The 72 oxygen positions of Model 2'L

(disordered x2x2x1 superstructure of cubic Model 2')

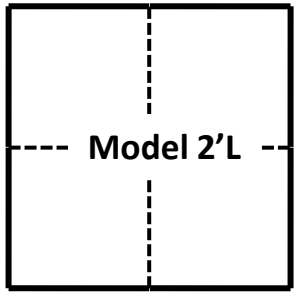
	Model 1L				Model 2'L			
		x	y	z		x	y	z
O1	O32	0.09175	0.34175	0.8165	O32	0.09175	0.34175	0.8165
	O33	0.15825	0.15825	0.3165	O33	0.15825	0.15825	0.3165
	O34	0.34175	0.40825	0.1835	O34	0.34175	0.40825	0.1835
	O35	0.40825	0.09175	0.6835	O35	0.40825	0.09175	0.6835
	O36	0.59175	0.34175	0.8165	O36	0.59175	0.34175	0.8165
	O37	0.65825	0.15825	0.3165	O37	0.65825	0.15825	0.3165
	O38	0.84175	0.40825	0.1835	O38	0.84175	0.40825	0.1835
	O39	0.90825	0.09175	0.6835	O39	0.90825	0.09175	0.6835
	O40	0.09175	0.84175	0.8165	O40	0.09175	0.84175	0.8165
	O41	0.15825	0.65825	0.3165	O41	0.15825	0.65825	0.3165
	O42	0.34175	0.90825	0.1835	O42	0.34175	0.90825	0.1835
	O43	0.40825	0.59175	0.6835	O43	0.40825	0.59175	0.6835
	O44	0.59175	0.84175	0.8165	O44	0.59175	0.84175	0.8165
	O45	0.65825	0.65825	0.3165	O45	0.65825	0.65825	0.3165
	O46	0.84175	0.90825	0.1835	O46	0.84175	0.90825	0.1835
	O47	0.90825	0.59175	0.6835	O47	0.90825	0.59175	0.6835
O2	O48	0.0905	0.168	0.9928	O48	0.0905	0.168	0.9928
	O49	0.9964	0.0905	0.336	O49	0.9964	0.0905	0.336
	O50	0.168	0.9964	0.181	O50	0.168	0.9964	0.181
	O51	0.4095	0.418	0.5072	O51′	0.4555	0.321	0.551
	O52	0.332	0.2464	0.319	O52	0.332	0.2464	0.319
	O53	0.5036	0.3405	0.164	O53	0.5036	0.3405	0.164
	O54	0.3405	0.082	0.0072	O54	0.3405	0.082	0.0072
	O55	0.418	0.2536	0.819	O55	0.418	0.2536	0.819
	O56	0.2464	0.1595	0.664	O56	0.2464	0.1595	0.664
	O57	0.2536	0.4095	0.836	O57	0.2536	0.4095	0.836
	O58	0.1595	0.332	0.4928	O58′	0.2055	0.429	0.449
	O59	0.082	0.5036	0.681	O59	0.082	0.5036	0.681
	O60	0.0036	0.3405	0.164	O60	0.0036	0.3405	0.164
	O61	0.9095	0.418	0.5072	O61	0.9095	0.418	0.5072
	O62	0.832	0.2464	0.319	O62	0.832	0.2464	0.319
	O63	0.4964	0.0905	0.336	O63′	0.4745	0.0445	0.142
	O64	0.5905	0.168	0.9928	O64	0.5905	0.168	0.9928
	O65	0.668	0.9964	0.181	O65	0.668	0.9964	0.181
	O66	0.7536	0.4095	0.836	O66	0.7536	0.4095	0.836
	O67	0.6595	0.332	0.4928	O67	0.6595	0.332	0.4928
	O68	0.582	0.5036	0.681	O68	0.582	0.5036	0.681
	O69	0.8405	0.082	0.0072	O69	0.8405	0.082	0.0072
	O70	0.918	0.2536	0.819	O70′	0.821	0.2755	0.911
	O71	0.7464	0.1595	0.664	O71	0.7464	0.1595	0.664
	O72	0.3405	0.582	0.0072	O72	0.3405	0.582	0.0072
	O73	0.418	0.7536	0.819	O73	0.418	0.7536	0.819
	O74	0.2464	0.6595	0.664	O74	0.2464	0.6595	0.664
	O75	0.168	0.4964	0.181	O75	0.168	0.4964	0.181
	O76	0.0905	0.668	0.9928	O76	0.0905	0.668	0.9928
	O77	0.9964	0.5905	0.336	O77′	0.9745	0.5445	0.142
	O78	0.4095	0.918	0.5072	O78	0.4095	0.918	0.5072
	O79	0.332	0.7464	0.319	O79	0.332	0.7464	0.319
	O80	0.5036	0.8405	0.164	O80	0.5036	0.8405	0.164
	O81	0.082	0.0036	0.681	O81′	0.179	0.0255	0.589
	O82	0.2536	0.9095	0.836	O82	0.2536	0.9095	0.836
	O83	0.1595	0.832	0.4928	O83	0.1595	0.832	0.4928
	O84	0.668	0.4964	0.181	O84	0.668	0.4964	0.181
	O85	0.4964	0.5905	0.336	O85	0.4964	0.5905	0.336
	O86	0.5905	0.668	0.9928	O86	0.5905	0.668	0.9928
	O87	0.8405	0.582	0.0072	O87	0.8405	0.582	0.0072
	O88	0.918	0.7536	0.819	O88	0.918	0.7536	0.819
	O89	0.7464	0.6595	0.664	O89′	0.7245	0.7055	0.858
	O90	0.582	0.0036	0.681	O90	0.582	0.0036	0.681
	O91	0.7536	0.9095	0.836	O91	0.7536	0.9095	0.836
	O92	0.6595	0.832	0.4928	O92	0.6595	0.832	0.4928
	O93	0.0036	0.8405	0.164	O93′	0.0255	0.7945	0.358
	O94	0.9095	0.918	0.5072	O94	0.9095	0.918	0.5072
	O95	0.832	0.7464	0.319	O95	0.832	0.7464	0.319
O1 (belong to bipyramids)	O96	0.0125	0.0125	0.025	O96	0.0125	0.0125	0.025
	O97	0.2625	0.2375	0.975	O97	0.2625	0.2375	0.975
	O98	0.9875	0.2625	0.475	O98	0.9875	0.2625	0.475
	O99	0.7375	0.4875	0.525	O99	0.7375	0.4875	0.525
	O100	0.2625	0.7375	0.975	O100	0.2625	0.7375	0.975
	O101	0.4875	0.7625	0.475	O101	0.4875	0.7625	0.475
	O102	0.5125	0.5125	0.025	O102	0.5125	0.5125	0.025
	O103	0.7375	0.9875	0.525	O103	0.7375	0.9875	0.525

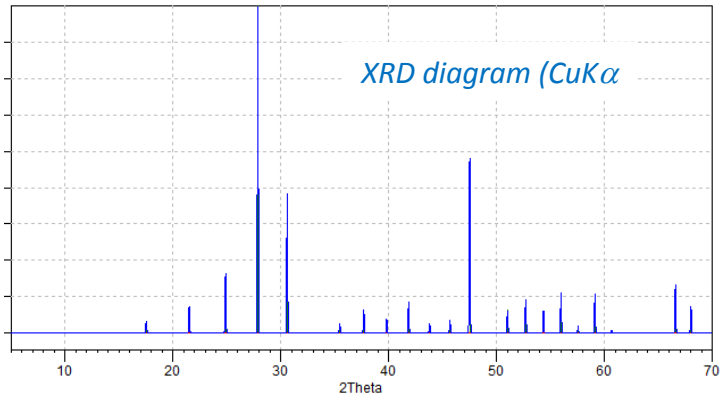
Shift of one O2 among three to position O3 resulting in asymmetric tetrahedra

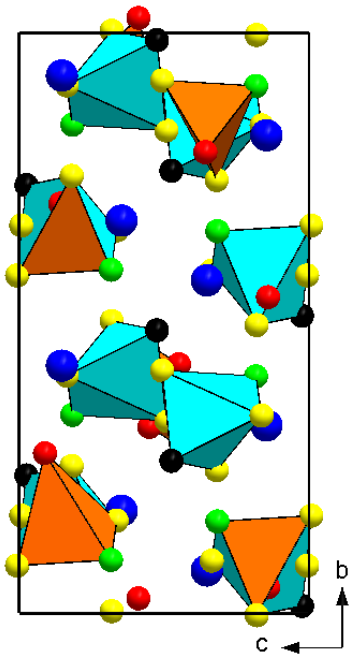
= O2 atoms in bipyramids

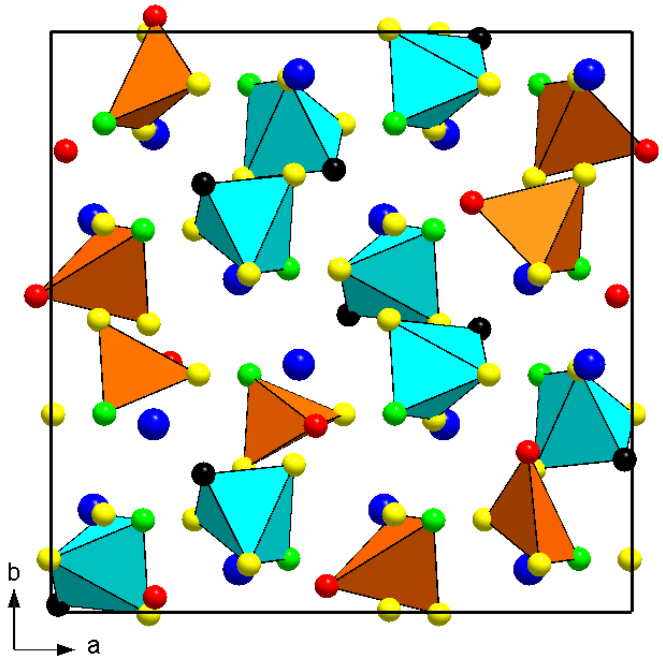
= O2&O3 atoms in asymmetric tetrahedra

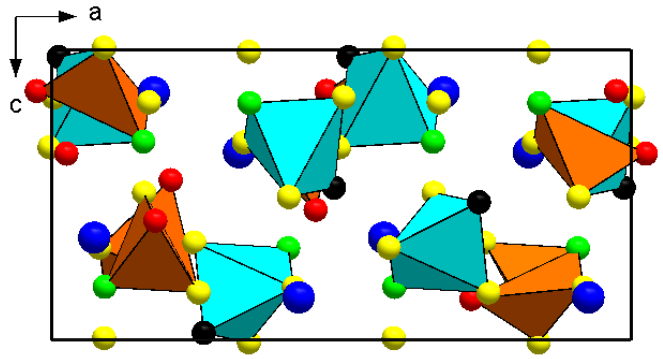
$La_2Mo_2O_9$ disordered **Model 2'L** (x2x2x1 cubic Model 2')

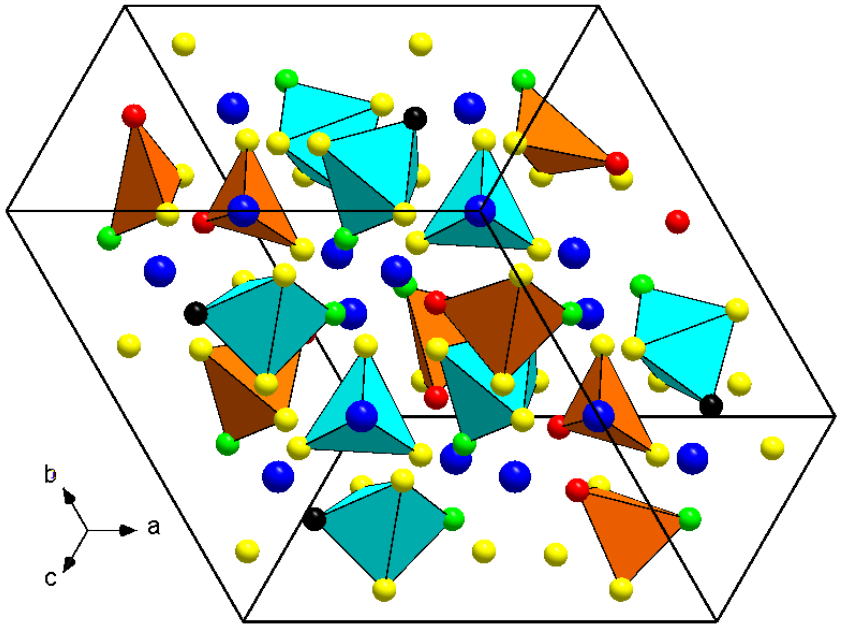












- La
- [MoO_5] bipyramids
- [MoO_4] asymmetrical tetrahedra
- O1
- O2
- O3
- O4