Initial Data						
Structure to fit to	Starting potential	Symmetry setup	Variables	Setup	Cycles to fit	Final sum of squares
ScCl3	Al-Cl	1	A, rho, k	fit conp simul opti nosymm com	247	0.44
ScCl3	Cu-Cl	1	A, rho, k	fit conp simul opti nosymm com	747	0.4
ScCl3	Pb-Cl	1	A, rho, k	fit conp simul opti nosymm com	33	7431.72
ScCl3	Mg-Cl	1	A, rho, k	fit conp simul opti nosymm com	345	0.35
ScCl3	Ca-Cl	1	A, rho, k	fit conp simul opti nosymm com	41	0.3
ScCl3	Sr-Cl	1	A, rho, k	fit conp simul opti nosymm com	45	0.33
ScCl3	Ba-Cl	1	A, rho, k	fit conp simul opti nosymm com	65	0.26
YCl3	Al-Cl	1	A, rho, k	fit conp simul opti nosymm com	56	0.1
YCl3	Cu-Cl	1	A, rho, k	fit conp simul opti nosymm com	38	0.1
YCl3	Pb-Cl	1	A, rho, k	fit conp simul opti nosymm com	21	0.1
YCl3	Mg-Cl	1	A, rho, k	fit conp simul opti nosymm com	39	0.1
YCl3	Ca-Cl	1	A, rho, k	fit conp simul opti nosymm com	21	0.1
YCl3	Sr-Cl	1	A, rho, k	fit conp simul opti nosymm com	21	0.1
YCl3	Ba-Cl	1	A, rho, k	fit conp simul opti nosymm com	35	0.1
InCl3	Al-Cl	1	A, rho, k	fit conp simul opti nosymm com	61	0.1
InCl3	Cu-Cl	1	A, rho, k	fit conp simul opti nosymm com	Shell has bee	
InCl3	Pb-Cl	1	A, rho, k	fit conp simul opti nosymm com	57	578.2
InCl3	Mg-Cl	1	A, rho, k	fit conp simul opti nosymm com	58	578.2
InCl3	Ca-Cl	1	A, rho, k	fit conp simul opti nosymm com	57	578.2
InCl3	Sr-Cl	1	A, rho, k	fit conp simul opti nosymm com	46	578.2
InCl3	Ba-Cl	1	A, rho, k	fit conp simul opti nosymm com	53	578.2

Fitting				Optimisation of MCl3 structure		
Values after fitting				Cycles for optimisation	Final energy [eV]	Lattice parameter var.
A	rho	C	k			
2456.22	0.3147	0	36.07	1	-94.2	<1% in all dimensions
2292.35	0.318	0.03	36.05	1	-94	<1% in all dimensions
2381.9	0.0337	0	12.07	Largest core-shell distance exceeds cutoff of cuts		
2057.6	0.3234	0	36.03	1	-93.8	<1% in all dimensions
1884	0.328	0	36.03	1	-93.6	<1% in all dimensions
2002.66	0.3248	0	36.4	1	-93.7	<1% in all dimensions
1701.3	0.3334	0	36.01	Too many failed attempts to optimise		
19216.6	0.2552	0	32.38	17	-91.6	10% var in c, <1% in other
12877.5	0.2672	0.03	32.38	17	-91	10% var in c, <1% in other
2008.4	0.3436	0	32.32	4	87.66	7% var in c, <1% in other
10507	0.2738	0	32.38	16	90.73	10% var in c, <1% in other
2015.1	0.3435	0	32.32	4	-87.7	7% var in c, <1% in other
1959.63	0.345	0	32.32	3	-87.6	7% var in c, <1% in other
2343.19	0.3355	0	32.34	5	-88	7% var in c, <1% in other
1879.22	0.3324	0	32.73	21	-91.43	4% var in a and b, <1% in c
n found with no matching core						
87.73	0.7111	0	18.39	Too many failed attempts to optimise		
87.73	0.7111	0	18.39	Conditions for minimum have not been satisfied		
87.73	0.7111	0	18.39	Largest core-shell distance exceeds cutoff of cuts		
87.74	0.7111	0	18.39	Largest core-shell distance exceeds cutoff of cuts		
87.74	0.7111	0	18.39	Largest core-shell distance exceeds cutoff of cuts		

Optimisation of halospinel (40% doped for Y/In)		
Cycles for optimisation	Final energy [eV]	Lattice parameter var.
29	-381.88	<4% in all dimensions
12	-378.23	<5% in all dimensions
11	-379.51	<4% in all dimensions