SUPPORTING INFORMATION

Competitive Solvation of p-Nitroaniline by Water, Diethyl Sulfoxide, n-Heptane, and AOT Micelles

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Table S1. The optimized coordinates for NA in vacuo, E(RM11) = -492.080916 hartree.

C	1.35349700	1.20729500	0.00025300
C	2.06711000	-0.00000400	-0.00026900
C	1.35344300	-1.20727900	0.00040500
C	-0.02348500	-1.20671700	0.00147000
C	-0.70113300	0.00004200	0.00201100
C	-0.02343700	1.20678100	0.00134800
H	1.89749300	2.14820700	-0.00018600
H	1.89740400	-2.14821100	0.00010700
H	-0.59139700	-2.13113600	0.00197800
H	-0.59130600	2.13122000	0.00180900
N	-2.15976300	0.00000800	0.00323900
N	3.43079800	-0.00002500	-0.00092700
H	3.94693200	0.85979200	-0.00436000
H	3.94692200	-0.85984400	-0.00447300
O	-2.72235300	-1.07511700	-0.00281500
O	-2.72255500	1.07503900	-0.00248100

Table S2. The optimized coordinates for NA in implicit solvent n-heptane, E(RM11) = -492.085982 hartree.

C	1.35429600	1.20982000	-0.00183000
C	2.06805400	0.00005000	0.00004500
C	1.35423200	-1.20969900	0.00139800
C	-0.02185400	-1.20882500	0.00110500
C	-0.69882800	0.00014500	-0.00029400
C	-0.02171700	1.20910300	-0.00171500
H	1.89793800	2.15064700	-0.00328900
H	1.89764400	-2.15066400	0.00311700
H	-0.58576500	-2.13551200	0.00173100
H	-0.58565200	2.13575500	-0.00299900
N	-2.15573400	-0.00000700	0.00008600
N	3.42769000	-0.00011300	0.00096200
H	3.94500500	0.86011100	-0.00158900
H	3.94419600	-0.86083200	-0.00073600
O	-2.72612500	-1.07238100	-0.00373200
O	-2.72664500	1.07210200	0.00425400

Table S3. The optimized coordinates for NA in implicit solvent DESO, E(RM11) = -492.094714 hartree.

C	1.35316100	1.21351800	0.00013500
C	2.06860800	0.00000100	0.00008200
C	1.35316400	-1.21351800	0.00017300
C	-0.02081200	-1.21224200	0.00018800
C	-0.69885400	-0.00000100	0.00016100
C	-0.02081500	1.21223900	0.00015900
H	1.89677200	2.15386400	0.00013900
H	1.89677800	-2.15386200	0.00022500
H	-0.57903100	-2.14235200	0.00019300
H	-0.57903600	2.14234900	0.00013400
N	-2.14723200	-0.00000100	0.00008500
N	3.42059400	0.00000000	0.00042500
H	3.93849100	0.86178800	-0.00287200
H	3.93849000	-0.86178800	-0.00290700
O	-2.72704900	-1.07069000	-0.00028600
O	-2.72704000	1.07069300	-0.00019700

Table S4. The optimized coordinates for NA in implicit solvent water, E(RM11) = -492.094907 hartree.

C	1.35355800	1.21191900	-0.00056400
C	2.06942500	0.00011100	0.00015800
C	1.35374600	-1.21183300	0.00021100
C	-0.02073600	-1.21053500	0.00008200
C	-0.70028000	-0.00009200	-0.00021700
C	-0.02090100	1.21042600	-0.00055200
H	1.89725200	2.15250400	-0.00117300
H	1.89748500	-2.15239200	0.00047400
H	-0.58050300	-2.13968000	0.00002700
H	-0.58095200	2.13942300	-0.00104800
N	-2.14972000	-0.00005200	-0.00001300
N	3.42365600	0.00000900	0.00100400
H	3.94237900	0.86052800	-0.00178000
H	3.94171700	-0.86093900	-0.00172200
O	-2.72795200	-1.07105200	-0.00071700
O	-2.72752300	1.07116300	0.00116600

Table S5. The optimized coordinates for Na-ion coordinates the AOT anion and the DESO molecule the presence of NA and water, E (RM11) = -2639.6 hartree.

S	-0.00967500	-1.18066400	0.67127300
O	-0.41263900	0.18956400	0.89563100
O	-0.84218300	-1.90234600	-0.29364800
O	0.20715500	-1.96506300	1.89168700
C	1.64579800	-1.09791700	-0.10879000
H	1.59127300	-0.29688800	-0.85385800
C	2.02264000	-2.45025400	-0.71461500
C	2.70338200	-0.73225100	0.92680100
C	3.64235800	-1.32236900	-2.17225000
H	3.74117900	-0.61253200	-1.35086000
C	5.01122100	-1.83518700	-2.56852900
H	5.62086600	-1.00255800	-2.93130600
H	5.51301900	-2.29079700	-1.71068500
H	4.92245900	-2.57798500	-3.36769600
C	3.07584500	2.28412700	2.81885100
H	3.73633100	2.66803600	3.60161000
H	3.25221700	2.85159300	1.90149400
H	2.03793000	2.43206900	3.13611300
O	1.54713500	-3.48570300	-0.30941100
O	3.68941800	-1.40728000	1.10101700
O	2.41039600	0.37127700	1.57561600
O	2.90448400	-2.48965800	-1.69079800
C	3.35019400	0.81159000	2.60541200
H	4.35350300	0.65399500	2.19782300
C	2.88621200	-0.69925600	-3.32861300
H	1.87831500	-0.39576300	-3.02975000
H	3.42310500	0.18845900	-3.67682300
H	2.80252100	-1.40883700	-4.15773400
C	3.13105800	-0.02327400	3.85328800
H	3.82994700	0.29298900	4.63315400
H	2.10983700	0.11990100	4.22194800
H	3.29352700	-1.08436800	3.64779200
Na	-0.39290600	-4.08435700	0.85310900
S	-5.05502400	-0.56435800	-0.25842600
O	-5.18827100	0.64979100	-1.16063300
C	-3.65622400	-0.20832600	0.81948900
H	-3.83195600	0.78819600	1.23938000
H	-2.79419200	-0.15648400	0.14584600
C	-3.45350400	-1.27453800	1.88655800
H	-2.49471700	-1.10259300	2.38316200
H	-4.24005800	-1.24612500	2.64528600
H	-3.42558700	-2.27562400	1.44343100
C	-6.39189900	-0.41575400	0.94469900
H	-6.29199500	-1.26556700	1.62633300
H	-6.22314700	0.51527400	1.49640200
C	-7.73267900	-0.42206800	0.22550700
H	-7.78781800	0.40621200	-0.48557000
H	-7.88444300	-1.36013000	-0.31714500

H	-8.54255200	-0.31070200	0.95093100
C	-2.13892200	2.34111100	-0.94242900
C	-1.73790100	1.45090300	-1.96167600
C	-0.37299300	1.38926100	-2.31350400
C	0.55375000	2.15656800	-1.65515700
C	0.13365100	3.00443600	-0.63293000
C	-1.21141000	3.10257400	-0.28338500
H	-3.19379900	2.39948200	-0.68678400
H	-0.07052300	0.73220600	-3.12430500
H	1.60440500	2.11115600	-1.93081300
H	-1.50917800	3.78226500	0.50797600
N	1.09358600	3.80993700	0.06324000
N	-2.65208900	0.68922100	-2.59059200
H	-2.36973900	0.03905400	-3.30432000
H	-3.62201000	0.69770600	-2.28320200
O	2.27513200	3.74250000	-0.26934400
O	0.71726200	4.54332100	0.95619200
O	3.94882100	1.46712200	-0.63906900
H	3.38021400	2.23431300	-0.47920200
H	4.64057600	1.76373900	-1.23721800

Table S6. The optimized coordinates for AOT + NA + DESO subsystem, E(RM11) = -2563.1 hartree.

S	2.18150200	0.75349600	-1.07127000
O	1.24989000	-0.26507400	-1.54638000
O	2.64029000	1.66956900	-2.09731500
O	3.23931400	0.21264000	-0.22433900
C	1.14017100	1.79908800	0.01545500
H	0.23421200	1.97285200	-0.55992700
C	1.92501300	3.06764900	0.32645200
C	0.78873900	1.06477900	1.30192700
C	0.12804200	4.44895400	-0.64748800
H	-0.58010800	3.75856400	-0.17765800
C	-0.25696300	5.87263600	-0.30323400
H	-0.29784600	6.01339100	0.77967400
H	0.47072700	6.57047200	-0.72853400
H	-1.24127600	6.09213700	-0.72563300
C	-2.52180700	0.46103000	2.55857200
H	-2.96143600	0.18094300	3.52011800
H	-2.75643900	1.50998400	2.35760700
H	-2.96682800	-0.16224200	1.77598300
O	2.99096900	3.00650500	0.89330400
O	1.59109800	0.81834400	2.17070100
O	-0.49233100	0.77153500	1.35190700
O	1.43979000	4.23733600	-0.03004400
C	-1.02535900	0.24250200	2.61658200
H	-0.56894000	0.84681700	3.40759900
C	0.23555900	4.21389600	-2.14139400
H	0.94201600	4.92936500	-2.57415800
H	0.58329700	3.20375400	-2.37680600
H	-0.74387400	4.36687600	-2.60337200
C	-0.64588200	-1.21503400	2.77706200
H	0.43795500	-1.33056100	2.84641900
H	-1.09659900	-1.60126300	3.69611600
H	-1.02685600	-1.79555600	1.93020400
Na	4.00583400	1.06198800	1.80762900
S	1.84577700	-4.29721100	-0.29361800
O	0.37178000	-4.65459100	-0.35112400
C	2.20486900	-3.52830400	-1.88812900
H	1.39886400	-2.81024400	-2.07247700
H	2.12286700	-4.34906000	-2.60654400
C	3.57523300	-2.86886100	-1.91902600
H	4.35573600	-3.54995800	-1.56308800
H	3.81892300	-2.58734300	-2.94708300
H	3.58588100	-1.96132000	-1.30898100
C	1.94999000	-2.84185600	0.79011900
H	1.71527000	-1.94191700	0.21022800
H	1.13370200	-3.03653300	1.49089700
C	3.28367300	-2.72949100	1.51470600
H	3.53533400	-3.66535300	2.02228800
H	4.09681700	-2.46954100	0.83281200

H	3.21159000	-1.94185200	2.27163100
C	-3.24605100	-2.34204900	-0.14735800
C	-2.18565300	-1.56453300	-0.66052400
C	-2.45380300	-0.23676500	-1.06199400
C	-3.71746200	0.28451800	-0.96231100
C	-4.74336000	-0.50591000	-0.45072200
C	-4.51086900	-1.81517700	-0.04413600
H	-3.05076500	-3.36352700	0.16792000
H	-1.63751500	0.36235000	-1.45775400
H	-3.92888600	1.30215500	-1.27337700
H	-5.33043400	-2.40600100	0.35121500
N	-6.07257900	0.04406500	-0.34153900
N	-0.94052900	-2.06191900	-0.76752400
H	-0.18517000	-1.44275300	-1.03573600
H	-0.71196900	-3.02430500	-0.52999600
O	-6.25943400	1.19227400	-0.70724400
O	-6.96031600	-0.65981500	0.10938400

Table S7. The optimized coordinates of the AOT + NA + n-heptane composition, E(RM11) = -1813.4 hartree.

Na	-0.09422400	1.37967500	-0.93331200
S	0.87246300	-1.93924700	-0.97954100
O	1.96546400	-1.07956900	2.21677700
O	0.10827800	-0.78473400	-1.46732600
O	0.19082400	-2.69288200	0.06444900
O	1.46592700	-2.73096000	-2.03318700
O	1.11285800	0.58469200	1.01108600
O	3.72893700	1.61439000	0.07307100
O	2.13434900	1.89153400	-1.45721400
C	2.30016100	-1.18167900	-0.11842800
C	1.74046600	-0.45470900	1.07859900
C	3.09103300	-0.30703300	-1.11867200
C	2.91832700	1.17214000	-0.87955900
C	1.40120600	-0.47802100	3.39375100
C	3.54188700	2.98027000	0.47518100
H	2.89784200	-2.02574600	0.22638500
H	2.76124400	-0.53730200	-2.13415400
H	4.15399500	-0.53859900	-1.02702100
H	1.64400300	-1.14888100	4.21647600
H	1.84228000	0.50995000	3.54930300
H	4.28641900	3.17070800	1.24738200
H	3.68650700	3.64424500	-0.38045600
C	-1.96899700	-0.87516500	1.05913400
C	-2.90227000	-1.69458400	0.39554800
C	-3.97901100	-1.09002400	-0.27676300
C	-4.05378100	0.27952500	-0.38824200
C	-3.05313200	1.05314500	0.17985500
C	-2.03354600	0.48656700	0.93855400
H	-1.16594900	-1.34786900	1.61525600
H	-1.29837700	1.12061300	1.42752900
N	-3.00273000	2.46869700	-0.09999200
N	-2.74799200	-3.04390200	0.43233400
H	-1.79550900	-3.36983600	0.54671200
H	-3.32002600	-3.59941700	-0.18260400
O	-4.01726100	3.05413400	-0.39201800
O	-1.89528200	3.00461800	-0.06107400
H	-4.84872300	0.75968500	-0.95082700
H	-4.72543300	-1.71484600	-0.75940100
H	0.31822100	-0.37943900	3.27757900
H	2.52880900	3.10233000	0.87028000