Supporting Information for:

Partial Atomic Charges and Screened Charge Models of the Electrostatic Potential

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This supporting information was prepared on March 11, 2012 and consists of 10 pages. We calculated the charges, dipole moments, ε_{all}, and ε_{outer} of several molecules. Tables S1–S3 show the results of 3 charged molecules without s-block and d-block elements, and Tables S4–S17 show the results of 14 molecules that contain s-block and d-block elements. All electrostatic potentials are from M06/def2-TZVP calculations.

Table S1. Charges, dipole moments, ε_{all}, and ε_{outer} of ClO_3^- derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 9.30 Debye.

charge model	point charge		ODS		FDS	
point selection scheme	MK	ChElPG	MK	ChElPG	MK	ChElPG
O	-0.46	-0.47	-0.46	-0.46	-0.46	-0.46
O	-0.46	-0.47	-0.46	-0.46	-0.46	-0.47
O	-0.46	-0.47	-0.46	-0.46	-0.46	-0.46
Cl	0.38	0.41	0.37	0.39	0.38	0.39
Dipole	9.35	9.38	9.34	9.36	9.35	9.36
ε_{all}	0.51	0.51	0.37	0.37	0.10	0.10
ε_{outer}	0.03	0.03	0.03	0.03	0.03	0.03

Table S2. Charges, dipole moments, ε_{all}, and ε_{outer} of H_3O^+ derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 15.11 Debye.

charge model	point charge		ODS		FDS	
point selection scheme	MK	ChElPG	MK	ChElPG	MK	ChElPG
O	-0.93	-0.91	-0.93	-0.92	-0.94	-0.94
H	0.64	0.64	0.64	0.64	0.65	0.65
H	0.64	0.64	0.64	0.64	0.65	0.65
H	0.64	0.64	0.64	0.64	0.65	0.65
Dipole	15.11	15.11	15.11	15.11	15.11	15.11
ε_{all}	0.21	0.21	0.16	0.16	0.02	0.02
ε_{outer}	0.01	0.01	0.00	0.00	0.00	0.00

Table S3. Charges, dipole moments, ε_{all}, and ε_{outer} of NO_3^- derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 8.86 Debye.

charge model	point charge		ODS		FDS	
point selection scheme	MK	ChElPG	MK	ChElPG	MK	ChElPG
O	-0.68	-0.69	-0.67	-0.68	-0.67	-0.67
N	1.03	1.06	1.02	1.04	1.01	1.02
O	-0.68	-0.69	-0.67	-0.68	-0.67	-0.68
O	-0.67	-0.69	-0.67	-0.68	-0.67	-0.67
Dipole	8.86	8.87	8.86	8.87	8.86	8.87
ε_{all}	0.48	0.48	0.34	0.34	0.05	0.05
ε_{outer}	0.02	0.02	0.02	0.02	0.02	0.02

Table S4. Charges, dipole moments, ε_{all}, and ε_{outer} of BeO derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 6.36 Debye.

charge model	**point charge**		**ODS**		**FDS**		**ODS (H and p-block)**	
point selection scheme	**MK**	**ChElPG**	**MK**	**ChElPG**	**MK**	**ChElPG**	**MK**	**ChElPG**
O	-1.01	-1.01	-1.01	-1.00	-0.96	-0.91	-1.01	-1.01
Be	1.01	1.01	1.01	1.00	0.96	0.91	1.01	1.01
Dipole	6.40	6.37	6.40	6.35	6.08	5.78	6.41	6.39
ε_{all}	0.45	0.45	0.37	0.37	0.31	0.30	0.39	0.39
ε_{outer}	0.19	0.19	0.19	0.19	0.24	0.24	0.19	0.19

Table S5. Charges, dipole moments, ε_{all}, and ε_{outer} of CaO derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 9.12 Debye.

charge model	**point charge**		**ODS**		**FDS**		**ODS (H and p-block)**	
point selection scheme	**MK**	**ChElPG**	**MK**	**ChElPG**	**MK**	**ChElPG**	**MK**	**ChElPG**
Ca	1.05	1.06	1.05	1.03	1.05	1.06	1.05	1.06
O	-1.05	-1.06	-1.05	-1.03	-1.05	-1.06	-1.05	-1.06
Dipole	9.15	9.21	9.14	8.93	9.17	9.27	9.15	9.22
ε_{all}	0.35	0.35	0.31	0.31	0.24	0.24	0.31	0.31
ε_{outer}	0.07	0.07	0.10	0.11	0.20	0.20	0.07	0.07

Table S6. Charges, dipole moments, ε_{all}, and ε_{outer} of $Co(CN)_6^{3-}$ derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 26.00 Debye.

Charge model	**point charge**		**ODS**		**FDS**		**ODS (H and p-block)**	
point selection scheme	**MK**	**ChElPG**	**MK**	**ChElPG**	**MK**	**ChElPG**	**MK**	**ChElPG**
Co	-2.35	-0.89	-3.00	-1.94	-3.74	-3.33	-2.50	-1.13
C	0.72	0.45	0.83	0.63	0.96	0.87	0.74	0.48
C	0.74	0.45	0.86	0.63	0.99	0.87	0.76	0.48
C	0.74	0.45	0.87	0.63	1.01	0.87	0.77	0.48
C	0.74	0.45	0.86	0.63	0.99	0.87	0.76	0.48
C	0.71	0.45	0.83	0.63	0.96	0.87	0.74	0.48
C	0.74	0.45	0.87	0.63	1.01	0.87	0.77	0.48
N	-0.84	-0.80	-0.85	-0.80	-0.87	-0.82	-0.84	-0.79
N	-0.83	-0.80	-0.84	-0.80	-0.85	-0.82	-0.83	-0.79
N	-0.84	-0.80	-0.85	-0.80	-0.87	-0.82	-0.84	-0.79
N	-0.85	-0.80	-0.86	-0.80	-0.87	-0.82	-0.85	-0.79
N	-0.84	-0.80	-0.84	-0.80	-0.85	-0.82	-0.83	-0.79
N	-0.85	-0.80	-0.86	-0.80	-0.87	-0.82	-0.85	-0.79
dipole	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00
ε_{all}	0.78	0.69	0.59	0.51	0.14	0.12	0.65	0.54
ε_{outer}	0.01	0.01	0.01	0.01	0.00	0.01	0.01	0.01

Table S7. Charges, dipole moments, ε_{all}, and ε_{outer} of $Cu(NH_3)_2^+$ derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 12.32 Debye.

charge model	**point charge**		**ODS**		**FDS**		**ODS (H and p-block)**	
point selection scheme	**MK**	**ChElPG**	**MK**	**ChElPG**	**MK**	**ChElPG**	**MK**	**ChElPG**
Cu	0.45	0.35	0.50	0.36	0.51	0.48	0.38	0.32
N	-0.91	-0.72	-1.11	-1.04	-1.07	-1.13	-0.76	-0.64
H	0.40	0.35	0.45	0.46	0.44	0.46	0.36	0.33
H	0.40	0.35	0.45	0.46	0.44	0.46	0.36	0.33
N	-0.93	-0.72	-1.10	-1.04	-1.08	-1.13	-0.77	-0.64
H	0.40	0.35	0.45	0.46	0.44	0.46	0.36	0.33
H	0.40	0.35	0.45	0.46	0.44	0.46	0.36	0.33
H	0.40	0.35	0.45	0.46	0.44	0.46	0.36	0.33
H	0.40	0.35	0.45	0.46	0.44	0.46	0.36	0.33
Dipole	12.32	12.32	12.32	12.32	12.32	12.32	12.32	12.32
ε_{all}	0.26	0.25	0.20	0.19	0.04	0.04	0.21	0.20
ε_{outer}	0.01	0.01	0.03	0.03	0.02	0.02	0.01	0.01

Table S8. Charges, dipole moments, ε_{all}, and ε_{outer} of $Fe(CO)_4$ derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 0.00 Debye.

charge model	**point charge**		**ODS**		**FDS**		**ODS (H and p-block)**	
point selection scheme	**MK**	**ChElPG**	**MK**	**ChElPG**	**MK**	**ChElPG**	**MK**	**ChElPG**
Fe	-0.66	-0.65	-0.67	-0.80	-0.63	-0.68	-0.62	-0.56
C	0.39	0.40	0.37	0.37	0.34	0.29	0.37	0.35
C	0.39	0.40	0.37	0.37	0.34	0.29	0.37	0.35
C	0.39	0.40	0.36	0.37	0.33	0.29	0.37	0.35
C	0.39	0.40	0.37	0.37	0.33	0.29	0.37	0.35
O	-0.22	-0.24	-0.20	-0.18	-0.18	-0.12	-0.21	-0.21
O	-0.22	-0.24	-0.20	-0.18	-0.18	-0.12	-0.21	-0.21
O	-0.22	-0.24	-0.20	-0.18	-0.18	-0.12	-0.21	-0.21
O	-0.22	-0.24	-0.20	-0.18	-0.18	-0.12	-0.21	-0.21
Dipole	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.00
ε_{all}	0.47	0.49	0.34	0.38	0.39	0.46	0.34	0.34
ε_{outer}	0.13	0.19	0.20	0.31	0.30	0.53	0.11	0.11

Table S9. Charges, dipole moments, ε_{all}, and ε_{outer} of $Fe(CO)_5$ derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 0.00 Debye.

charge model	**point charge**		**ODS**		**FDS**		**ODS (H and p-block)**	
point selection scheme	**MK**	**ChElPG**	**MK**	**ChElPG**	**MK**	**ChElPG**	**MK**	**ChElPG**
Fe	-1.71	-1.42	-1.93	-1.99	-1.97	-2.37	-1.67	-1.39
C	0.56	0.49	0.61	0.62	0.60	0.68	0.54	0.47
O	-0.26	-0.26	-0.25	-0.25	-0.24	-0.21	-0.25	-0.24
C	0.67	0.65	0.68	0.68	0.67	0.68	0.65	0.60
O	-0.26	-0.28	-0.25	-0.24	-0.23	-0.19	-0.26	-0.25
C	0.67	0.65	0.68	0.68	0.67	0.68	0.65	0.60
O	-0.26	-0.28	-0.25	-0.24	-0.23	-0.19	-0.26	-0.25
C	0.56	0.49	0.61	0.62	0.60	0.67	0.54	0.47
O	-0.26	-0.26	-0.25	-0.25	-0.24	-0.21	-0.25	-0.24
C	0.56	0.49	0.61	0.62	0.60	0.67	0.54	0.47
O	-0.26	-0.26	-0.25	-0.25	-0.24	-0.21	-0.25	-0.24
Dipole	0.00	0.01	0.00	0.00	0.00	0.01	0.00	0.00
ε_{all}	0.52	0.51	0.30	0.33	0.33	0.41	0.40	0.35
ε_{outer}	0.11	0.16	0.09	0.13	0.23	0.45	0.09	0.07

Table S10. Charges, dipole moments, ε_{all}, and ε_{outer} of $MgBr_2$ derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 0.00 Debye.

charge model	point charge		ODS		FDS		ODS (H and p-block)	
point selection scheme	MK	ChElPG	MK	ChElPG	MK	ChElPG	MK	ChElPG
Mg	0.77	0.72	0.74	0.71	0.65	0.61	0.76	0.74
Br	-0.38	-0.36	-0.37	-0.36	-0.32	-0.30	-0.38	-0.37
Br	-0.38	-0.36	-0.37	-0.36	-0.32	-0.30	-0.38	-0.37
Dipole	0.01	0.00	0.00	0.00	0.00	0.00	0.01	0.00
ε_{all}	0.54	0.54	0.39	0.39	0.24	0.24	0.43	0.43
ε_{outer}	0.27	0.26	0.25	0.25	0.24	0.24	0.27	0.26

Table S11. Charges, dipole moments, ε_{all}, and ε_{outer} of $MgCl_2$ derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 0.00 Debye.

charge model	point charge		ODS		FDS		ODS (H and p-block)	
point selection scheme	MK	ChElPG	MK	ChElPG	MK	ChElPG	MK	ChElPG
Mg	0.96	0.89	0.90	0.86	0.76	0.75	0.95	0.89
Cl	-0.48	-0.44	-0.45	-0.43	-0.38	-0.37	-0.48	-0.45
Cl	-0.48	-0.44	-0.45	-0.43	-0.38	-0.37	-0.48	-0.45
Dipole	0.01	0.00	0.01	0.00	0.00	0.00	0.01	0.00
ε_{all}	0.46	0.45	0.32	0.31	0.20	0.20	0.36	0.35
ε_{outer}	0.22	0.19	0.19	0.17	0.17	0.18	0.21	0.19

Table S12. Charges, dipole moments, ε_{all}, and ε_{outer} of MgS derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 7.54 Debye.

charge model	point charge		ODS		FDS		ODS (H and p-block)	
point selection scheme	MK	ChElPG	MK	ChElPG	MK	ChElPG	MK	ChElPG
S	-0.79	-0.75	-0.77	-0.75	-0.71	-0.71	-0.80	-0.77
Mg	0.79	0.75	0.77	0.75	0.71	0.71	0.80	0.77
Dipole	8.10	7.68	7.90	7.70	7.20	7.25	8.14	7.84
ε_{all}	0.56	0.55	0.43	0.42	0.25	0.25	0.47	0.47
ε_{outer}	0.27	0.27	0.27	0.26	0.29	0.29	0.27	0.27

Table S13. Charges, dipole moments, ε_{all}, and ε_{outer} of MnO_4^- derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 9.66 Debye.

charge model	point charge		ODS		FDS		ODS (H and p-block)	
point selection scheme	MK	ChElPG	MK	ChElPG	MK	ChElPG	MK	ChElPG
Mn	0.94	1.11	0.72	0.51	0.75	0.55	0.95	1.10
O	-0.49	-0.53	-0.43	-0.38	-0.44	-0.39	-0.49	-0.53
O	-0.49	-0.53	-0.43	-0.38	-0.44	-0.39	-0.49	-0.53
O	-0.49	-0.53	-0.43	-0.38	-0.44	-0.39	-0.49	-0.53
O	-0.49	-0.53	-0.43	-0.38	-0.44	-0.39	-0.49	-0.53
Dipole	9.66	9.66	9.66	9.66	9.66	9.66	9.66	9.66
ε_{all}	0.49	0.47	0.27	0.28	0.05	0.05	0.40	0.39
ε_{outer}	0.01	0.01	0.01	0.01	0.02	0.02	0.01	0.01

Table S14. Charges, dipole moments, ε_{all}, and ε_{outer} of $NaCH_3COO$ derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 5.90 Debye.

charge model	point charge		ODS		FDS		ODS (H and p-block)	
point selection scheme	MK	ChElPG	MK	ChElPG	MK	ChElPG	MK	ChElPG
C	-0.37	-0.26	-0.47	-0.44	-0.49	-0.49	-0.25	-0.21
H	0.09	0.06	0.13	0.12	0.13	0.13	0.06	0.05
H	0.10	0.07	0.13	0.13	0.14	0.14	0.07	0.06
H	0.10	0.06	0.13	0.13	0.14	0.14	0.07	0.05
C	0.84	0.84	0.79	0.78	0.80	0.79	0.79	0.78
O	-0.81	-0.82	-0.77	-0.76	-0.78	-0.77	-0.80	-0.80
O	-0.80	-0.81	-0.76	-0.75	-0.77	-0.76	-0.79	-0.79
Na	0.86	0.86	0.81	0.80	0.83	0.83	0.86	0.86
Dipole	5.81	5.79	5.27	5.11	5.45	5.37	5.85	5.85
ε_{all}	0.43	0.42	0.32	0.32	0.11	0.11	0.28	0.27
ε_{outer}	0.05	0.06	0.08	0.09	0.06	0.07	0.04	0.05

Table S15. Charges, dipole moments, ε_{all}, and ε_{outer} of NaCl derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 8.87 Debye.

charge model	point charge		ODS		FDS		ODS (H and p-block)	
point selection scheme	MK	ChElPG	MK	ChElPG	MK	ChElPG	MK	ChElPG
Cl	-0.78	-0.77	-0.74	-0.73	-0.76	-0.75	-0.79	-0.78
Na	0.78	0.77	0.74	0.73	0.76	0.75	0.79	0.78
Dipole	8.93	8.84	8.48	8.28	8.62	8.52	8.96	8.94
ε_{all}	0.50	0.50	0.40	0.40	0.14	0.14	0.38	0.38
ε_{outer}	0.11	0.11	0.13	0.13	0.12	0.12	0.11	0.11

Table S16. Charges, dipole moments, ε_{all}, and ε_{outer} of $Ni(CO)_4$ derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 0.00 Debye.

charge model	point charge		ODS		FDS		ODS (H and p-block)	
point selection scheme	MK	ChElPG	MK	ChElPG	MK	ChElPG	MK	ChElPG
Ni	-1.12	-0.86	-1.35	-1.41	-1.37	-1.71	-1.10	-0.84
C	0.52	0.45	0.57	0.58	0.57	0.64	0.50	0.42
O	-0.24	-0.23	-0.23	-0.23	-0.22	-0.21	-0.23	-0.21
C	0.52	0.45	0.57	0.58	0.57	0.64	0.50	0.42
C	0.52	0.45	0.57	0.58	0.57	0.64	0.50	0.42
C	0.52	0.45	0.57	0.58	0.57	0.64	0.50	0.42
O	-0.24	-0.23	-0.24	-0.23	-0.23	-0.21	-0.23	-0.21
O	-0.24	-0.23	-0.24	-0.23	-0.23	-0.21	-0.23	-0.21
O	-0.24	-0.23	-0.23	-0.23	-0.22	-0.21	-0.23	-0.21
Dipole	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ε_{all}	0.53	0.55	0.30	0.33	0.32	0.40	0.39	0.37
ε_{outer}	0.11	0.22	0.10	0.15	0.23	0.44	0.06	0.10

Table S17. Charges, dipole moments, ε_{all}, and ε_{outer} of $TiCl_4$ derived from the point-charge model and the ODS and FDS models. The MK and ChElPG point selection schemes are tested. The directly calculated dipole moment is 0.00 Debye.

charge model	**point charge**		**ODS**		**FDS**		**ODS (H and p-block)**	
point selection scheme	**MK**	**ChElPG**	**MK**	**ChElPG**	**MK**	**ChElPG**	**MK**	**ChElPG**
Ti	0.20	0.46	0.08	0.16	-0.30	-0.42	0.17	0.39
Cl	-0.05	-0.11	-0.02	-0.04	0.07	0.11	-0.04	-0.10
Cl	-0.05	-0.11	-0.02	-0.04	0.08	0.11	-0.04	-0.10
Cl	-0.05	-0.11	-0.02	-0.04	0.08	0.11	-0.04	-0.10
Cl	-0.05	-0.11	-0.02	-0.04	0.08	0.11	-0.04	-0.10
dipole	0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.00
ε_{all}	0.86	1.03	0.56	0.57	0.62	0.70	0.73	0.85
ε_{outer}	0.79	1.16	0.60	0.62	1.00	1.16	0.73	1.02