Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Data

Relationships between dipole moments of diatomic molecules

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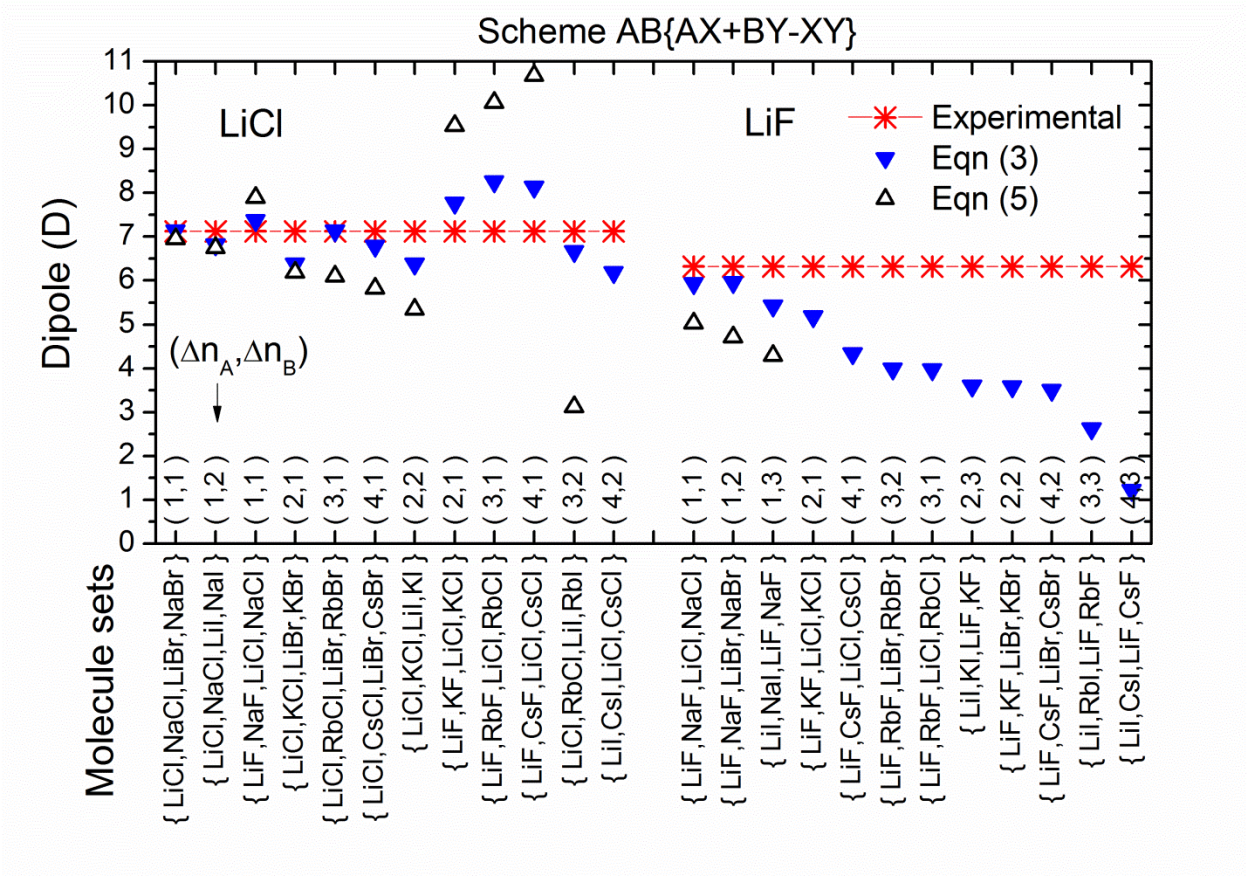

Figure S1. LiF & LiCl. The $(\Delta n_A,\Delta n_B)=(4,2)$ result from Eqn (5) for LiCl, and similar results from nine of the LiF schemes are unphysical.

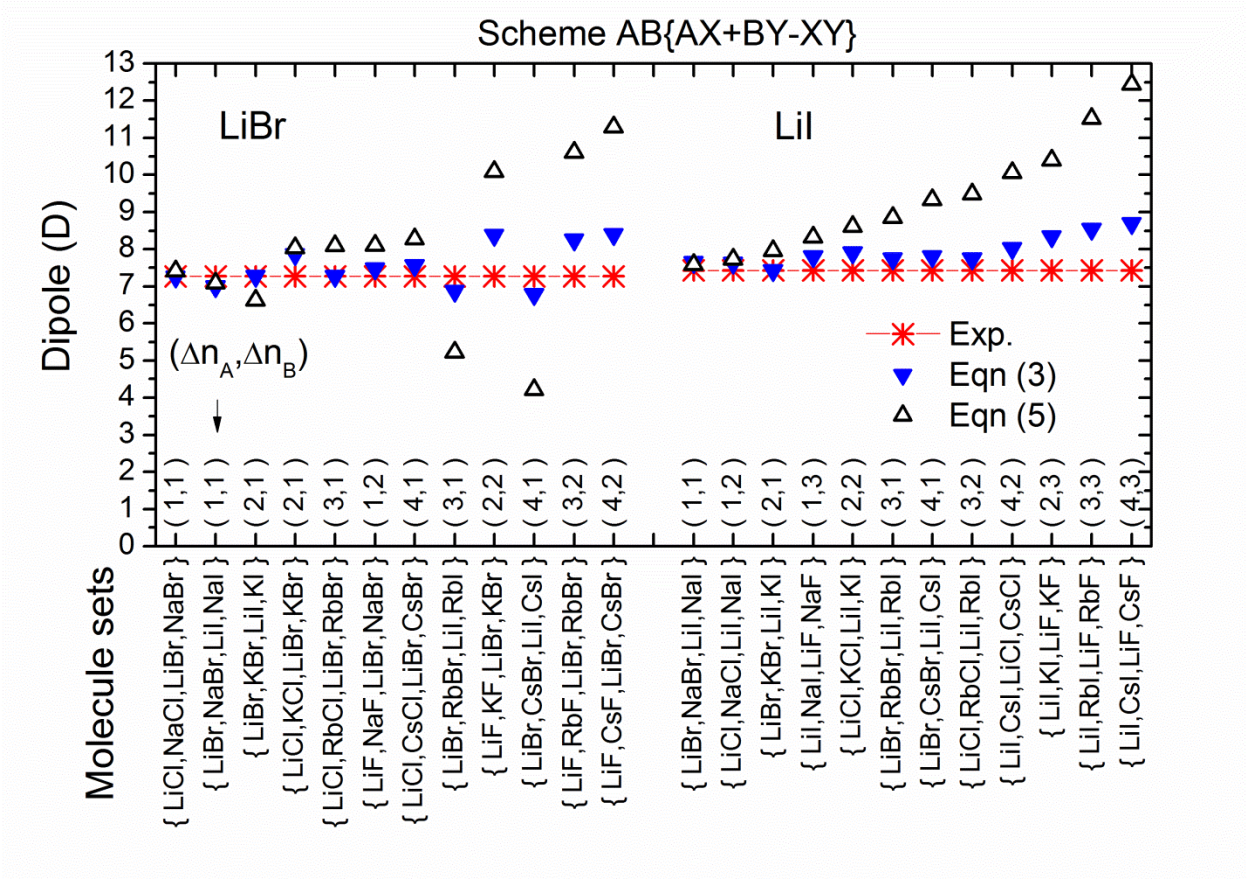

Figure S2. LiBr & LiI

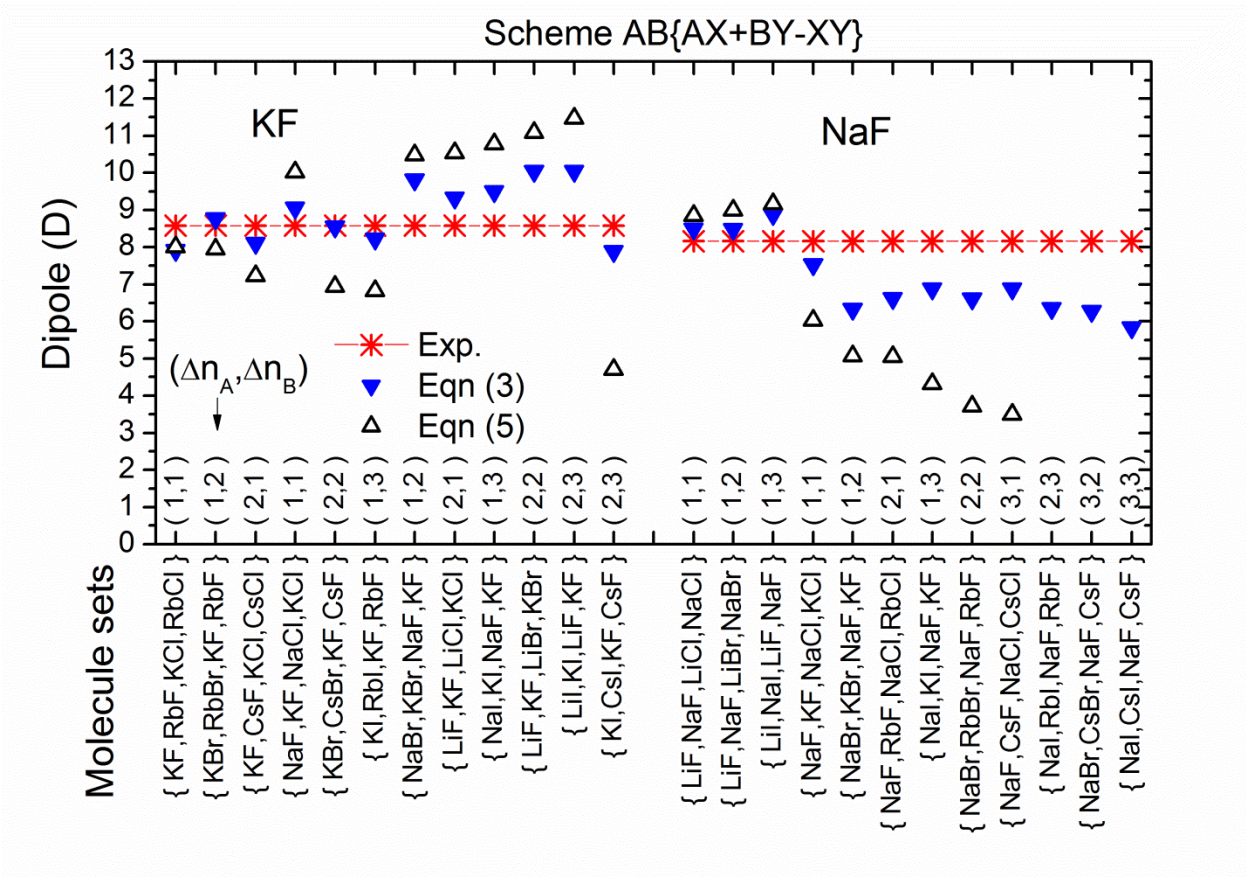

Figure S3. KF & NaF. The results from Eqn (5) for $(\Delta n_A,\Delta n_B)$ = (2,3), (3,2), and (3,3) schemes are unphysical.

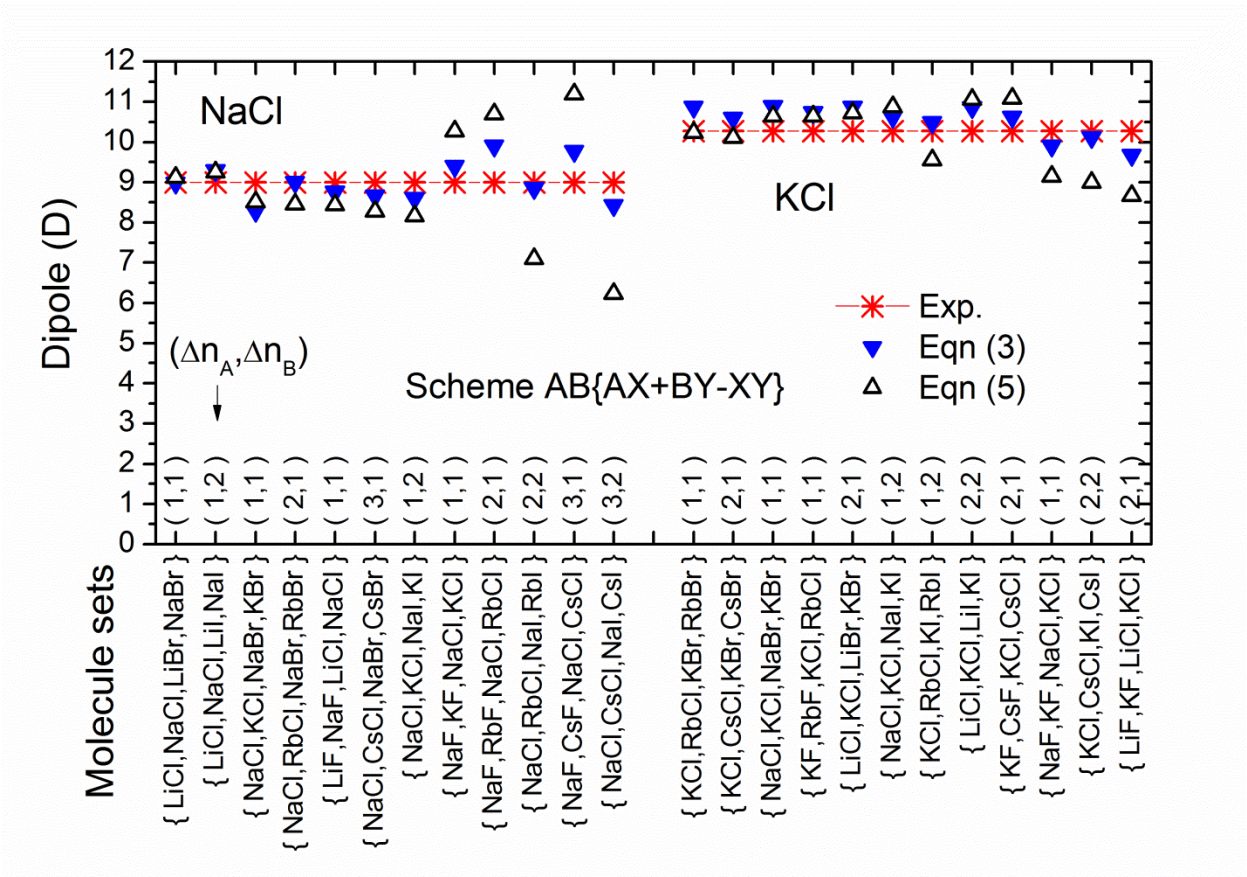

Figure S4. KCl & NaCl

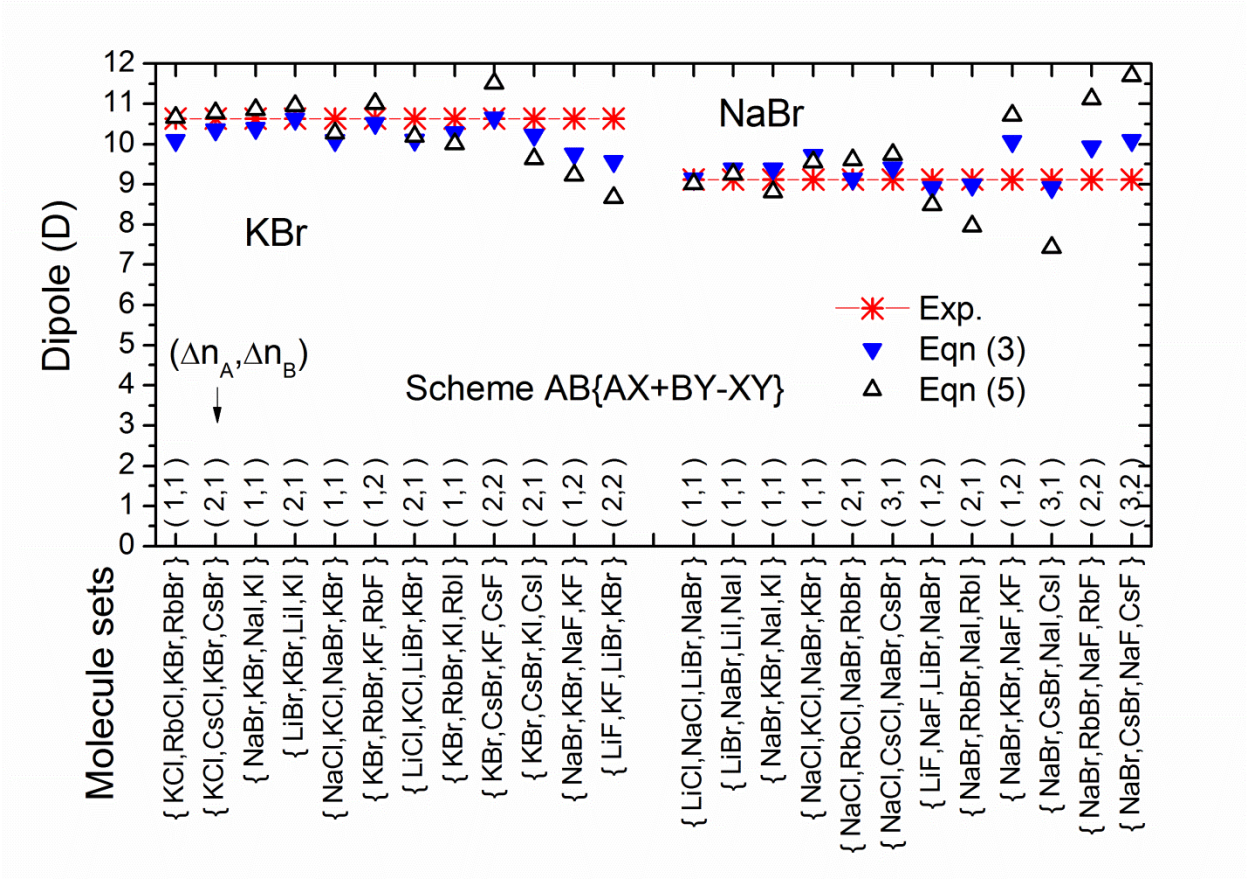

Figure S5. KBr & NaBr

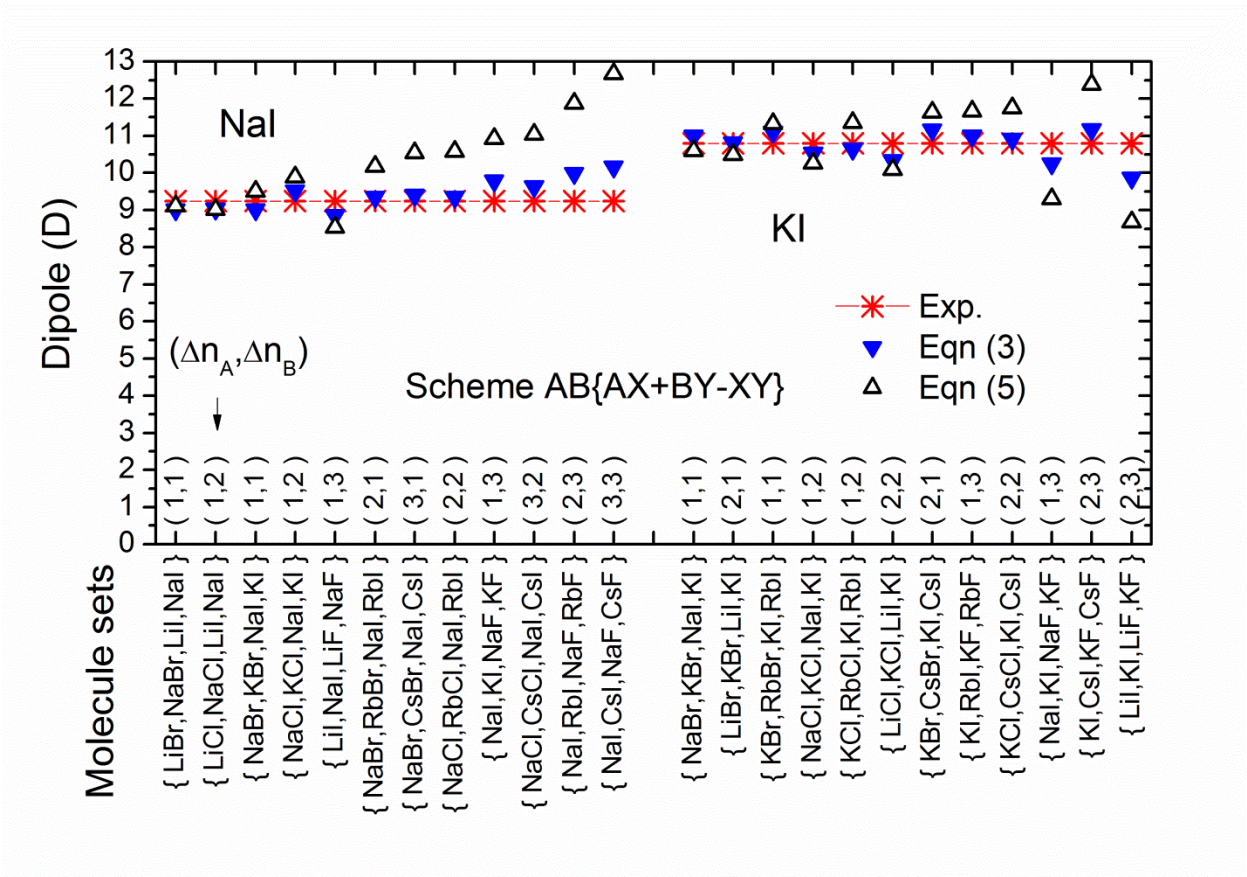

Figure S6. KI & NaI

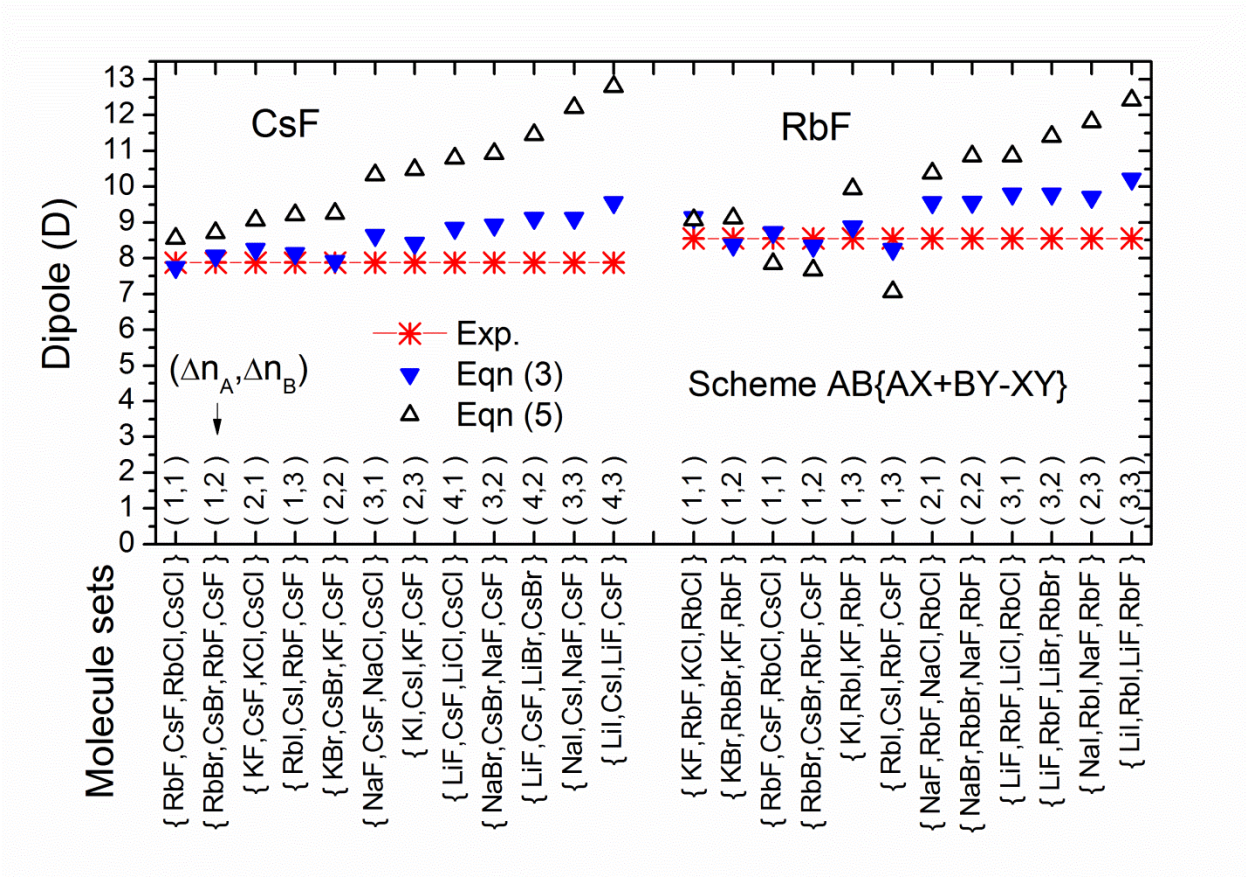

Figure S7. CsF & RbF

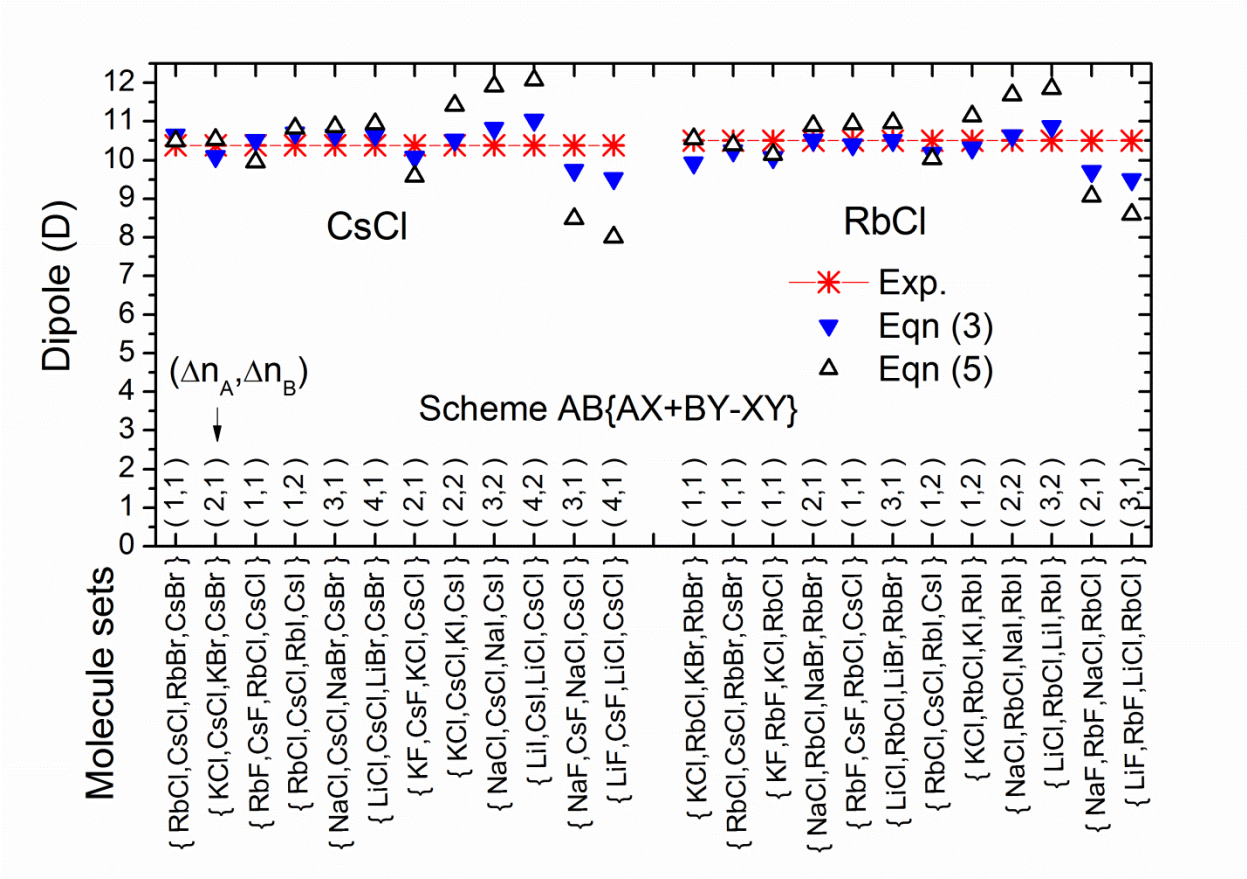

Figure S8. CsCl & RbCl

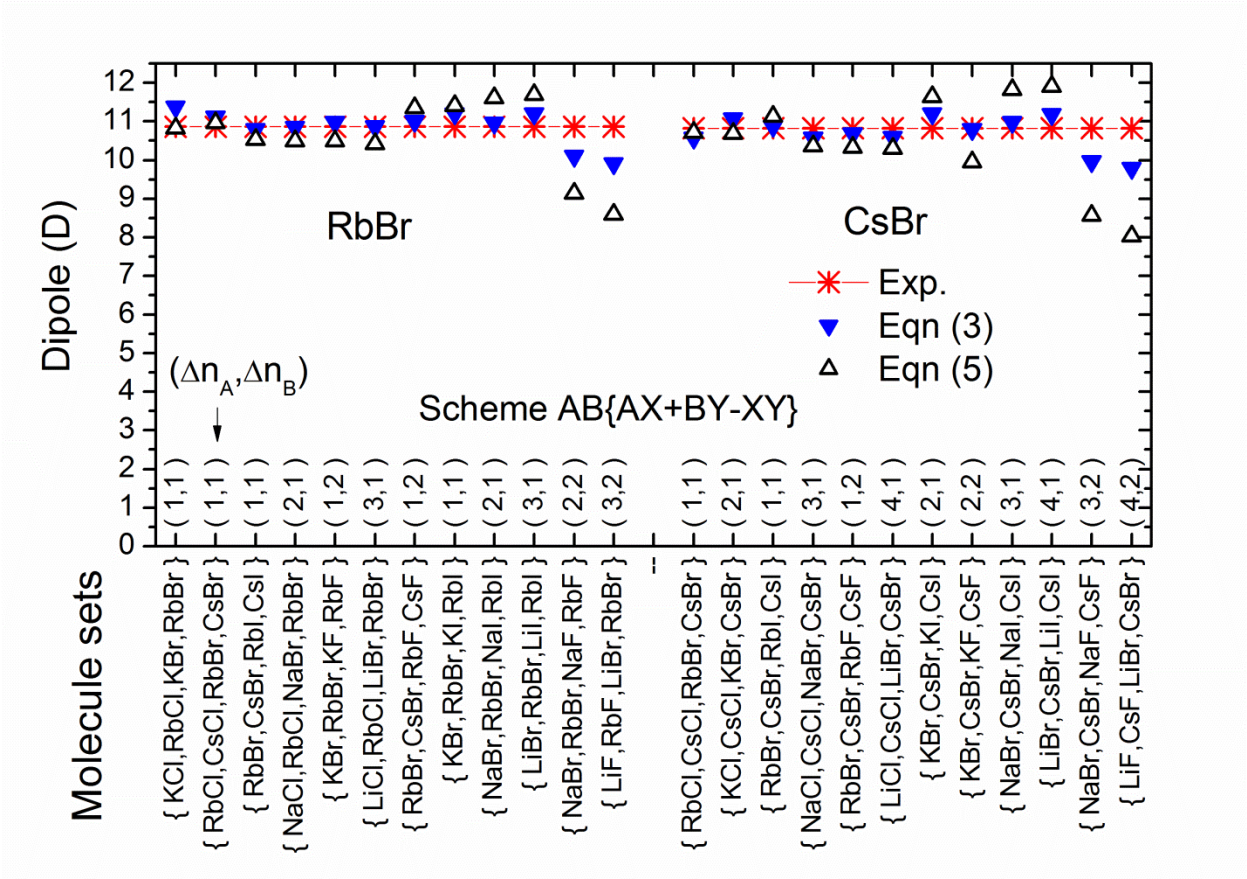

Figure S9. RbBr and CsBr.

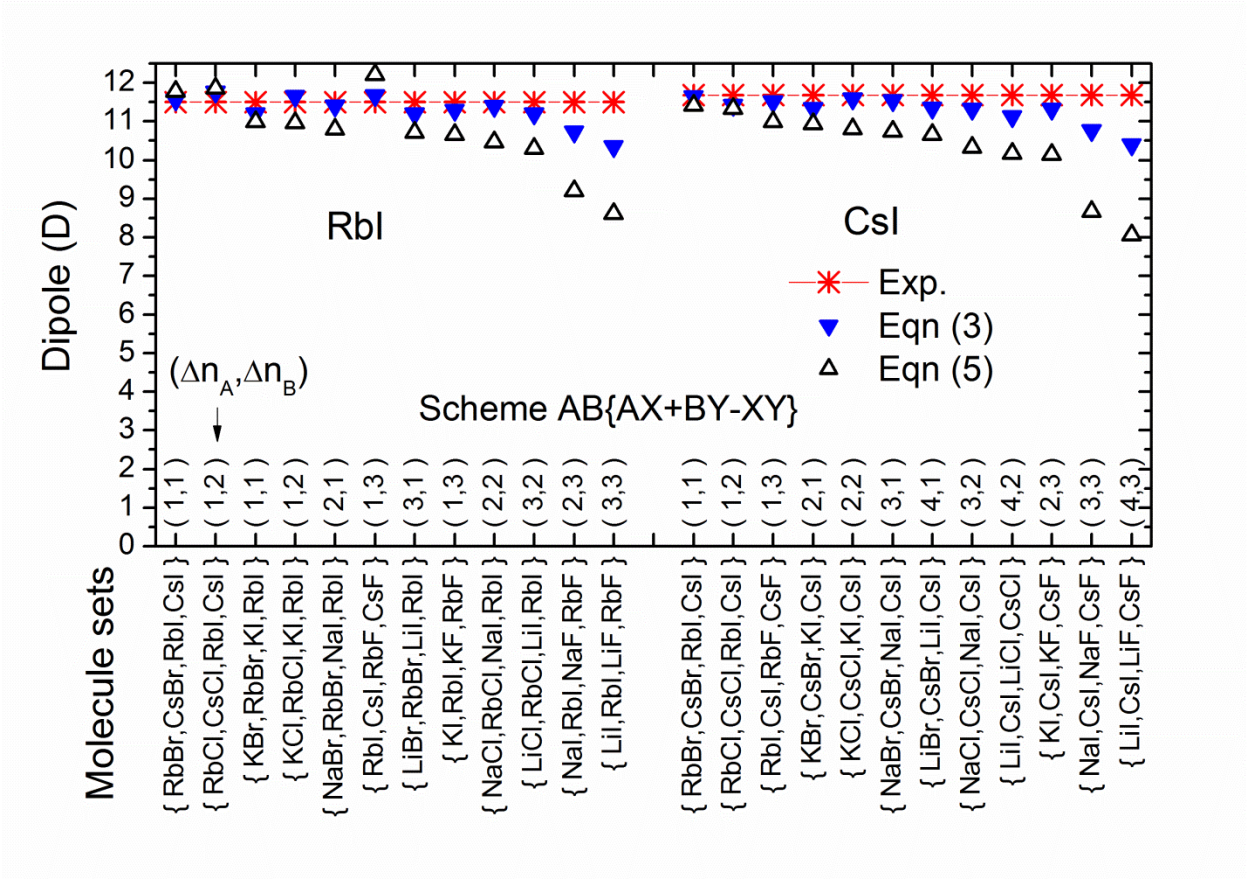

Figure S10. CsI & RbI

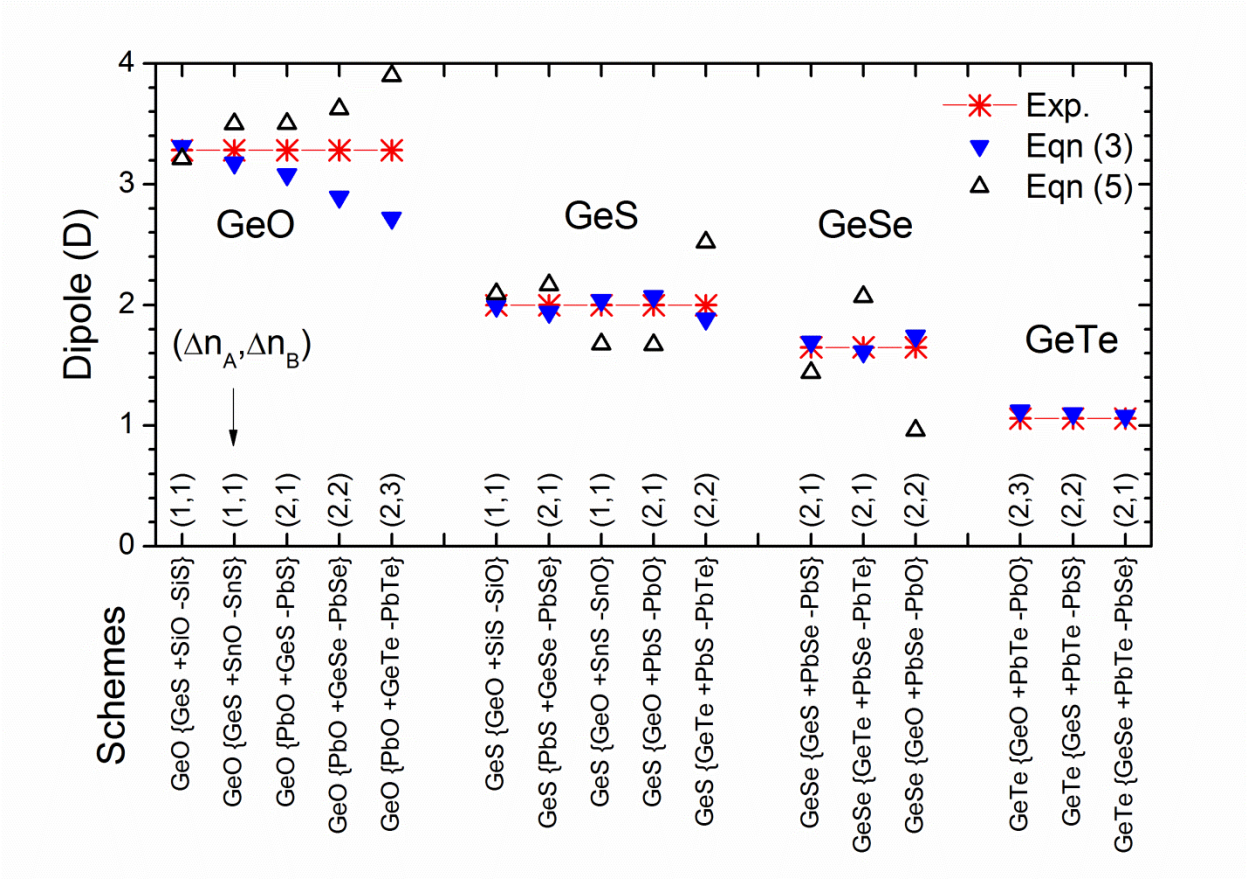

Figure S11. Results for GeX(X=O,S,Se,Te). The results for GeTe from Eqn (5) are unphysical.

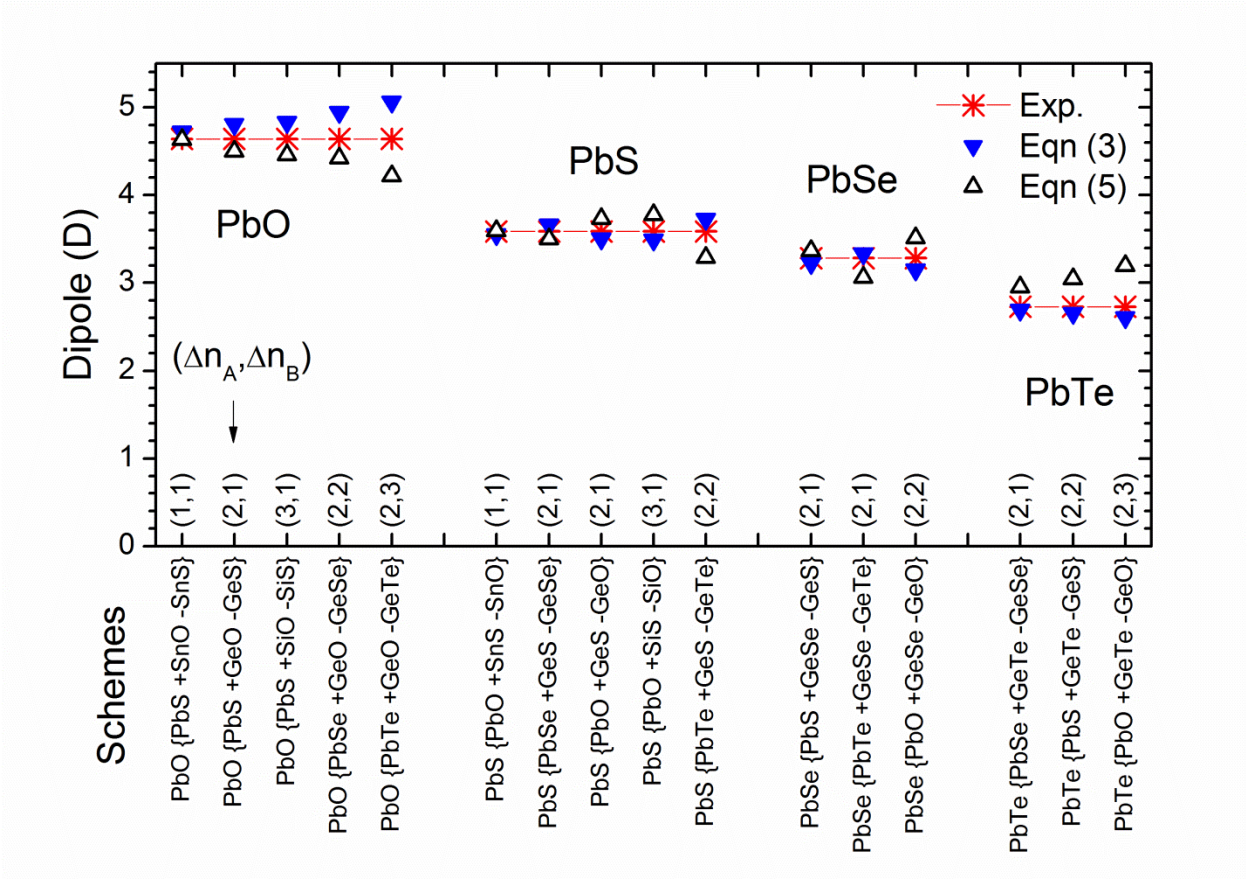

Figure S12. Results for the ground states of PbX (X=O, S, Se, Te).

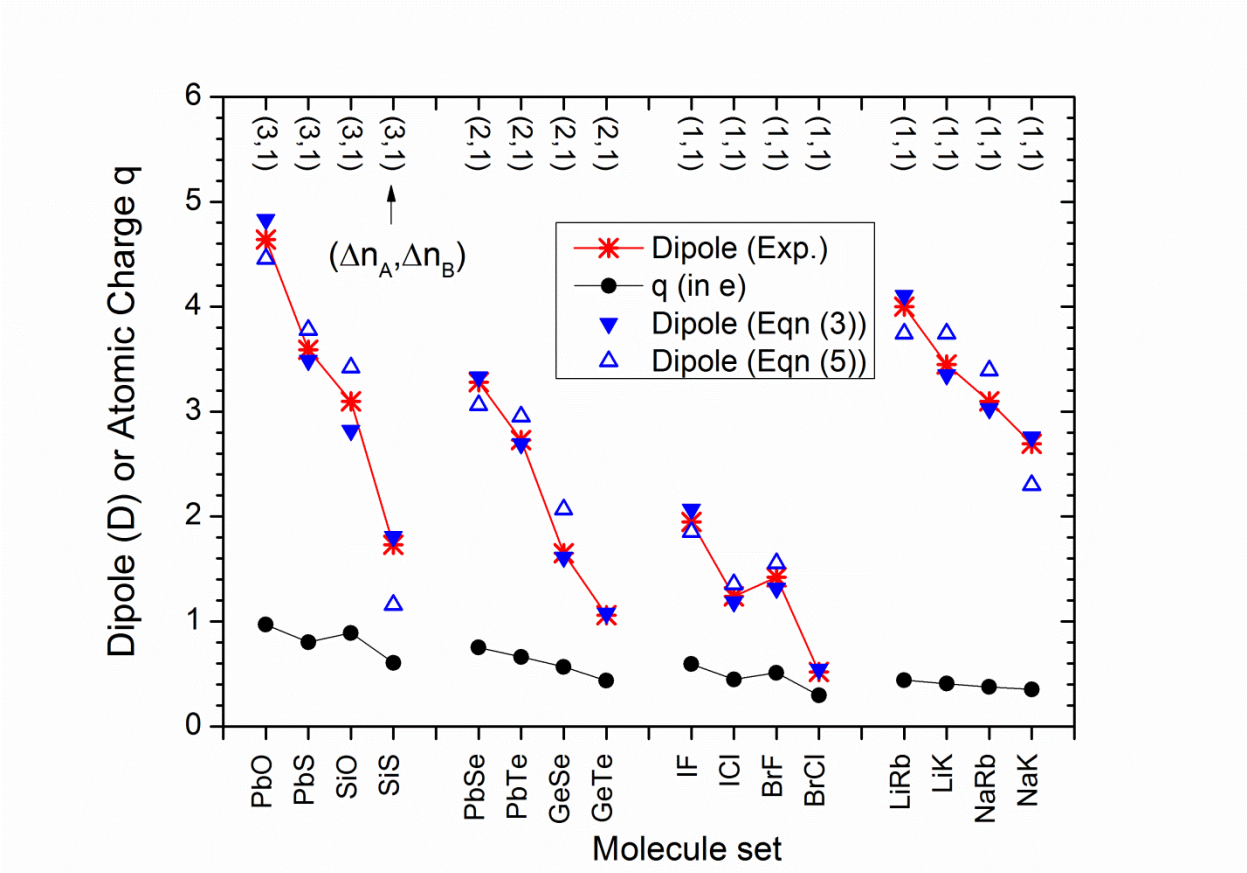

Figure S13. Results for general molecules from different molecule sets. The results for BrCl and GeTe are unphysical. This figure also shows that molecules in the same set with larger polar charges have relative smaller errors.

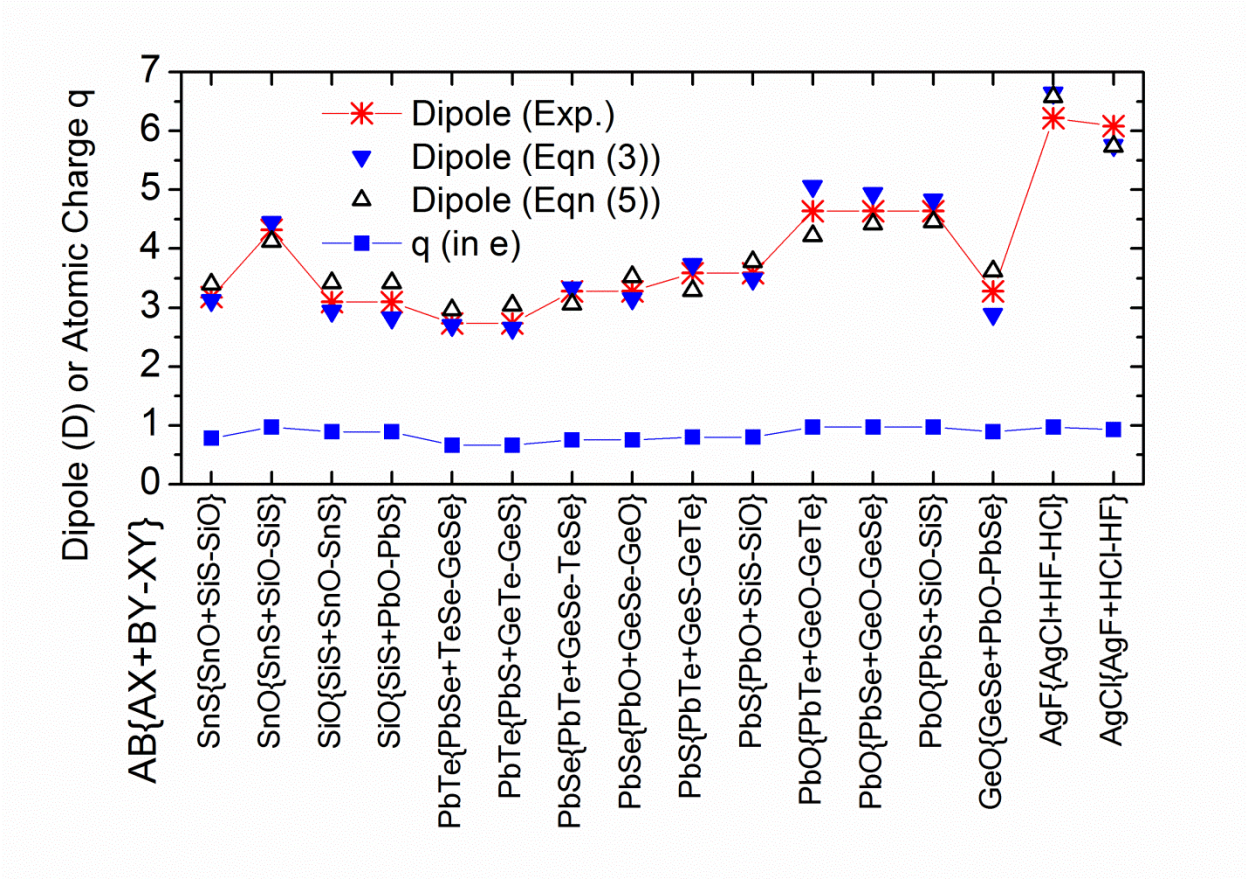

Figure S14. A collection of some results some general molecules from $(\Delta n_A,\Delta n_B)\neq(1,1)$ schemes. AgF and AgCl can be seemed as exceptions, since H and Ag are not in the same group (but they have kind of similarity in electron configurations and electronegativities).

Table S2. Predicted dipole moments from Eqns (3) and (5) for dozens of general molecules.

	Ref.17	Ref.17	Ref.13	Dipole (charge=q)			Dipole (charge=1e)							
Mole	Re/Å	Dipole/D	q(in e)	Eqn(3)	δ(Eqn(3))	δ%[a]	Eqn(5)	δ(Eqn(5))	δ%[b]	{AB,AX,BY,XY}				(Δn_A,Δn_B)
SnS	2.20898	3.18	0.780	3.2213	0.0413	1.30	3.1770	-0.0030	-0.09	SnO	PbO	SnS	PbS	(1,1)
PbO	1.9218359	4.64	0.970	4.7175	0.0775	1.67	4.6377	-0.0023	-0.05	SnO	PbO	SnS	PbS	(1,1)
SnO	1.83251	4.32	0.975	4.2292	-0.0908	-2.10	4.3226	0.0026	0.06	SnO	PbO	SnS	PbS	(1,1)
PbS	2.2868898	3.59	0.803	3.5498	-0.0402	-1.12	3.5925	0.0025	0.07	SnO	PbO	SnS	PbS	(1,1)
SnO	1.83251	4.32	0.975	4.4224	0.1024	2.37	4.1652	-0.1548	-3.58	GeO	SnO	GeS	SnS	(1,1)
SnS	2.20898	3.18	0.780	3.1317	-0.0483	-1.52	3.3469	0.1669	5.25	GeO	SnO	GeS	SnS	(1,1)
GeO	1.62464	3.2823	0.887	3.1749	-0.1074	-3.27	3.5007	0.2184	6.65	GeO	SnO	GeS	SnS	(1,1)
GeS	2.0120982	2	0.637	2.0369	0.0369	1.84	1.6745	-0.3255	-16.27	GeO	SnO	GeS	SnS	(1,1)
GeO	1.62464	3.2823	0.887	3.3133	0.0310	0.94	3.2125	-0.0698	-2.13	SiO	GeO	SiS	GeS	(1,1)
SiO	1.50975	3.0982	0.891	3.0620	-0.0362	-1.17	3.1760	0.0778	2.51	SiO	GeO	SiS	GeS	(1,1)
GeS	2.0120982	2	0.637	1.9890	-0.0110	-0.55	2.0896	0.0896	4.48	SiO	GeO	SiS	GeS	(1,1)
SiS	1.92926	1.73	0.605	1.7407	0.0107	0.62	1.6158	-0.1142	-6.60	SiO	GeO	SiS	GeS	(1,1)
SnO	1.83251	4.32	0.975	4.4522	0.1322	3.06	4.1167	-0.2033	-4.71	SiO	SnO	SiS	SnS	(2,1)
SnS	2.20898	3.18	0.780	3.1173	-0.0627	-1.97	3.3964	0.2164	6.80	SiO	SnO	SiS	SnS	(2,1)
SiO	1.50975	3.0982	0.891	2.9357	-0.1625	-5.25	3.4177	0.3195	10.31	SiO	SnO	SiS	SnS	(2,1)
SiS	1.92926	1.73	0.605	1.7766	0.0466	2.69	1.1678	-0.5622	-32.50	SiO	SnO	SiS	SnS	(2,1)
PbO	1.9218359	4.64	0.970	4.8308	0.1908	4.11	4.4578	-0.1822	-3.93	SiO	PbO	SiS	PbS	(3,1)
PbS	2.2868898	3.59	0.803	3.4890	-0.1010	-2.81	3.7790	0.1890	5.26	SiO	PbO	SiS	PbS	(3,1)
SiO	1.50975	3.0982	0.891	2.8217	-0.2765	-8.93	3.4218	0.3236	10.44	SiO	PbO	SiS	PbS	(3,1)
SiS	1.92926	1.73	0.605	1.8071	0.0771	4.46	1.1585	-0.5715	-33.04	SiO	PbO	SiS	PbS	(3,1)
PbO	1.9218359	4.64	0.970	4.8053	0.1653	3.56	4.5006	-0.1394	-3.00	GeO	PbO	GeS	PbS	(2,1)

PbS	2.2868898	3.59	0.803	3.5029	-0.0871	-2.43	3.7361	0.1461	4.07	GeO	PbO	GeS	PbS	(2,1)
GeO	1.62464	3.2823	0.887	3.0788	-0.2035	-6.20	3.5043	0.2220	6.76	GeO	PbO	GeS	PbS	(2,1)
GeS	2.0120982	2	0.637	2.0683	0.0683	3.42	1.6683	-0.3317	-16.58	GeO	PbO	GeS	PbS	(2,1)
PbO	1.9218359	4.64	0.970	4.9433	0.3033	6.54	4.4194	-0.2206	-4.75	GeO	PbO	GeSe	PbSe	(2,2)
PbSe	2.4022637	3.28	0.751	3.1498	-0.1302	-3.97	3.5153	0.2353	7.17	GeO	PbO	GeSe	PbSe	(2,2)
GeO	1.62464	3.2823	0.887	2.8919	-0.3904	-11.89	3.6245	0.3422	10.43	GeO	PbO	GeSe	PbSe	(2,2)
GeSe	2.1346561	1.65	0.567	1.7401	0.0901	5.46	0.9610	-0.6890	-41.76	GeO	PbO	GeSe	PbSe	(2,2)
PbO	1.9218359	4.64	0.970	5.0607	0.4207	9.07	4.2193	-0.4207	-9.07	GeO	PbO	GeTe	PbTe	(2,3)
PbTe	2.595006	2.73	0.662	2.6068	-0.1232	-4.51	3.1958	0.4658	17.06	GeO	PbO	GeTe	PbTe	(2,3)
GeO	1.62464	3.2823	0.887	2.7182	-0.5641	-17.19	3.8964	0.6141	18.71	GeO	PbO	GeTe	PbTe	(2,3)
GeTe	2.3401928	1.06	0.435	1.1225	0.0625	5.89	Unphysical	-		GeO	PbO	GeTe	PbTe	(2,3)
PbS	2.2868898	3.59	0.803	3.6634	0.0734	2.04	3.5042	-0.0858	-2.39	GeS	PbS	GeSe	PbSe	(2,1)
PbSe	2.4022637	3.28	0.751	3.2204	-0.0596	-1.82	3.3672	0.0872	2.66	GeS	PbS	GeSe	PbSe	(2,1)
GeS	2.0120982	2	0.637	1.9392	-0.0608	-3.04	2.1661	0.1661	8.31	GeS	PbS	GeSe	PbSe	(2,1)
GeSe	2.1346561	1.65	0.567	1.6923	0.0423	2.56	1.4388	-0.2112	-12.80	GeS	PbS	GeSe	PbSe	(2,1)
PbS	2.2868898	3.59	0.803	3.7263	0.1363	3.80	3.2904	-0.2996	-8.35	GeS	PbS	GeTe	PbTe	(2,2)
PbTe	2.595006	2.73	0.662	2.6546	-0.0754	-2.76	3.0446	0.3146	11.52	GeS	PbS	GeTe	PbTe	(2,2)
GeS	2.0120982	2	0.637	1.8845	-0.1155	-5.78	2.5185	0.5185	25.93	GeS	PbS	GeTe	PbTe	(2,2)
GeTe	2.3401928	1.06	0.435	1.0990	0.0390	3.68	Unphysical	-		GeS	PbS	GeTe	PbTe	(2,2)
PbSe	2.4022637	3.28	0.751	3.3312	0.0512	1.56	3.0619	-0.2181	-6.65	GeSe	GeTe	PbSe	PbTe	(2,1)
PbTe	2.595006	2.73	0.662	2.6951	-0.0349	-1.28	2.9552	0.2252	8.25	GeSe	GeTe	PbSe	PbTe	(2,1)
GeSe	2.1346561	1.65	0.567	1.6122	-0.0378	-2.29	2.0685	0.4185	25.36	GeSe	GeTe	PbSe	PbTe	(2,1)
GeTe	2.3401928	1.06	0.435	1.0784	0.0184	1.73	Unphysical	-		GeSe	GeTe	PbSe	PbTe	(2,1)
InF	1.9854	3.4	0.738	3.3700	-0.0300	-0.88	3.2110	-0.1890	-5.56	InF	TlF	InCl	TlCl	(1,1)
TlCl	2.48483	4.54299	0.766	4.5223	-0.0207	-0.46	4.4318	-0.1112	-2.45	InF	TlF	InCl	TlCl	(1,1)

TlF	2.08439	4.2282	0.799	4.2595	0.0313	0.74	4.3667	0.1385	3.27	InF	TlF	InCl	TlCl	(1,1)
InCl	2.40117	3.79	0.713	3.8092	0.0192	0.51	3.9239	0.1339	3.53	InF	TlF	InCl	TlCl	(1,1)
IF	1.90976	1.948	0.593	2.0677	0.1197	6.14	1.8519	-0.0961	-4.93	BrF	IF	BrCl	ICl	(1,1)
ICl	2.32088	1.24	0.447	1.1872	-0.0528	-4.26	1.3557	0.1157	9.33	BrF	IF	BrCl	ICl	(1,1)
BrF	1.75894	1.422	0.510	1.3174	-0.1046	-7.36	1.5551	0.1331	9.36	BrF	IF	BrCl	ICl	(1,1)
BrCl	2.13607	0.519	0.295	0.5439	0.0249	4.81	Unphysical	-		BrF	IF	BrCl	ICl	(1,1)
LiRb	3.46615*	4	0.441	4.1071	0.1071	2.68	3.7428	-0.2572	-6.43	LiK	LiRb	NaK	NaRb	(1,1)
LiK	3.27	3.45	0.407	3.3520	-0.0980	-2.84	3.7435	0.2935	8.51	LiK	LiRb	NaK	NaRb	(1,1)
NaRb	3.6435#	3.1	0.376	3.0288	-0.0712	-2.30	3.3918	0.2918	9.41	LiK	LiRb	NaK	NaRb	(1,1)
NaK	3.49958	2.693	0.354	2.7581	0.0651	2.42	2.2978	-0.3952	-14.68	LiK	LiRb	NaK	NaRb	(1,1)
AgF	1.983203	6.22	0.975	6.6473	0.4273	6.87	6.5777	0.3577	5.75	HF	HCl	AgF	AgCl	
AgCl	2.280819	6.08	0.923	5.7555	-0.3245	-5.34	5.7433	-0.3367	-5.54	HF	HCl	AgF	AgCl	
HCl	1.2745717	1.1086	0.441	1.2605	0.1519	13.70	2.8900	1.7814	160.69	HF	HCl	AgF	AgCl	
HF	0.91682	1.82653	0.610	1.2284	-0.5981	-32.75	Unphysical	-		HF	HCl	AgF	AgCl	

[a] δ%=[Dipole(Eqn (3))-Diploe(exp.)]/Diploe(exp)×100%.

[b] δ%=[Dipole(Eqn (5))-Diploe(exp.)]/Diploe(exp)×100%

* M. Ivanova, A. Stein, A. Pashov, H. Knöckel, and E. Tiemann, The $X^1\Sigma^+$ state of LiRb studied by Fourier-transform spectroscopy, J. Chem. Phys. 134, 024321 (9pp) (2011)

S. Kasahara, T. Ebi, M. Tanimura, H. Ikoma, K. Matsubara, M. Baba, and H. Kato, High-resolution laser spectroscopy of the $X^1\Sigma^+$ and $(1)^3\Sigma^+$ states of $^{23}Na^{85}Rb$ molecule, J. Chem. Phys. 105, 1341-1347 (1996)

Table S3. Dipole moments (in D) for some ground-state molecules. CCSD data are calculated using Gaussian 09 package.[18] All experimental data involved in Eqn (5) are from Ref. 17.

AB	Exp.[17]	CCSD/ 6-311++G(3df)	δ/D[a]	Eqn (5)	δ/D[b]	Scheme	(Δn_A,Δn_B)
LiCl	7.12887	7.2326	0.10	6.9604	-0.17	{LiBr+NaCl-NaBr}	(1,1)
NaCl	9.00117	9.2876	0.29	9.1133	0.11	{NaBr+LiCl-LiBr}	(1,1)
KCl	10.269	10.6485	0.38	10.2312	-0.04	{KBr+RbCl-RbBr}	(1,1)
LiBr	7.268	7.4029	0.13	7.4184	0.15	{LiCl+NaBr-NaCl}	(1,1)
NaBr	9.1183	9.4559	0.34	9.0126	-0.11	{NaCl+LiBr-LiCl}	(1,1)
KBr	10.628	11.0439	0.42	10.6624	0.03	{KCl+RbBr-RbCl}	(1,1)
BrF	1.422	1.4405	0.02	1.5551	0.13	{BrCl+IF-ICl}	(1,1)
NaK	2.693	2.7862	0.09	2.2978	-0.40	{NaRb+LiK-LiRb}	(1,1)
LiK	3.45	3.8859	0.44	3.7435	0.29	{LiRb+NaK-NaRb}	(1,1)
SiS	1.73	1.7733	0.04	1.6158	-0.11	{SiO+GeS-GeO}	(1,1)
SiO	3.0982	3.2492	0.15	3.1760	0.08	{SiS+GeO-GeS}	(1,1)
GeO	3.2823	3.5904	0.31	3.2125	-0.07	{GeS+SiO-SiS}	(1,1)
GeS	2	2.223	0.22	2.0896	0.09	{GeO+SiS-SiO}	(1,1)
GeSe	1.65	1.8784	0.23	1.4388	-0.21	{GeS+PbSe-PbS}	(2,1)
IF	1.948			1.8519	-0.10	{ICl +BrF -BrCl}	(1,1)
ICl	1.24			1.3557	0.12	{IF +BrCl -BrF}	(1,1)
LiRb	4			3.7428	-0.26	{LiK+NaRb-NaK}	(1,1)
NaRb	3.1			3.3918	0.29	{NaK+LiRb-LiK}	(1,1)
CsBr	10.82			10.7197	-0.10	{CsCl+RbBr-RbCl}	(1,1)
RbBr	10.86			10.8277	-0.03	{RbCl+KBr-KCl}	(1,1)
CsCl	10.387			10.4964	0.11	{CsBr +RbCl-RbBr}	(1,1)
RbCl	10.51			10.5452	0.04	{RbBr+KCl-KBr}	(1,1)
RbI	11.5			11.7775	0.28	{RbBr+CsI-CsBr}	(1,1)
CsI	11.69			11.4221	-0.27	{CsBr+RbI-RbBr}	(1,1)
NaI	9.236			9.1165	-0.12	{NaBr+LiI -LiBr}	(1,1)
KI	10.8			10.5912	-0.21	{KBr+NaI -NaBr}	(1,1)
LiI	7.428			7.5934	0.17	{LiBr+NaI-NaBr}	(1,1)
InF	3.4			3.2110	-0.19	{InCl +TlF -TlCl}	(1,1)
TlCl	4.54299			4.4318	-0.11	{TlF +InCl -InF}	(1,1)
TlF	4.2282			4.3667	0.14	{TlCl +InF -InCl}	(1,1)
InCl	3.79			3.9239	0.13	{InF +TlCl -TlF}	(1,1)
SnS	3.18			3.1770	-0.01	{SnO+PbS-PbO}	(1,1)
PbO	4.64			4.6377	-0.01	{PbS+SnO-SnS}	(1,1)

SnO	4.32		4.3226	0.01	{SnS+PbO-PbS}	(1,1)
PbS	3.59		3.5925	0.01	{PbO+SnS-SnO}	(1,1)
PbSe	3.28		3.3672	0.09	{PbS+GeSe-GeS}	(2,1)
PbTe	2.73		2.9552	0.23	{PbSe+GeTe-GeSe}	(2,1)
Average [c]		0.23		0.14		

[a] δ=Dipole(CCSD)-Diploe(exp).

[b] δ=Dipole(Eqn (5))-Diploe(exp).

[c] The mean absolute deviation.

Table S4. Data adopted for predicted dipole moments using Eqn (5) for GaCl, InBr, SrCl, SrS, CuCl, and CuBr ground state molecules. All experimental data are from Ref. 17 except those indicated. The atomic charges are also presented for references.

AB	R_e/Å	μ_d/D (Predicted)	BY	Re/Å	μ_d/D	q(e)	AX	Re/Å	μ_d/D	q(e)	XY	μ_d/D	Re/Å	q(e)
GaCl	2.20169	3.17469	InCl	2.40117	3.79	0.71	GaF	1.77437	2.45	0.76	InF	1.9854	3.4	0.74
InBr	2.54315	3.761849	$Tl^{81}Br$	2.61817	4.49	0.75	InCl	2.40117	3.79	0.71	TlCl	2.48483	4.54299	0.77
SrCl	2.575848[a]	3.847601	CaCl	2.43676	3.6	0.69	SrF	2.074685	3.4676	0.72	CaF	1.951639	3.07	0.69
SrS	2.441[b]	11.54003	BaS	2.5074	10.86	1.32	SrO	1.91983	8.9	1.25	BaO	1.939712	7.954	1.22
CuCl	2.05118	5.658725	AgF	1.983203	6.22	0.97	CuF	1.744951	5.77	0.98	AgCl	2.280819	6.08	0.92
CuBr	2.17344	5.203706	AgCl	2.280819	6.08	0.92	CuCl	2.05118	5.74[c]	~0.92	AgBr	2.393138	5.62	0.88

a From Ref. 19.
b From Ref. 20.
c. Theoretical data from Ref.13.