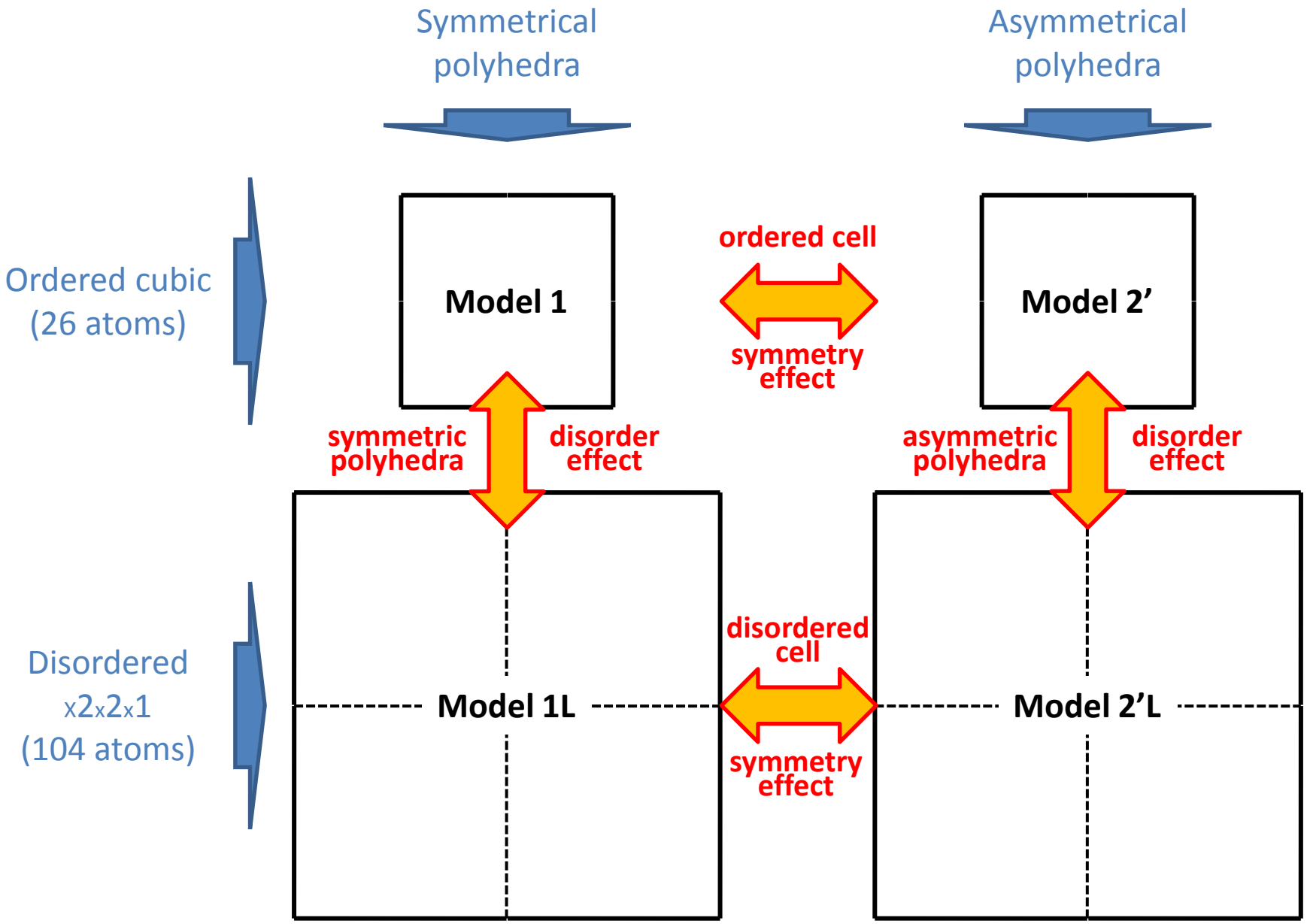
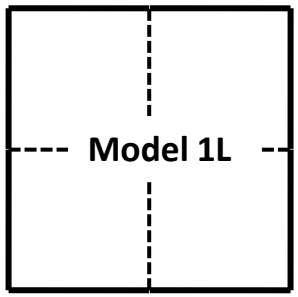
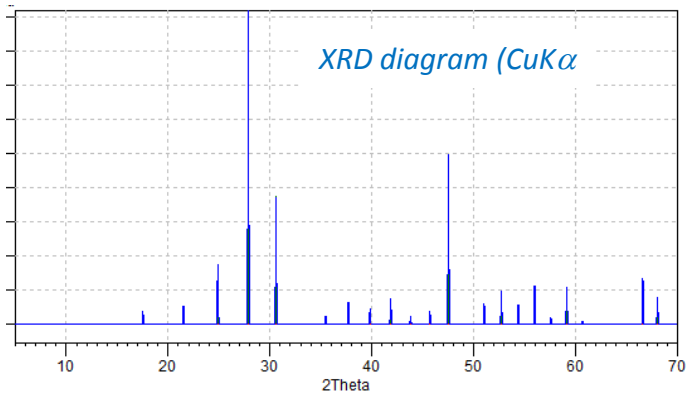
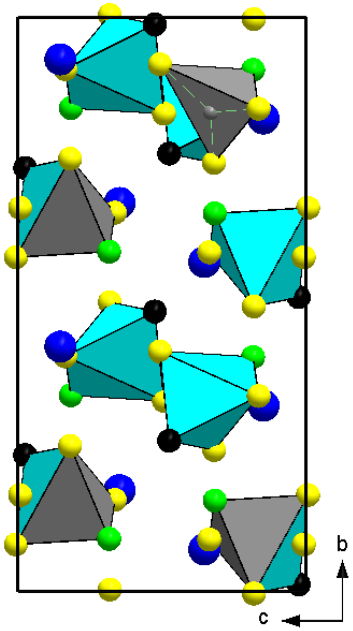
Modelisation of $La_2Mo_2O_9$ with 26 atoms cubic cell and 104 atoms superstructure

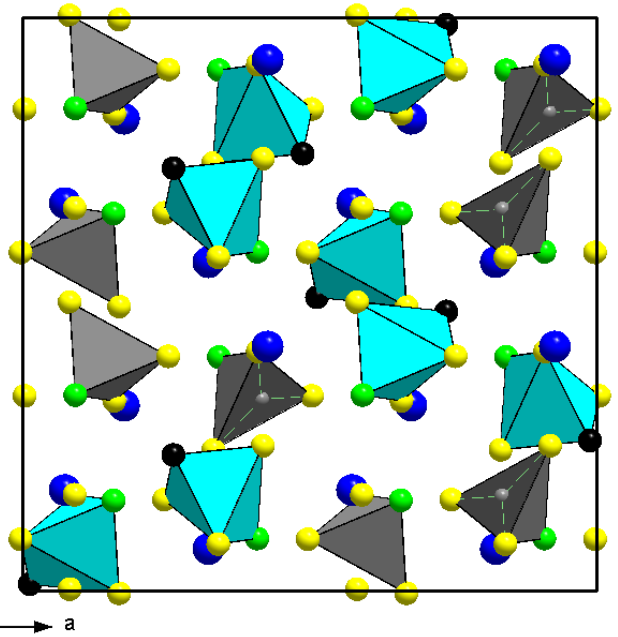


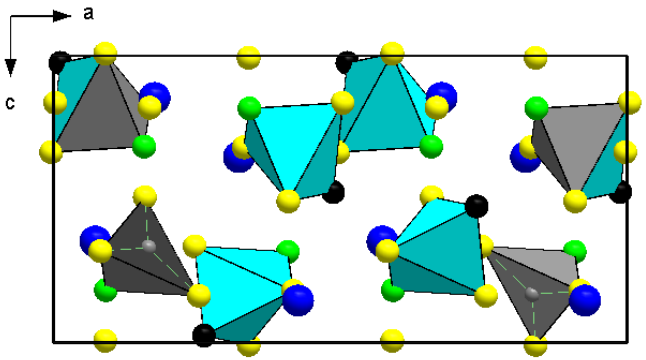
$La_2Mo_2O_9$ disordered Model 1L (x2x2x1 cubic Model 1)

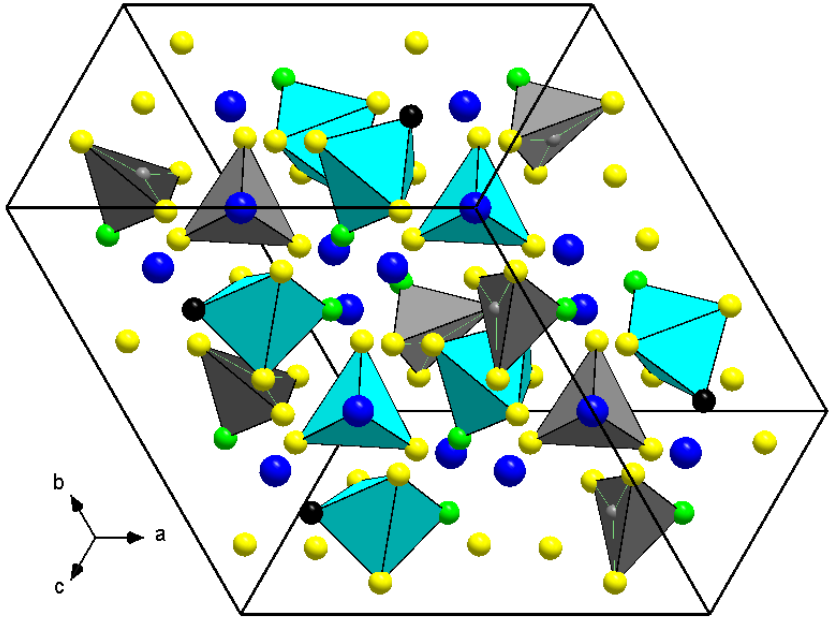








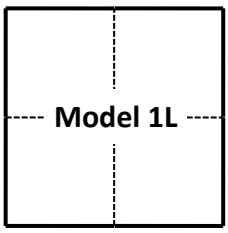




- La
- [MoO_5] bipyramids
- [MoO_4] symmetrical tetrahedra
- O1
- O2
- O4

The 72 oxygen positions of Model 1L

(disordered x2x2x1 superstructure of simple cubic Model 1)

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_cell_length_a    14.30940000
_cell_length_b    14.30940000
_cell_length_c    7.15470000
```

	x	y	z
O32	0.09175	0.34175	0.8165
O33	0.15825	0.15825	0.3165
O34	0.34175	0.40825	0.1835
O35	0.40825	0.09175	0.6835
O36	0.59175	0.34175	0.8165
O37	0.65825	0.15825	0.3165
O38	0.84175	0.40825	0.1835
O39	0.90825	0.09175	0.6835
O40	0.09175	0.84175	0.8165
O41	0.15825	0.65825	0.3165
O42	0.34175	0.90825	0.1835
O43	0.40825	0.59175	0.6835
O44	0.59175	0.84175	0.8165
O45	0.65825	0.65825	0.3165
O46	0.84175	0.90825	0.1835
O47	0.90825	0.59175	0.6835
O48	0.0905	0.168	0.9928
O49	0.9964	0.0905	0.336
O50	0.168	0.9964	0.181
O51	0.4095	0.418	0.5072
O52	0.332	0.2464	0.319
O53	0.5036	0.3405	0.164
O54	0.3405	0.082	0.0072
O55	0.418	0.2536	0.819
O56	0.2464	0.1595	0.664
O57	0.2536	0.4095	0.836
O58	0.1595	0.332	0.4928
O59	0.082	0.5036	0.681
O60	0.0036	0.3405	0.164
O61	0.9095	0.418	0.5072
O62	0.832	0.2464	0.319
O63	0.4964	0.0905	0.336
O64	0.5905	0.168	0.9928
O65	0.668	0.9964	0.181
O66	0.7536	0.4095	0.836
O67	0.6595	0.332	0.4928
O68	0.582	0.5036	0.681
O69	0.8405	0.082	0.0072
O70	0.918	0.2536	0.819
O71	0.7464	0.1595	0.664
O72	0.3405	0.582	0.0072
O73	0.418	0.7536	0.819
O74	0.2464	0.6595	0.664
O75	0.168	0.4964	0.181
O76	0.0905	0.668	0.9928
O77	0.9964	0.5905	0.336
O78	0.4095	0.918	0.5072
O79	0.332	0.7464	0.319
O80	0.5036	0.8405	0.164
O81	0.082	0.0036	0.681
O82	0.2536	0.9095	0.836
O83	0.1595	0.832	0.4928
O84	0.668	0.4964	0.181
O85	0.4964	0.5905	0.336
O86	0.5905	0.668	0.9928
O87	0.8405	0.582	0.0072
O88	0.918	0.7536	0.819
O89	0.7464	0.6595	0.664
O90	0.582	0.0036	0.681
O91	0.7536	0.9095	0.836
O92	0.6595	0.832	0.4928
O93	0.0036	0.8405	0.164
O94	0.9095	0.918	0.5072
O95	0.832	0.7464	0.319
O96	0.0125	0.0125	0.025
O97	0.2625	0.2375	0.975
O98	0.9875	0.2625	0.475
O99	0.7375	0.4875	0.525
O100	0.2625	0.7375	0.975
O101	0.4875	0.7625	0.475
O102	0.5125	0.5125	0.025
O103	0.7375	0.9875	0.525

O1

O2

O1
(belong to bipyramids)

O2 belonging to tetrahedra
(one per group of three will be shifted to O3 position in Model 2'L)

= O2 atoms belonging to bipyramids