exponential decay.

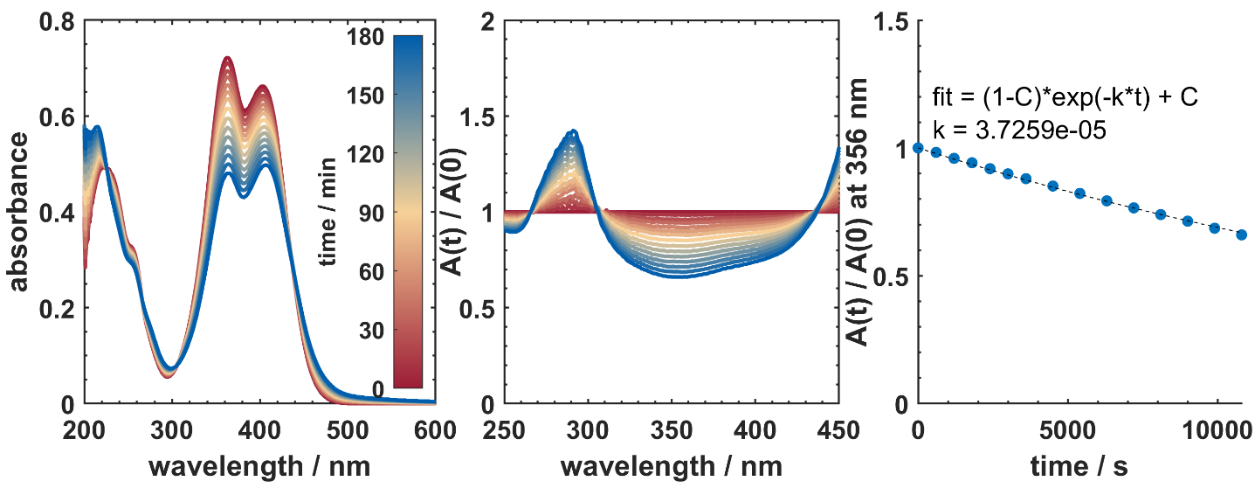

Figure S7. (a) The absorption spectrum of 24DNP collected over 3 h of exposure to photochemical radiation, (b) the absorption spectrum of 24DNP normalized to the absorption spectrum obtained before photolysis began, and (c) the decrease in the normalized absorbance at 356 nm, indicating loss of 24DNP, fit to an exponential decay.

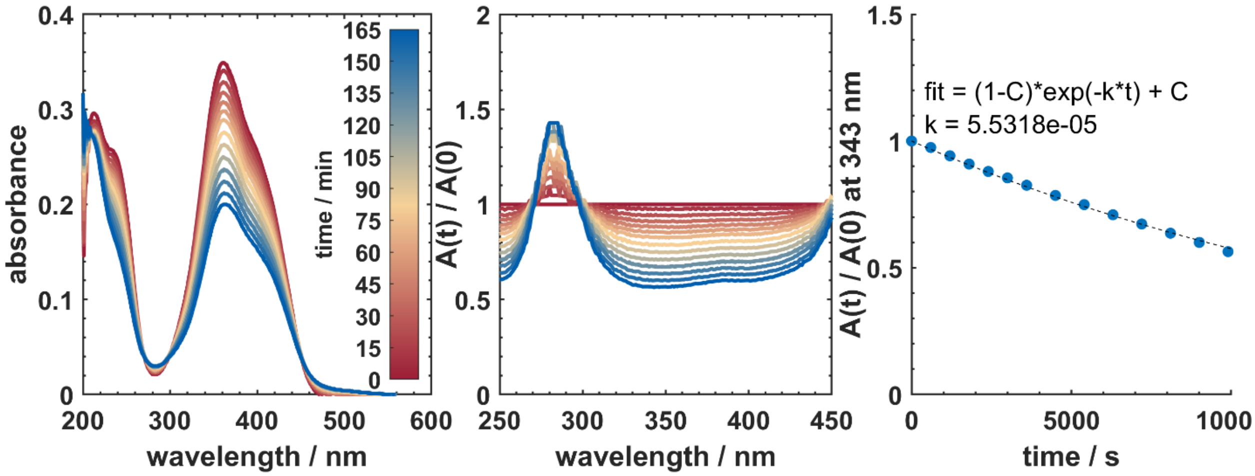

Figure S8. (a) The absorption spectrum of 246TNP collected over 3 h of exposure to photochemical radiation, (b) the absorption spectrum of 246TNP normalized to the absorption spectrum obtained before photolysis began, and (c) the decrease in the normalized absorbance at 343 nm, indicating loss of 246TNP, fit to an exponential decay.

Referenced Photochemical Yields in Aqueous Solutions

Table S1. Photochemical yields of undissociated nitrophenols in aqueous solutions.

Molecule	Quantum Yield	Reference	Conditions
2NP	$(6.8 \pm 0.3) \times 10^{-6}$	This work	$[HCl] = 10^{-3}$ M, broadband
	1×10^{-4}	Barsotti et al., 2017	pH = 3, broadband
	4.7×10^{-6}	Alif et al., 1991	pH = 2.2, monochromatic (365 nm)
4NP	$(9.9 \pm 0.1) \times 10^{-5}$	This work	$[HCl] = 10^{-3}$ M, broadband
	$(3.3 \text{ to } 21) \times 10^{-5}$	Lemaire et al., 1985	pH = 2, broadband
	4.3×10^{-4}	Einschlag et al., 2002	pH = 2.5, broadband
	$(7.3 \pm 0.5) \times 10^{-4}$	Barsotti et al., 2017	pH = 3, broadband
	$(1.4 \pm 0.1) \times 10^{-4}$	Braman et al., 2020	pH = 3.5, broadband
24DNP	1.3×10^{-4}	Einschlag et al., 2002	pH = 2.5, broadband
	$(8.1 \pm 0.4) \times 10^{-5}$	Albinet et al., 2010	pH = 2.5, broadband
	$(3.6 \text{ to } 4.4) \times 10^{-6}$	Lignell et al., 2014	Broadband
	$(2.1 \pm 0.1) \times 10^{-4}$	Barsotti et al., 2017	pH = 3, broadband

Simulated Absorption Spectra

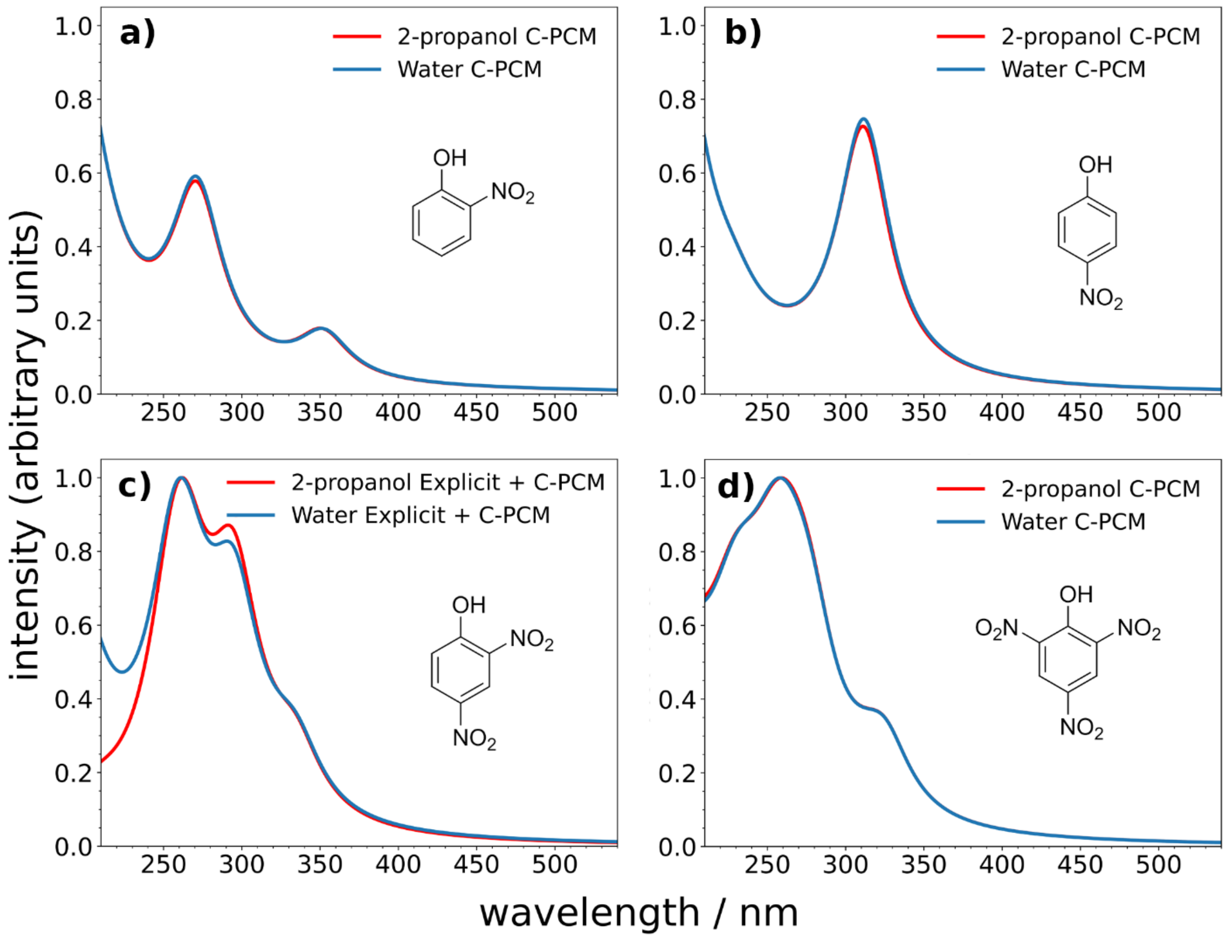

Figure S9. Simulated absorption spectra for 2NP (a), 4NP (b), 24DNP (c) and 246TNP (d) employing solvation models for 2-propanol (red) and aqueous (blue) solutions. The 24DNP spectrum required explicit solvation by three solvent molecules, as described in the main text. Subtle (i.e., less than 1 nm) changes in peak position were observed for only some absorption bands. Variations in intensity for the 24DNP spectra are the most notable result.

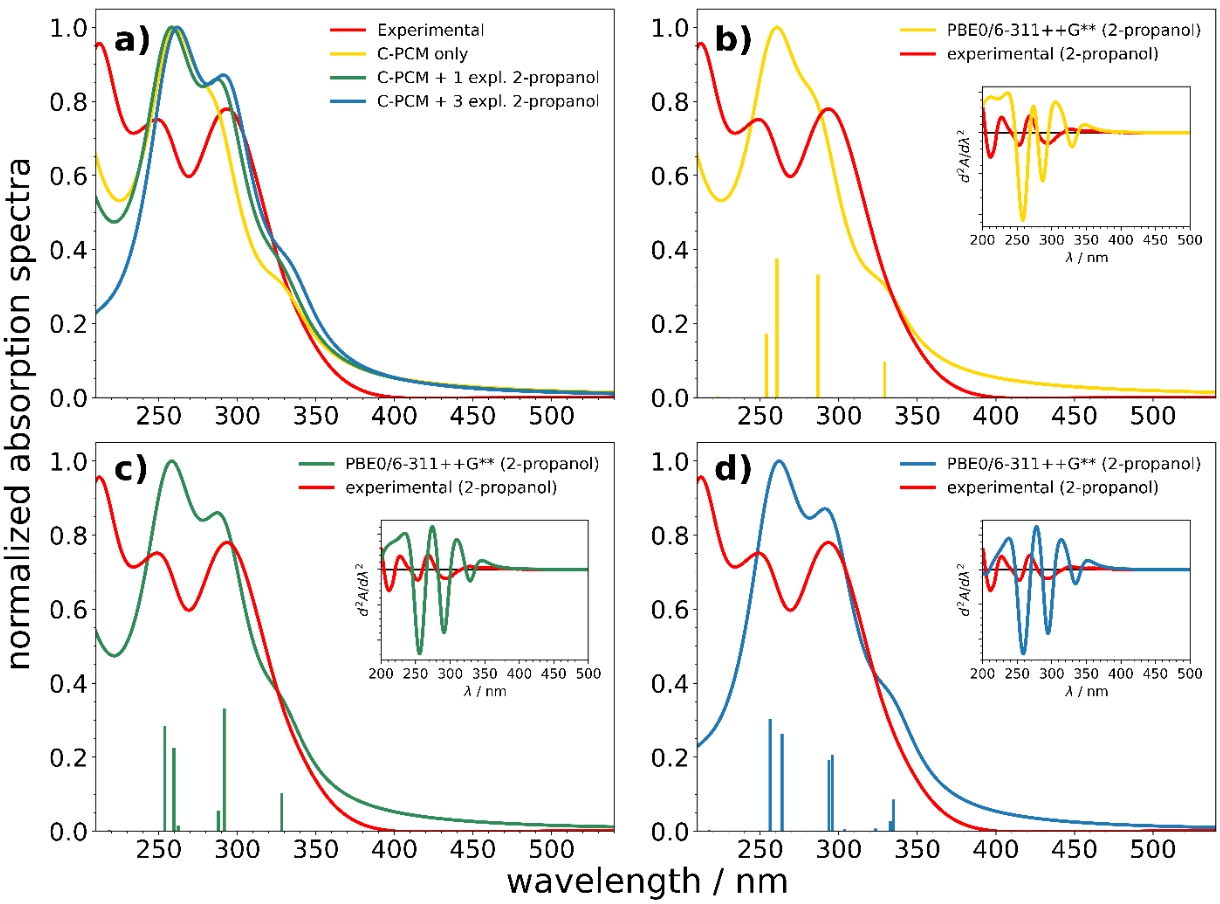

Figure S10. The experimental and theoretical spectra of 24DNP in 2-propanol as solvent. Panel (a) shows the spectra overlayed on each other, and panels (b), (c), and (d) show the individual spectra and oscillator strengths from simulations with C-PCM only, and one and three explicit 2-propanol solvent molecules, respectively. Explicit solvation affects the relative intensities of individual excitations within each absorption band. The notation in the figure legends represent the number of explicit solvent molecules used, i.e. “1x” for 1 explicit 2-propanol solvent molecule.

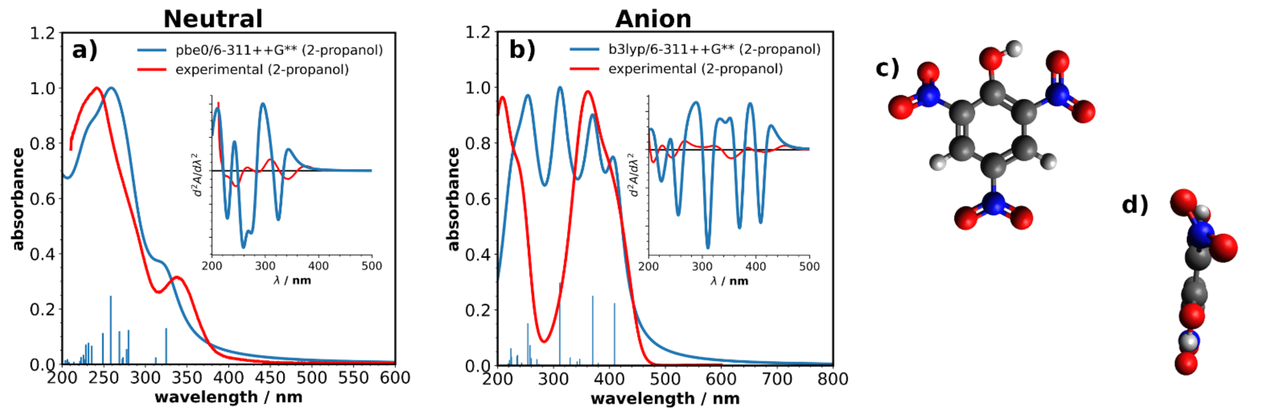

Figure S11. The experimental and theoretical absorption spectra of 246TNP as a neutral (a) and anionic (b) species in isopropanol. The insets of these plots show the second derivatives of the absorption spectra. The optimized structures of the neutral form of 246TNP are shown in (c) and (d), with the latter having been rotated to show the rotation of the non-planar NO_2 group.

Output Data from TDDFT/TDA Calculations

The numerical values used to create the theoretical excitation spectra are in Table S1 below. Spectra were created by finding 35 roots (all singlets) and assigning Lorentzian functions to each excitation wavelength, but only those with an excitation energy less than 6.7 eV are listed here. Minimal differences were observed by using expanded basis sets, i.e. 6-311++G** vs. 6-311++G**, so only the results from 6-311++G**, aug-cc-pVDZ, and def2-TZVPD are reported.

Table S2. Simulated spectral data for 2-nitrophenol, 4-nitrophenol, 2,4-dinitrophenol, and 2,4,6-trinitrophenol.

Nitrophenol	Exchange	Basis	Energy (eV)	Wavelength (nm)	Oscillator Strength
2-nitrophenol	B3LYP	6-311++G**	3.351	370.0	8.48E-02
	B3LYP	6-311++G**	3.936	315.0	8.06E-06
	B3LYP	6-311++G**	4.428	280.0	3.95E-01
	B3LYP	6-311++G**	4.493	275.9	4.47E-04
	B3LYP	6-311++G**	5.632	220.2	1.68E-02
	B3LYP	6-311++G**	5.973	207.6	9.83E-02
	B3LYP	6-311++G**	6.020	205.9	3.31E-04
	B3LYP	6-311++G**	6.158	201.3	3.74E-03
	B3LYP	6-311++G**	6.417	193.2	2.93E-01
	B3LYP	6-311++G**	6.492	191.0	2.19E-02
	B3LYP	6-311++G**	6.517	190.2	2.59E-03
2-nitrophenol	B3LYP	aug-cc-pVTZ	3.377	367.2	8.47E-02
	B3LYP	aug-cc-pVTZ	3.953	313.6	6.65E-06
	B3LYP	aug-cc-pVTZ	4.448	278.7	3.90E-01
	B3LYP	aug-cc-pVTZ	4.490	276.1	5.00E-04
	B3LYP	aug-cc-pVTZ	5.616	220.8	1.65E-02
	B3LYP	aug-cc-pVTZ	5.981	207.3	1.16E-01
	B3LYP	aug-cc-pVTZ	6.012	206.2	2.53E-03
	B3LYP	aug-cc-pVTZ	6.020	206.0	1.53E-03
	B3LYP	aug-cc-pVTZ	6.385	194.2	2.82E-01
	B3LYP	aug-cc-pVTZ	6.388	194.1	2.66E-03
	B3LYP	aug-cc-pVTZ	6.463	191.8	9.14E-03
	B3LYP	aug-cc-pVTZ	6.579	188.4	8.68E-03

2-nitrophenol	B3LYP	def2-TZVPPD	3.376	367.3	8.44E-02
	B3LYP	def2-TZVPPD	3.951	313.8	6.82E-06
	B3LYP	def2-TZVPPD	4.449	278.7	3.89E-01
	B3LYP	def2-TZVPPD	4.489	276.2	5.04E-04
	B3LYP	def2-TZVPPD	5.625	220.4	1.53E-02
	B3LYP	def2-TZVPPD	5.987	207.1	1.09E-01
	B3LYP	def2-TZVPPD	6.017	206.1	3.77E-04
	B3LYP	def2-TZVPPD	6.246	198.5	3.00E-03
	B3LYP	def2-TZVPPD	6.398	193.8	2.94E-01
	B3LYP	def2-TZVPPD	6.466	191.7	1.10E-02
	B3LYP	def2-TZVPPD	6.629	187.0	3.97E-03
2-nitrophenol	PBE0	6-311++G**	3.525	351.8	9.95E-02
	PBE0	6-311++G**	4.011	309.1	6.09E-06
	PBE0	6-311++G**	4.564	271.6	6.68E-04
	PBE0	6-311++G**	4.573	271.1	3.88E-01
	PBE0	6-311++G**	5.776	214.6	1.61E-02
	PBE0	6-311++G**	6.169	201.0	4.29E-04
	PBE0	6-311++G**	6.177	200.7	1.44E-01
	PBE0	6-311++G**	6.414	193.3	3.39E-03
	PBE0	6-311++G**	6.569	188.7	2.80E-01
	PBE0	6-311++G**	6.647	186.5	3.14E-02
2-nitrophenol	PBE0	aug-cc-pVTZ	3.551	349.2	9.90E-02
	PBE0	aug-cc-pVTZ	4.032	307.5	5.08E-06
	PBE0	aug-cc-pVTZ	4.559	272.0	4.67E-04
	PBE0	aug-cc-pVTZ	4.595	269.8	3.83E-01
	PBE0	aug-cc-pVTZ	5.760	215.2	1.67E-02
	PBE0	aug-cc-pVTZ	6.161	201.2	4.66E-04
	PBE0	aug-cc-pVTZ	6.173	200.8	1.66E-01
	PBE0	aug-cc-pVTZ	6.265	197.9	3.34E-03
	PBE0	aug-cc-pVTZ	6.530	189.9	2.38E-01
	PBE0	aug-cc-pVTZ	6.643	186.6	4.51E-02

	PBE0	aug-cc-pVTZ	6.656	186.3	3.63E-03
2-nitrophenol	PBE0	def2-TZVPPD	3.550	349.2	9.85E-02
	PBE0	def2-TZVPPD	4.030	307.7	5.16E-06
	PBE0	def2-TZVPPD	4.558	272.0	4.68E-04
	PBE0	def2-TZVPPD	4.596	269.7	3.82E-01
	PBE0	def2-TZVPPD	5.767	215.0	1.54E-02
	PBE0	def2-TZVPPD	6.159	201.3	4.74E-04
	PBE0	def2-TZVPPD	6.182	200.5	1.58E-01
	PBE0	def2-TZVPPD	6.495	190.9	2.54E-03
	PBE0	def2-TZVPPD	6.539	189.6	2.46E-01
	PBE0	def2-TZVPPD	6.647	186.5	5.11E-02
4-nitrophenol	B3LYP	6-311++G**	3.829	323.8	1.30E-07
	B3LYP	6-311++G**	3.980	311.5	5.02E-01
	B3LYP	6-311++G**	4.159	298.1	1.60E-02
	B3LYP	6-311++G**	4.504	275.3	3.26E-04
	B3LYP	6-311++G**	5.438	228.0	6.89E-02
	B3LYP	6-311++G**	6.117	202.7	1.61E-03
	B3LYP	6-311++G**	6.143	201.8	1.51E-04
	B3LYP	6-311++G**	6.376	194.4	1.24E-01
	B3LYP	6-311++G**	6.450	192.2	1.12E-01
	B3LYP	6-311++G**	6.479	191.4	1.58E-02
	B3LYP	6-311++G**	6.530	189.9	3.28E-04
	B3LYP	6-311++G**	6.595	188.0	2.33E-06
4-nitrophenol	B3LYP	aug-cc-pVTZ	3.855	321.6	9.12E-08
	B3LYP	aug-cc-pVTZ	4.003	309.7	4.98E-01
	B3LYP	aug-cc-pVTZ	4.193	295.7	1.46E-02
	B3LYP	aug-cc-pVTZ	4.508	275.0	3.83E-04
	B3LYP	aug-cc-pVTZ	5.413	229.0	6.92E-02
	B3LYP	aug-cc-pVTZ	6.004	206.5	1.67E-03
	B3LYP	aug-cc-pVTZ	6.148	201.7	5.82E-05

	B3LYP	aug-cc-pVTZ	6.358	195.0	9.76E-02
	B3LYP	aug-cc-pVTZ	6.403	193.6	1.09E-01
	B3LYP	aug-cc-pVTZ	6.405	193.6	3.66E-04
	B3LYP	aug-cc-pVTZ	6.488	191.1	5.32E-02
	B3LYP	aug-cc-pVTZ	6.551	189.2	3.47E-05
	B3LYP	aug-cc-pVTZ	6.639	186.7	2.43E-05
4-nitrophenol	B3LYP	def2-TZVPPD	3.853	321.8	9.28E-08
	B3LYP	def2-TZVPPD	4.003	309.7	4.97E-01
	B3LYP	def2-TZVPPD	4.193	295.7	1.44E-02
	B3LYP	def2-TZVPPD	4.506	275.2	3.86E-04
	B3LYP	def2-TZVPPD	5.423	228.6	6.74E-02
	B3LYP	def2-TZVPPD	6.145	201.7	2.54E-05
	B3LYP	def2-TZVPPD	6.212	199.6	1.62E-03
	B3LYP	def2-TZVPPD	6.381	194.3	1.05E-01
	B3LYP	def2-TZVPPD	6.406	193.5	1.14E-01
	B3LYP	def2-TZVPPD	6.498	190.8	4.03E-02
	B3LYP	def2-TZVPPD	6.559	189.0	4.29E-05
	B3LYP	def2-TZVPPD	6.626	187.1	5.72E-04
4-nitrophenol	PBE0	6-311++G**	3.902	317.8	1.14E-07
	PBE0	6-311++G**	4.127	300.4	5.14E-01
	PBE0	6-311++G**	4.367	283.9	1.47E-02
	PBE0	6-311++G**	4.574	271.1	2.97E-04
	PBE0	6-311++G**	5.568	222.7	8.15E-02
	PBE0	6-311++G**	6.297	196.9	3.52E-05
	PBE0	6-311++G**	6.386	194.1	2.11E-03
	PBE0	6-311++G**	6.534	189.7	9.32E-02
	PBE0	6-311++G**	6.572	188.6	1.41E-01
4-nitrophenol	PBE0	aug-cc-pVTZ	3.932	315.3	7.89E-08
	PBE0	aug-cc-pVTZ	4.153	298.5	5.09E-01
	PBE0	aug-cc-pVTZ	4.402	281.7	1.34E-02
	PBE0	aug-cc-pVTZ	4.578	270.8	3.57E-04

	PBE0	aug-cc-pVTZ	5.543	223.7	8.21E-02
	PBE0	aug-cc-pVTZ	6.267	197.8	1.96E-03
	PBE0	aug-cc-pVTZ	6.297	196.9	9.80E-05
	PBE0	aug-cc-pVTZ	6.501	190.7	8.74E-02
	PBE0	aug-cc-pVTZ	6.528	189.9	1.34E-01
	PBE0	aug-cc-pVTZ	6.690	185.3	1.81E-04
4-nitrophenol	PBE0	def2-TZVPPD	3.929	315.5	7.99E-08
	PBE0	def2-TZVPPD	4.153	298.5	5.09E-01
	PBE0	def2-TZVPPD	4.401	281.7	1.33E-02
	PBE0	def2-TZVPPD	4.575	271.0	3.59E-04
	PBE0	def2-TZVPPD	5.552	223.3	8.02E-02
	PBE0	def2-TZVPPD	6.295	196.9	3.53E-05
	PBE0	def2-TZVPPD	6.481	191.3	2.11E-03
	PBE0	def2-TZVPPD	6.526	190.0	8.55E-02
	PBE0	def2-TZVPPD	6.531	189.8	1.38E-01
2,4-dinitrophenol	B3LYP	6-311++G**	3.584	345.9	8.59E-02
	B3LYP	6-311++G**	3.847	322.2	8.13E-07
	B3LYP	6-311++G**	3.964	312.8	4.28E-06
	B3LYP	6-311++G**	4.155	298.4	3.03E-01
	B3LYP	6-311++G**	4.466	277.6	2.72E-07
	B3LYP	6-311++G**	4.495	275.8	6.31E-04
	B3LYP	6-311++G**	4.545	272.8	3.19E-01
	B3LYP	6-311++G**	4.700	263.8	2.33E-01
	B3LYP	6-311++G**	4.710	263.2	6.19E-06
	B3LYP	6-311++G**	5.260	235.7	3.78E-03
	B3LYP	6-311++G**	5.265	235.5	1.10E-05
	B3LYP	6-311++G**	5.302	233.8	5.17E-06
	B3LYP	6-311++G**	5.698	217.6	3.09E-05
	B3LYP	6-311++G**	5.772	214.8	9.89E-03
	B3LYP	6-311++G**	5.942	208.7	3.48E-02

	B3LYP	6-311++G**	6.347	195.3	9.77E-02
	B3LYP	6-311++G**	6.449	192.3	3.92E-04
	B3LYP	6-311++G**	6.469	191.6	9.13E-02
	B3LYP	6-311++G**	6.561	189.0	4.08E-02
2,4-dinitrophenol	B3LYP	aug-cc-pVTZ	3.604	344.0	8.63E-02
	B3LYP	aug-cc-pVTZ	3.875	319.9	3.74E-07
	B3LYP	aug-cc-pVTZ	3.982	311.4	3.79E-06
	B3LYP	aug-cc-pVTZ	4.175	297.0	3.03E-01
	B3LYP	aug-cc-pVTZ	4.466	277.6	5.74E-06
	B3LYP	aug-cc-pVTZ	4.495	275.8	7.03E-04
	B3LYP	aug-cc-pVTZ	4.569	271.3	3.24E-01
	B3LYP	aug-cc-pVTZ	4.719	262.7	2.35E-01
	B3LYP	aug-cc-pVTZ	4.728	262.2	1.34E-05
	B3LYP	aug-cc-pVTZ	5.259	235.8	6.65E-06
	B3LYP	aug-cc-pVTZ	5.295	234.1	3.82E-03
	B3LYP	aug-cc-pVTZ	5.314	233.3	8.56E-07
	B3LYP	aug-cc-pVTZ	5.689	217.9	3.50E-05
	B3LYP	aug-cc-pVTZ	5.806	213.5	1.05E-02
	B3LYP	aug-cc-pVTZ	5.925	209.2	3.39E-02
	B3LYP	aug-cc-pVTZ	6.341	195.5	1.10E-01
	B3LYP	aug-cc-pVTZ	6.435	192.7	8.98E-02
			6.441	192.5	4.76E-04
			6.548	189.3	2.64E-02
	B3LYP	aug-cc-pVTZ	6.554	189.2	1.93E-04
2,4-dinitrophenol	B3LYP	def2-TZVPPD	3.603	344.1	8.60E-02
	B3LYP	def2-TZVPPD	3.873	320.2	4.06E-07
	B3LYP	def2-TZVPPD	3.980	311.5	3.83E-06
	B3LYP	def2-TZVPPD	4.175	297.0	3.02E-01
	B3LYP	def2-TZVPPD	4.464	277.7	3.94E-06
	B3LYP	def2-TZVPPD	4.493	275.9	7.11E-04
	B3LYP	def2-TZVPPD	4.569	271.4	3.23E-01

	B3LYP	def2-TZVPPD	4.719	262.7	2.35E-01
	B3LYP	def2-TZVPPD	4.726	262.3	1.50E-05
	B3LYP	def2-TZVPPD	5.257	235.8	6.86E-06
	B3LYP	def2-TZVPPD	5.295	234.2	3.83E-03
	B3LYP	def2-TZVPPD	5.312	233.4	1.09E-06
	B3LYP	def2-TZVPPD	5.687	218.0	3.45E-05
	B3LYP	def2-TZVPPD	5.805	213.6	1.05E-02
	B3LYP	def2-TZVPPD	5.930	209.1	3.28E-02
	B3LYP	def2-TZVPPD	6.342	195.5	1.10E-01
	B3LYP	def2-TZVPPD	6.436	192.6	9.03E-02
	B3LYP	def2-TZVPPD	6.438	192.6	5.17E-04
	B3LYP	def2-TZVPPD	6.551	189.3	2.72E-02
2,4-dinitrophenol	PBE0	6-311++G**	3.766	329.2	9.74E-02
	PBE0	6-311++G**	3.924	315.9	8.03E-07
	PBE0	6-311++G**	4.041	306.8	3.15E-06
	PBE0	6-311++G**	4.322	286.8	3.32E-01
	PBE0	6-311++G**	4.543	272.9	1.38E-06
	PBE0	6-311++G**	4.570	271.3	5.77E-04
	PBE0	6-311++G**	4.755	260.7	3.76E-01
	PBE0	6-311++G**	4.884	253.8	1.72E-01
	PBE0	6-311++G**	5.056	245.2	1.23E-07
	PBE0	6-311++G**	5.561	222.9	3.34E-03
	PBE0	6-311++G**	5.586	222.0	1.61E-05
	PBE0	6-311++G**	5.661	219.0	1.43E-05
	PBE0	6-311++G**	6.008	206.4	3.47E-05
	PBE0	6-311++G**	6.092	203.5	1.01E-02
	PBE0	6-311++G**	6.116	202.7	3.53E-02
	PBE0	6-311++G**	6.535	189.7	1.60E-01
	PBE0	6-311++G**	6.599	187.9	1.09E-01
	PBE0	6-311++G**	6.627	187.1	5.07E-04
2,4-dinitrophenol	PBE0	aug-cc-pVTZ	3.785	327.6	9.73E-02

	PBE0	aug-cc-pVTZ	3.957	313.3	3.91E-07
	PBE0	aug-cc-pVTZ	4.063	305.1	2.81E-06
	PBE0	aug-cc-pVTZ	4.343	285.5	3.30E-01
	PBE0	aug-cc-pVTZ	4.542	273.0	7.18E-06
	PBE0	aug-cc-pVTZ	4.569	271.4	6.59E-04
	PBE0	aug-cc-pVTZ	4.781	259.3	3.89E-01
	PBE0	aug-cc-pVTZ	4.905	252.7	1.69E-01
	PBE0	aug-cc-pVTZ	5.075	244.3	2.60E-06
	PBE0	aug-cc-pVTZ	5.573	222.5	1.21E-05
	PBE0	aug-cc-pVTZ	5.599	221.4	3.50E-03
	PBE0	aug-cc-pVTZ	5.672	218.6	3.93E-06
	PBE0	aug-cc-pVTZ	5.994	206.9	4.02E-05
	PBE0	aug-cc-pVTZ	6.098	203.3	3.32E-02
	PBE0	aug-cc-pVTZ	6.131	202.2	1.32E-02
	PBE0	aug-cc-pVTZ	6.512	190.4	1.58E-01
	PBE0	aug-cc-pVTZ	6.566	188.8	1.07E-01
	PBE0	aug-cc-pVTZ	6.610	187.6	5.98E-04
2,4-dinitrophenol	PBE0	def2-TZVPPD	3.784	327.6	9.70E-02
	PBE0	def2-TZVPPD	3.954	313.6	4.17E-07
	PBE0	def2-TZVPPD	4.061	305.3	2.82E-06
	PBE0	def2-TZVPPD	4.343	285.5	3.30E-01
	PBE0	def2-TZVPPD	4.540	273.1	5.05E-06
	PBE0	def2-TZVPPD	4.567	271.5	6.64E-04
	PBE0	def2-TZVPPD	4.781	259.3	3.87E-01
	PBE0	def2-TZVPPD	4.906	252.7	1.70E-01
	PBE0	def2-TZVPPD	5.073	244.4	2.34E-06
	PBE0	def2-TZVPPD	5.571	222.5	1.21E-05
	PBE0	def2-TZVPPD	5.599	221.4	3.51E-03
	PBE0	def2-TZVPPD	5.671	218.6	4.48E-06
	PBE0	def2-TZVPPD	5.993	206.9	3.95E-05
	PBE0	def2-TZVPPD	6.102	203.2	3.17E-02

	PBE0	def2-TZVPPD	6.129	202.3	1.34E-02
	PBE0	def2-TZVPPD	6.514	190.3	1.58E-01
	PBE0	def2-TZVPPD	6.568	188.8	1.07E-01
	PBE0	def2-TZVPPD	6.608	187.6	5.78E-04
2,4,6-trinitrophenol	PBE0	6-311++G**	3.815	324.9	1.30E-01
	PBE0	6-311++G**	3.948	314.1	1.16E-04
	PBE0	6-311++G**	3.969	312.4	2.49E-02
	PBE0	6-311++G**	4.048	306.3	8.05E-04
	PBE0	6-311++G**	4.431	279.8	1.24E-01
	PBE0	6-311++G**	4.468	277.5	5.52E-02
	PBE0	6-311++G**	4.540	273.1	2.52E-02
	PBE0	6-311++G**	4.551	272.4	1.94E-02
	PBE0	6-311++G**	4.614	268.7	1.20E-01
	PBE0	6-311++G**	4.799	258.4	2.48E-01
	PBE0	6-311++G**	4.918	252.1	1.50E-03
	PBE0	6-311++G**	4.984	248.8	1.13E-01
	PBE0	6-311++G**	5.264	235.5	6.73E-02
	PBE0	6-311++G**	5.351	231.7	7.75E-02
	PBE0	6-311++G**	5.430	228.3	7.11E-02
	PBE0	6-311++G**	5.469	226.7	1.80E-02
	PBE0	6-311++G**	5.495	225.6	3.42E-02
	PBE0	6-311++G**	5.566	222.8	2.60E-02
	PBE0	6-311++G**	5.599	221.4	1.24E-02
	PBE0	6-311++G**	5.651	219.4	2.70E-03
	PBE0	6-311++G**	5.738	216.1	1.81E-03
	PBE0	6-311++G**	5.794	214.0	9.04E-03
	PBE0	6-311++G**	5.844	212.2	5.19E-04
	PBE0	6-311++G**	5.958	208.1	8.10E-03
	PBE0	6-311++G**	6.012	206.2	1.87E-02
	PBE0	6-311++G**	6.079	204.0	1.47E-02

	PBE0	6-311++G**	6.116	202.7	2.44E-03
	PBE0	6-311++G**	6.225	199.2	2.37E-02
	PBE0	6-311++G**	6.230	199.0	5.34E-03
	PBE0	6-311++G**	6.424	193.0	6.01E-03
	PBE0	6-311++G**	6.437	192.6	1.61E-02
	PBE0	6-311++G**	6.628	187.1	1.69E-01
2,4,6-trinitrophenol		**aug-cc-pVTZ failed to converge after 300 SCF cycles**			
	PBE0	aug-cc-pVDZ	3.821	324.5	1.36E-01
	PBE0	aug-cc-pVDZ	3.967	312.5	1.31E-04
	PBE0	aug-cc-pVDZ	3.985	311.2	1.95E-02
	PBE0	aug-cc-pVDZ	4.064	305.1	7.08E-04
	PBE0	aug-cc-pVDZ	4.434	279.6	1.30E-01
	PBE0	aug-cc-pVDZ	4.475	277.0	4.82E-02
	PBE0	aug-cc-pVDZ	4.548	272.6	4.04E-02
	PBE0	aug-cc-pVDZ	4.561	271.8	1.25E-02
	PBE0	aug-cc-pVDZ	4.620	268.3	1.10E-01
	PBE0	aug-cc-pVDZ	4.810	257.7	2.60E-01
	PBE0	aug-cc-pVDZ	4.920	252.0	1.68E-03
	PBE0	aug-cc-pVDZ	4.991	248.4	1.11E-01
	PBE0	aug-cc-pVDZ	5.271	235.2	5.98E-02
	PBE0	aug-cc-pVDZ	5.369	230.9	1.05E-01
	PBE0	aug-cc-pVDZ	5.449	227.5	6.88E-02
	PBE0	aug-cc-pVDZ	5.497	225.6	2.57E-02
	PBE0	aug-cc-pVDZ	5.527	224.3	9.63E-03
	PBE0	aug-cc-pVDZ	5.569	222.6	3.07E-02
	PBE0	aug-cc-pVDZ	5.604	221.2	1.39E-02
	PBE0	aug-cc-pVDZ	5.655	219.2	2.73E-03
	PBE0	aug-cc-pVDZ	5.745	215.8	1.49E-03
	PBE0	aug-cc-pVDZ	5.805	213.6	8.43E-03
	PBE0	aug-cc-pVDZ	5.884	210.7	6.46E-04
	PBE0	aug-cc-pVDZ	5.957	208.1	8.42E-03

	PBE0	aug-cc-pVDZ	6.044	205.1	2.20E-02
	PBE0	aug-cc-pVDZ	6.112	202.8	1.27E-03
	PBE0	aug-cc-pVDZ	6.120	202.6	1.65E-02
	PBE0	aug-cc-pVDZ	6.228	199.1	2.76E-03
	PBE0	aug-cc-pVDZ	6.249	198.4	2.68E-02
	PBE0	aug-cc-pVDZ	6.415	193.3	6.00E-03
	PBE0	aug-cc-pVDZ	6.432	192.8	1.51E-02
	PBE0	aug-cc-pVDZ	6.618	187.3	1.62E-01
2,4,6-trinitrophenol	PBE0	def2-TZVPPD	3.977	311.8	1.09E-04
	PBE0	def2-TZVPPD	3.996	310.3	1.88E-02
	PBE0	def2-TZVPPD	4.068	304.8	6.85E-04
	PBE0	def2-TZVPPD	4.448	278.7	1.12E-01
	PBE0	def2-TZVPPD	4.469	277.4	6.05E-02
	PBE0	def2-TZVPPD	4.538	273.2	3.04E-02
	PBE0	def2-TZVPPD	4.551	272.4	1.15E-02
	PBE0	def2-TZVPPD	4.625	268.1	1.23E-01
	PBE0	def2-TZVPPD	4.821	257.2	2.67E-01
	PBE0	def2-TZVPPD	4.934	251.3	1.60E-03
	PBE0	def2-TZVPPD	5.005	247.7	1.12E-01
	PBE0	def2-TZVPPD	5.267	235.4	5.34E-02
	PBE0	def2-TZVPPD	5.371	230.8	9.88E-02
	PBE0	def2-TZVPPD	5.452	227.4	7.48E-02
	PBE0	def2-TZVPPD	5.493	225.7	2.39E-02
	PBE0	def2-TZVPPD	5.524	224.5	1.23E-02
	PBE0	def2-TZVPPD	5.572	222.5	3.40E-02
	PBE0	def2-TZVPPD	5.601	221.3	1.56E-02
	PBE0	def2-TZVPPD	5.675	218.5	2.36E-03
	PBE0	def2-TZVPPD	5.746	215.8	7.56E-04
	PBE0	def2-TZVPPD	5.811	213.4	9.31E-03
	PBE0	def2-TZVPPD	5.883	210.7	5.98E-04
	PBE0	def2-TZVPPD	5.966	207.8	9.23E-03

PBE0	def2-TZVPPD	6.042	205.2	2.25E-02
PBE0	def2-TZVPPD	6.108	203.0	1.62E-03
PBE0	def2-TZVPPD	6.119	202.6	1.73E-02
PBE0	def2-TZVPPD	6.221	199.3	2.48E-03
PBE0	def2-TZVPPD	6.246	198.5	2.83E-02
PBE0	def2-TZVPPD	6.409	193.4	7.04E-03
PBE0	def2-TZVPPD	6.437	192.6	1.15E-02
PBE0	def2-TZVPPD	6.609	187.6	1.64E-01

END OF TABLE