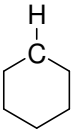
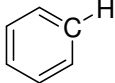
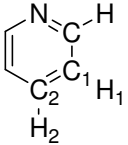
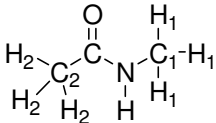



Supporting Information for:

"Integrated Continuum Dielectric Approaches to treat Molecular Polarizability and the Condensed Phase: Refractive Index and Implicit Solvation"

Jean-François Truchon, Anthony Nicholls, Benoît Roux, Radu I. Iftimie and Christopher I. Bayly

Table S1. The atomic partial charges (atomic units) fitted with DRESP<sup>1</sup> on B3LYP/6-311++G(3df,3pd) electrostatic potential

																							
	cyclohexane		benzene		pyridine							N-methylacetamide								dimethylsulfone			
Model	C	H	C	H	N	C	H	C <sub>1</sub>	H <sub>1</sub>	C <sub>2</sub>	H <sub>2</sub>	O	C	N	H	C <sub>1</sub>	H <sub>1</sub>	C <sub>2</sub>	H <sub>2</sub>	S	O	C	H
$\epsilon_{in}=1$	0.05	-0.02	-0.12	0.12	-0.73	0.59	0.00	-0.66	0.21	0.40	0.05	-0.57	0.80	-0.44	0.28	-0.19	0.11	-0.96	0.25	1.03	-0.50	-0.77	0.25
G1-4	0.05	-0.02	-0.25	0.25	-1.31	1.05	0.02	-1.19	0.39	0.66	0.10	-0.93	1.49	-0.90	0.52	-0.39	0.19	-1.63	0.41	1.75	-0.81	-1.11	0.35
G1-12	0.14	-0.07	-0.42	0.42	-2.11	1.72	0.03	-1.93	0.65	0.99	0.17	-1.40	2.71	-1.59	0.85	-0.81	0.35	-2.97	0.73	3.02	-1.20	-2.24	0.64
G1-24	-0.23	0.12	-0.54	0.54	-2.63	2.27	-0.02	-2.57	0.87	1.35	0.17	-1.72	3.51	-2.01	1.08	-1.23	0.49	-4.33	1.08	4.14	-1.50	-3.51	0.98

<sup>1</sup>Truchon, J.-F.; Nicholls, A.; Grant, J. A.; Iftimie, R. I.; Roux, B.; Bayly, C. I. *Submitted 2008*