

The Alkali Halides Dimer Data [01.04.20]

Molecule	Dissociation[eV]	L[Å]	Atom Positions[Å]	Electron Positions[Å]
Li2F2	{Li1, F1} {Li2, F2} -2.5 {Li1, F2} {Li2, F1} -2.5	1.69	<Obj> <X> <Y> <Z> Li1 -1.137 0 0 Li2 1.137 0 0 F1 0 0 -1.25 F2 0 0 1.25	<Obj> <X> <Y> <Z> F1 -0.195 0.678 -1.036 Li1 -0.195 -0.678 -1.036 F1 0.195 0.678 -1.036 F1 0.195 -0.678 -1.036 F2 -0.195 0.678 1.036 F2 -0.195 -0.678 1.036 F2 0.195 0.678 1.036 Li2 0.195 -0.678 1.036
Li2Cl2	{Li1, Cl1} {Li2, Cl2} -2.37 {Li1, Cl2} {Li2, Cl1} -2.37	2.23	<Obj> <X> <Y> <Z> Li1 -1.31 0 0 Li2 1.31 0 0 Cl1 0 0 -1.805 Cl2 0 0 1.805	<Obj> <X> <Y> <Z> Cl1 -0.278 0.929 -1.421 Li1 -0.278 -0.929 -1.421 Cl1 0.278 0.929 -1.421 Cl1 0.278 -0.929 -1.421 Cl2 -0.278 0.929 1.421 Cl2 -0.278 -0.929 1.421 Cl2 0.278 0.929 1.421 Li2 0.278 -0.929 1.421
Li2Br2	{Li1, Br1} {Li2, Br2} -2.27 {Li1, Br2} {Li2, Br1} -2.27	2.35	<Obj> <X> <Y> <Z> Li1 -1.348 0 0 Li2 1.348 0 0 Br1 0 0 -1.925 Br2 0 0 1.925	<Obj> <X> <Y> <Z> Br1 -0.3 0.992 -1.496 Li1 -0.3 -0.992 -1.496 Br1 0.3 0.992 -1.496 Br1 0.3 -0.992 -1.496 Br2 -0.3 0.992 1.496 Br2 -0.3 -0.992 1.496 Br2 0.3 0.992 1.496 Li2 0.3 -0.992 1.496
Li2I2	{Li1, I1} {Li2, I2} -2.12 {Li1, I2} {Li2, I1} -2.12	2.54	<Obj> <X> <Y> <Z> Li1 -1.352 0 0 Li2 1.352 0 0 I1 0 0 -2.15 I2 0 0 2.15	<Obj> <X> <Y> <Z> I1 -0.351 1.119 -1.593 Li1 -0.351 -1.119 -1.593 I1 0.351 1.119 -1.593 I1 0.351 -1.119 -1.593 I2 -0.351 1.119 1.593 I2 -0.351 -1.119 1.593 I2 0.351 1.119 1.593 Li2 0.351 -1.119 1.593
Na2F2	{Na1, F1} {Na2, F2} -2.42 {Na1, F2} {Na2, F1} -2.42	1.99	<Obj> <X> <Y> <Z> Na1 -1.373 0 0 Na2 1.373 0 0 F1 0 0 -1.44 F2 0 0 1.44	<Obj> <X> <Y> <Z> F1 -0.212 0.742 -1.218 Na1 -0.212 -0.742 -1.218 F1 0.212 0.742 -1.218 F1 0.212 -0.742 -1.218 F2 -0.212 0.742 1.218 F2 -0.212 -0.742 1.218 F2 0.212 0.742 1.218 Na2 0.212 -0.742 1.218
Na2Cl2	{Na1, Cl1} {Na2, Cl2} -2.3 {Na1, Cl2} {Na2, Cl1} -2.3	2.51	<Obj> <X> <Y> <Z> Na1 -1.712 0 0 Na2 1.712 0 0 Cl1 0 0 -1.835 Cl2 0 0 1.835	<Obj> <X> <Y> <Z> Cl1 -0.246 0.866 -1.571 Na1 -0.246 -0.866 -1.571 Cl1 0.246 0.866 -1.571 Cl1 0.246 -0.866 -1.571 Cl2 -0.246 0.866 1.571 Cl2 -0.246 -0.866 1.571 Cl2 0.246 0.866 1.571 Na2 0.246 -0.866 1.571
Na2Br2	{Na1, Br1} {Na2, Br2} -2.24 {Na1, Br2} {Na2, Br1} -2.24	2.65	<Obj> <X> <Y> <Z> Na1 -1.811 0 0 Na2 1.811 0 0 Br1 0 0 -1.935 Br2 0 0 1.935	<Obj> <X> <Y> <Z> Br1 -0.254 0.896 -1.663 Na1 -0.254 -0.896 -1.663 Br1 0.254 0.896 -1.663 Br1 0.254 -0.896 -1.663 Br2 -0.254 0.896 1.663 Br2 -0.254 -0.896 1.663 Br2 0.254 0.896 1.663 Na2 0.254 -0.896 1.663
Na2I2	{Na1, I1} {Na2, I2} -2.09 {Na1, I2} {Na2, I1} -2.09	2.88	<Obj> <X> <Y> <Z> Na1 -1.944 0 0 Na2 1.944 0 0 I1 0 0 -2.125 I2 0 0 2.125	<Obj> <X> <Y> <Z> I1 -0.279 0.981 -1.819 Na1 -0.279 -0.981 -1.819 I1 0.279 0.981 -1.819 I1 0.279 -0.981 -1.819 I2 -0.279 0.981 1.819 I2 -0.279 -0.981 1.819 I2 0.279 0.981 1.819 Na2 0.279 -0.981 1.819
K2F2	{K1, F1} {K2, F2} -2.09 {K1, F2} {K2, F1} -2.09	2.33	<Obj> <X> <Y> <Z> K1 -1.655 0 0 K2 1.655 0 0 F1 0 0 -1.64 F2 0 0 1.64	<Obj> <X> <Y> <Z> F1 -0.236 0.835 -1.406 K1 -0.236 -0.835 -1.406 F1 0.236 0.835 -1.406 F1 0.236 -0.835 -1.406 F2 -0.236 0.835 1.406 F2 -0.236 -0.835 1.406 F2 0.236 0.835 1.406 K2 0.236 -0.835 1.406
K2Cl2	{K1, Cl1} {K2, Cl2} -2.06 {K1, Cl2} {K2, Cl1} -2.06	2.84	<Obj> <X> <Y> <Z> K1 -1.981 0 0 K2 1.981 0 0 Cl1 0 0 -2.035 Cl2 0 0 2.035	<Obj> <X> <Y> <Z> Cl1 -0.266 0.942 -1.762 K1 -0.266 -0.942 -1.762 Cl1 0.266 0.942 -1.762 Cl1 0.266 -0.942 -1.762 Cl2 -0.266 0.942 1.762 Cl2 -0.266 -0.942 1.762 Cl2 0.266 0.942 1.762 K2 0.266 -0.942 1.762

K2Br2	{K1, Br1} {K2, Br2} -2.02 {K1, Br2} {K2, Br1} -2.02	2.97	<Obj> <X> <Y> <Z> K1 -2.059 0 0 K2 2.059 0 0 Br1 0 0 -2.14 Br2 0 0 2.14	<Obj> <X> <Y> <Z> Br1 -0.276 0.976 -1.853 K1 -0.276 -0.976 -1.853 Br1 0.276 0.976 -1.853 Br1 0.276 -0.976 -1.853 Br2 -0.276 0.976 1.853 Br2 -0.276 -0.976 1.853 Br2 0.276 0.976 1.853 K2 0.276 -0.976 1.853
K2I2	{K1, I1} {K2, I2} -1.93 {K1, I2} {K2, I1} -1.93	3.21	<Obj> <X> <Y> <Z> K1 -2.24 0 0 K2 2.24 0 0 I1 0 0 -2.3 I2 0 0 2.3	<Obj> <X> <Y> <Z> I1 -0.287 1.019 -2.005 K1 -0.287 -1.019 -2.005 I1 0.287 1.019 -2.005 I1 0.287 -1.019 -2.005 I2 -0.287 1.019 2.005 I2 -0.287 -1.019 2.005 I2 0.287 1.019 2.005 K2 0.287 -1.019 2.005
Rb2F2	{Rb1, F1} {Rb2, F2} -1.93 {Rb1, F2} {Rb2, F1} -1.93	2.47	<Obj> <X> <Y> <Z> Rb1 -1.778 0 0 Rb2 1.778 0 0 F1 0 0 -1.715 F2 0 0 1.715	<Obj> <X> <Y> <Z> F1 -0.248 0.878 -1.476 Rb1 -0.248 -0.878 -1.476 F1 0.248 0.878 -1.476 F1 0.248 -0.878 -1.476 F2 -0.248 0.878 1.476 F2 -0.248 -0.878 1.476 F2 0.248 0.878 1.476 Rb2 0.248 -0.878 1.476
Rb2Cl2	{Rb1, Cl1} {Rb2, Cl2} -1.96 {Rb1, Cl2} {Rb2, Cl1} -1.96	2.96	<Obj> <X> <Y> <Z> Rb1 -2.076 0 0 Rb2 2.076 0 0 Cl1 0 0 -2.11 Cl2 0 0 2.11	<Obj> <X> <Y> <Z> Cl1 -0.276 0.979 -1.829 Rb1 -0.276 -0.979 -1.829 Cl1 0.276 0.979 -1.829 Cl1 0.276 -0.979 -1.829 Cl2 -0.276 0.979 1.829 Cl2 -0.276 -0.979 1.829 Cl2 0.276 0.979 1.829 Rb2 0.276 -0.979 1.829
Rb2Br2	{Rb1, Br1} {Rb2, Br2} -1.94 {Rb1, Br2} {Rb2, Br1} -1.94	3.11	<Obj> <X> <Y> <Z> Rb1 -2.188 0 0 Rb2 2.188 0 0 Br1 0 0 -2.21 Br2 0 0 2.21	<Obj> <X> <Y> <Z> Br1 -0.28 0.995 -1.927 Rb1 -0.28 -0.995 -1.927 Br1 0.28 0.995 -1.927 Br1 0.28 -0.995 -1.927 Br2 -0.28 0.995 1.927 Br2 -0.28 -0.995 1.927 Br2 0.28 0.995 1.927 Rb2 0.28 -0.995 1.927
Rb2I2	{Rb1, I1} {Rb2, I2} -1.84 {Rb1, I2} {Rb2, I1} -1.84	3.35	<Obj> <X> <Y> <Z> Rb1 -2.337 0 0 Rb2 2.337 0 0 I1 0 0 -2.4 I2 0 0 2.4	<Obj> <X> <Y> <Z> I1 -0.301 1.068 -2.091 Rb1 -0.301 -1.068 -2.091 I1 0.301 1.068 -2.091 I1 0.301 -1.068 -2.091 I2 -0.301 1.068 2.091 I2 -0.301 -1.068 2.091 I2 0.301 1.068 2.091 Rb2 0.301 -1.068 2.091
Cs2F2	{Cs1, F1} {Cs2, F2} -1.72 {Cs1, F2} {Cs2, F1} -1.72	2.6	<Obj> <X> <Y> <Z> Cs1 -1.881 0 0 Cs2 1.881 0 0 F1 0 0 -1.795 F2 0 0 1.795	<Obj> <X> <Y> <Z> F1 -0.266 0.943 -1.541 Cs1 -0.266 -0.943 -1.541 F1 0.266 0.943 -1.541 F1 0.266 -0.943 -1.541 F2 -0.266 0.943 1.541 F2 -0.266 -0.943 1.541 F2 0.266 0.943 1.541 Cs2 0.266 -0.943 1.541
Cs2Cl2	{Cs1, Cl1} {Cs2, Cl2} -1.83 {Cs1, Cl2} {Cs2, Cl1} -1.83	3.12	<Obj> <X> <Y> <Z> Cs1 -2.197 0 0 Cs2 2.197 0 0 Cl1 0 0 -2.215 Cl2 0 0 2.215	<Obj> <X> <Y> <Z> Cl1 -0.292 1.037 -1.92 Cs1 -0.292 -1.037 -1.92 Cl1 0.292 1.037 -1.92 Cl1 0.292 -1.037 -1.92 Cl2 -0.292 1.037 1.92 Cl2 -0.292 -1.037 1.92 Cl2 0.292 1.037 1.92 Cs2 0.292 -1.037 1.92
Cs2Br2	{Cs1, Br1} {Cs2, Br2} -1.81 {Cs1, Br2} {Cs2, Br1} -1.81	3.26	<Obj> <X> <Y> <Z> Cs1 -2.295 0 0 Cs2 2.295 0 0 Br1 0 0 -2.315 Br2 0 0 2.315	<Obj> <X> <Y> <Z> Br1 -0.298 1.059 -2.014 Cs1 -0.298 -1.059 -2.014 Br1 0.298 1.059 -2.014 Br1 0.298 -1.059 -2.014 Br2 -0.298 1.059 2.014 Br2 -0.298 -1.059 2.014 Br2 0.298 1.059 2.014 Cs2 0.298 -1.059 2.014
Cs2I2	{Cs1, I1} {Cs2, I2} -1.74 {Cs1, I2} {Cs2, I1} -1.74	3.49	<Obj> <X> <Y> <Z> Cs1 -2.455 0 0 Cs2 2.455 0 0 I1 0 0 -2.48 I2 0 0 2.48	<Obj> <X> <Y> <Z> I1 -0.312 1.111 -2.165 Cs1 -0.312 -1.111 -2.165 I1 0.312 1.111 -2.165 I1 0.312 -1.111 -2.165 I2 -0.312 1.111 2.165 I2 -0.312 -1.111 2.165 I2 0.312 1.111 2.165 Cs2 0.312 -1.111 2.165