

Supplementary Material

Bond Length and Bond Valence Relationships for Chromium Oxides, Chromium Sulfides, Molybdenum Oxides, and Molybdenum Sulfides, by Labrecque and Hardcastle

a0	0.529177	Kantor, A.; Kantor, I.; Merlini, M.; Glazyrin, K.; Prescher, C.; Hanfland, M.; Dubrovinsky, L.		
		High-pressure structural studies of eskolaite by means of single-crystal X-ray diffraction Note: P = 63.9 GPa		
COD: 9014067		American Mineralogist, 2012, 97, 1764-1770		
Cr2O3		1.963	0.553939238	
		1.963	0.553939238	
		1.963	0.553939238	
		2.012	0.477527918	
		2.012	0.477527918	
		2.012	0.477527918	
		3.37	0.007806255	Cr-Cr
		3.37	0.007806255	
		3.37	0.007806255	
		3.639	0.003455827	
		3.639	0.003455827	
		3.639	0.003455827	
		3.685	0.003006321	
		3.685	0.003006321	
		3.982	0.001222668	
		3.982	0.001222668	
		3.982	0.001222668	
		4.342	0.000410866	
		4.554	0.000216171	
		4.554	0.000216171	
		4.554	0.000216171	
		4.57	0.000205944	
		4.57	0.000205944	
		4.57	0.000205944	
		4.591	0.000193251	
		4.591	0.000193251	
		4.591	0.000193251	
		4.591	0.000193251	
		4.591	0.000193251	
		4.833	9.28434E-05	
		4.833	9.28434E-05	
		4.833	9.28434E-05	3.14079 0.019822

Belokoneva, E. L.; Shcherbakova, Y. K.

Electron density in synthetic eskolaite Cr2O3 with a corundum structure and its relation to antiferromagnetic properties

COD: 9016327		Russian Journal of Inorganic Chemistry, 2003, 48, 861-869		
Cr2O3		1.963	0.553939238	
		1.963	0.553939238	

Cr-O	1.963	0.553939238	Cr-Cr	
	2.012	0.477527918		
	2.012	0.477527918		
	2.0120	0.477527918		
	3.37	0.007806255		
	3.37	0.007806255		
	3.3700	0.007806255		
	3.637	0.003476828		
	3.637	0.003476828		
	3.637	0.003476828		
	3.684	0.003015442		
	3.6840	0.003015442		
	3.6840	0.003015442		
	3.9790	0.00123383		
	3.9790	0.00123383		
	3.9790	0.00123383		
	4.343	0.000409623		
	4.343	0.000409623		
	4.553	0.000216827		
	4.553	0.000216827		
	4.553	0.000216827		
	4.569	0.000206568		
	4.569	0.000206568		
	4.569	0.000206568		
	4.591	0.000193251		
	4.591	0.000193251		
	4.591	0.000193251		
	4.5910	0.000193251		
	4.5910	0.000193251		
	4.83	9.3691E-05		
	4.8300	9.3691E-05	3.144242	0.020806

Sawada, H.

Residual electron density study of chromium sesquioxide by crystal structure and scattering factor refinement

Materials Research Bulletin, 1994, 29, 239-245

	1.964	0.53889571		
COD: 9014036	1.964	0.552263767		
Cr ₂ O ₃	1.964	0.552263767	Cr-Cr	
	2.013	0.476083564		
	2.013	0.476083564		
	3.372	0.007759104		
Cr-O	3.372	0.007759104		
	3.372	0.007759104		

3.64	0.003445375		
3.64	0.003445375		
3.64	0.003445375		
3.687	0.002988163		
3.687	0.002988163		
3.687	0.002988163		
3.983	0.00121897		
3.983	0.00121897		
4.346	0.000405918		
4.346	0.000405918		
4.557	0.000214215		
4.557	0.000214215		
4.557	0.000214215		
4.573	0.00020408		
4.573	0.00020408		
4.573	0.00020408		
4.595	0.000190923		
4.595	0.000190923		
4.595	0.000190923		
4.595	0.000190923	2.643437	0.127137

Lu Zhonghua; Dahn, J.R.

Structure and electrochemistry of layered Li (Cr_x Li_(1/3-x/3) Mn_(2/3-2x/3)) O₂

Journal of the Electrochemical Society, 2002, 149, A1454-A1459

COD: 1532839

CrLiO₂

4.725	0.000128776	
4.561	0.000211635	Cr-Cr
4.561	0.000211635	
3.729	0.002631176	
3.52	0.00495571	
4.725	0.000128776	
4.561	0.000211635	
1.994	0.504288641	
4.561	0.000211635	
3.52	0.00495571	
3.52	0.00495571	
4.725	0.000128776	
4.561	0.000211635	
1.994	0.504288641	
4.561	0.000211635	
1.994	0.504288641	
1.994	0.504288641	

4.561	0.000211635		
4.561	0.000211635		
1.994	0.504288641		
4.561	0.000211635		
3.52	0.00495571		
3.52	0.00495571		
4.725	0.000128776		
4.561	0.000211635		
1.994	0.504288641		
4.725	0.000128776		
3.52	0.00495571		
3.729	0.002631176		
4.561	0.000211635		
4.725	0.000128776		
4.561	0.000211635		
4.725	0.000128776	3.06417	0.004118

Tarantino, Serena C.; Giannini, Mattia; Carpenter, Michael A.; Zema, Michele

Cooperative Jahn–Teller effect and the role of strain in the tetragonal-to-cubic phase transition in Mg

IUCrJ, 2016, 3

COD: 1543900

Cr2MgO4

4.783	0.000108026
4.783	0.000108026
4.617	0.000178614
4.617	0.000178614
3.604	0.003842353
3.444	0.00623864
1.993	0.505818565
3.664	0.003203779
4.614	0.000180245
3.604	0.003842353
4.617	0.000178614
4.617	0.000178614
4.617	0.000178614
4.617	0.000178614
1.993	0.505818565
1.993	0.505818565
4.617	0.000178614
4.783	0.000108026
3.664	0.003203779
3.664	0.003203779
1.993	0.505818565
3.444	0.00623864
4.783	0.000108026

3.664	0.003203779		
4.617	0.000178614		
4.617	0.000178614		
4.783	0.000108026		
4.783	0.000108026		
4.617	0.000178614	2.058687	

Weakley, T. J. R.; Ylvisaker, E. R.; Yager, R. J.; Stephens, J.E.; Wiegel, R.; Mengis, M.; Bauer, M. R.; Abrahams, S. C.

Phase transitions in $K_2Cr_2O_7$ and structural redeterminations of phase II

Acta Crystallographica, Section B, 2004, 60, 714-724

COD: 2102643
Cr₂K₂O₇

5.742	5.91411E-06		
4.535	0.000228978		
4.317	0.00044319		
5.134	3.73045E-05		
4.79	0.00010576		
4.346	0.000405918		
1.611	1.608962326		
4.661	0.000156326		
3.753	0.002446674		
1.614	1.594406803		
3.996	0.0011719		
4.003	0.001147311		
3.766	0.002352196		
1.787	0.944069577		
4.499	0.000255361		
5.395	1.69198E-05		
1.603	1.648429985		
3.667	0.003174796		
5.721	6.30256E-06		
4.331	0.000424787		
4.752	0.000118662		
4.542	0.000224174		
5.127	3.8104E-05		
3.993	0.001182598		
3.813	0.002040052		
5.001	5.58128E-05		
4.882	8.00364E-05	5.811988	0.035349

Crottaz, O.; Kubel, F.

Crystal structure of copper(I) chromium(III) oxide, $2HCuCrO_2$

Zeitschrift fuer Kristallographie (149,1979-), 1996, 211, 481-481

COD: 8104065

Cr-O	5	5.59821E-05		
	5	5.59821E-05		
	4.653	0.00016016		
	3.578	0.004157214		
	4.653	0.00016016		
	4.653	0.00016016		
	1.989	0.511984815		
	1.989	0.511984815		
	4.653	0.00016016		
	3.578	0.004157214		
	1.989	0.511984815		
	3.578	0.004157214		
	4.653	0.00016016		
	4.653	0.00016016		
	4.652	0.000160646		
	4.653	0.00016016		
	3.578	0.004157214		
	1.989	0.511984815		
	3.578	0.004157214		
	4.652	0.000160646		
	1.989	0.511984815		
	1.989	0.511984815		
	4.652	0.000160646		
	4.652	0.000160646		
	3.578	0.004157214		
	4.653	0.00016016		
	5	5.59821E-05		
	5	5.59821E-05		
	5	5.59821E-05	3.099056	0.009812

Jimenez, E.; Fernandez, M.T.; Isasi, J.; Saez-Puche, R.

Magnetic behavior of Er Cr O4 oxide

Journal of Alloys Compd., 2002, 2000, 369-374

COD: 1531650

CrErO4

Cr-O

4.639	0.000167099
5.499	1.23474E-05
5.271	2.46336E-05
4.205	0.000622206
5.92	3.44919E-06
3.643	0.003414206
3.788	0.002200548
5.271	2.46336E-05
3.788	0.002200548
4.639	0.000167099

4.639	0.000167099	
3.788	0.002200548	
1.692	1.258879005	
4.205	0.000622206	
3.788	0.002200548	
5.499	1.23474E-05	
5.463	1.37701E-05	
4.639	0.000167099	
1.692	1.258879005	
1.692	1.258879005	
5.92	3.44919E-06	
3.463	0.00588971	
3.758	0.002409895	
4.639	0.000167099	
3.788	0.002200548	
4.639	0.000167099	
4.639	0.000167099	
3.788	0.002200548	
3.463	0.00588971	
5.271	2.46336E-05	
5.271	2.46336E-05	3.810002

W.A. Dollase; H.St.C. O'Neill

The Spinel $\text{CuCr}_{2-2x}\text{O}_{4-4x}$ and $\text{CuRh}_{2-2x}\text{O}_{4-4x}$

COD: 2006190

Acta Crystallographica Section C, 1997, 53, 657-659

Cr-O

4.959	6.33852E-05
3.588	0.00403317
4.525	0.00023602
4.712	0.000133948
3.767	0.002345081
4.559	0.000212921
1.998	0.498215083
3.588	0.00403317
1.973	0.53741074
4.712	0.000133948
4.525	0.00023602
1.996	0.501242663
3.435	0.006411064
4.813	9.86421E-05
3.435	0.006411064
4.525	0.00023602
1.998	0.498215083
4.712	0.000133948

1.973	0.53741074		
1.998	0.498215083		
4.559	0.000212921		
3.767	0.002345081		
4.559	0.000212921		
4.712	0.000133948		
4.525	0.00023602		
4.498	0.000256136		
3.558	0.004416863		
4.813	9.86421E-05	3.10334	0.010679

Palatinus, Lukas; Dusek, Michal; El Bali, Brahim; Glaum, Robert

The incommensurately and commensurately modulated crystal structures of chromium(II) diphosphate

Acta Crystallographica Section B, 2006, 62, 556-566

COD: 2100549
Cr2O7P2

2.0699	0.400706838
5.899	3.67573E-06
4.898	7.62497E-05
4.139	0.000759911
3.976	0.001245093
5.27	2.47083E-05
4.099	0.000857799
3.081	0.018734625
4.379	0.000367302
5.01	5.43117E-05
2.768	0.04835275
3.504	0.005201818
4.124	0.000795236
4.654	0.000159676
4.124	0.000795236
3.925	0.001453103
4.475	0.000274617
2.02	0.46609467
5.422	1.5591E-05
5.674	7.2669E-06
2.069	0.401800779
3.674	0.003108184
5.01	5.43117E-05
4.158	0.000717409
4.158	0.000717409
2.069	0.401800779
3.081	0.018734625
4.654	0.000159676
4.139	0.000759911

4.778	0.000109675		
3.504	0.005201818		
4.778	0.000109675		
5.422	1.5591E-05		
4.475	0.000274617		
3.925	0.001453103		
4.39	0.000355265		
4.099	0.000857799		
5.659	7.60471E-06		
4.898	7.62497E-05		
5.27	2.47083E-05		
5.899	3.67573E-06	1.782323	0.047383

Weakley, T. J. R.; Ylvisaker, E. R.; Yager, R. J.; Stephens, J.E.; Wiegel, R.; Mengis, M.; Bauer, M. R.; Abrahams, S. C.

Phase transitions in $K\sim 2\sim Cr\sim 2\sim O\sim 7\sim$ and structural redeterminations of phase II

Acta Crystallographica, Section B, 2004, 60, 714-724

COD: 2102643

Cr-O

4.546	0.000221474
4.879	8.07671E-05
5.4	1.66655E-05
5.128	3.79888E-05
5.002	5.5644E-05
3.764	0.00236649
3.664	0.003203779
5.002	5.5644E-05
4.008	0.001130065
1.603	1.648429985
3.807	0.00207747
5.721	6.30256E-06
5.882	3.86998E-06
3.993	0.001182598
3.754	0.002439273
1.789	0.938367256
4.753	0.000118303
4.782	0.000108354
1.614	1.594406803
3.993	0.001182598
4.387	0.000358508
5.125	3.83356E-05
4.534	0.000229672
5.424	1.54969E-05
4.348	0.000403466
4.662	0.000155853
4.76	0.000115821

5.797	5.00649E-06		
5.738	5.98621E-06	4.196819	

Pérez-Cruz, María Ana; Elizalde-González, María de la Paz; Escudero, Roberto; Bernès, Sylvain;

At last! The single-crystal X-ray structure of a naturally occurring sample of the ilmenite-type oxide FeCrO₃

COD: 2107479

Acta Crystallographica Section B, 2015, 71, 555-561

CrFeO₃

5.807	4.8571E-06		
4.235	0.000568155		
5.023	5.22145E-05		
4.235	0.000568155		
4.235	0.000568155		
4.785	0.000107374		
3.795	0.002154377		
4.658	0.000157753		
5.807	4.8571E-06		
5.023	5.22145E-05		
4.658	0.000157753		
2.101	0.364680257		
2.101	0.364680257		
4.785	0.000107374		
4.405	0.000339483		
3.795	0.002154377		
2.101	0.364680257		
3.795	0.002154377		
3.479	0.005611056		
1.9	0.670414804		
3.479	0.005611056		
4.785	0.000107374		
4.658	0.000157753		
4.405	0.000339483		
1.9	0.670414804		
1.9	0.670414804		
4.683	0.000146247		
5.469	1.35221E-05		
4.7	0.000138907		
3.479	0.005611056		
4.405	0.000339483		
3.665	0.003194089		
3.665	0.003194089		
5.406	1.63653E-05		
3.665	0.003194089		
4.683	0.000146247		
5.406	1.63653E-05	3.142274	0.020242

Weil, Matthias; Stöger, Berthold

Spinel-type HgCr₂O₄ from single-crystal data

COD: 2210102

Acta Crystallographica Section E, 2006, 62, i199-i200

Cr-O	3.885	0.001640286		
	5.072	4.50119E-05		
	3.439	0.00633385		
	4.763	0.000114773		
	4.763	0.000114773		
	5.072	4.50119E-05		
	2.001	0.493707966		
	2.001	0.493707966		
	5.072	4.50119E-05		
	3.885	0.001640286		
	3.855	0.001796334		
	2.001	0.493707966		
	4.763	0.000114773		
	4.763	0.000114773		
	4.763	0.000114773		
	2.001	0.493707966		
	3.855	0.001796334		
	3.855	0.001796334		
	5.072	4.50119E-05		
	2.001	0.493707966		
	2.001	0.493707966		
	5.072	4.50119E-05		
	4.763	0.000114773		
	3.439	0.00633385		
	4.763	0.000114773		
	5.072	4.50119E-05		
	5.072	4.50119E-05		
	3.855	0.001796334		
	5.072	4.50119E-05	2.986545	0.000181

Levy, D.; Diella, V.; Pavese, A.; Dapiaggi, M.; Sani, A.

P-V equation of state, thermal expansion, and P-T stability of synthetic zincochromite (ZnCr₂O₄ spinel) Sample: T = 298 K

COD: 9003703

American Mineralogist, 2005, 90, 1157-1162

Cr ₂ O ₄ Zn	4.844	8.98007E-05		
	4.844	8.98007E-05		
	4.6	0.000188053		
	3.693	0.002934342		
	4.6	0.000188053		
	4.844	8.98007E-05		

4.844	8.98007E-05		
3.693	0.002934342		
4.6	0.000188053		
1.954	0.569249082		
1.954	0.569249082		
3.367	0.007877519		
1.954	0.569249082		
3.693	0.002934342		
4.844	8.98007E-05		
4.6	0.000188053		
4.6	0.000188053		
3.693	0.002934342		
4.844	8.98007E-05		
3.367	0.007877519		
1.954	0.569249082		
1.954	0.569249082		
1.954	0.569249082		
4.6	0.000188053		
3.693	0.002934342		
4.6	0.000188053		
4.844	8.98007E-05		
4.844	8.98007E-05		
3.693	0.002934342		
4.844	8.98007E-05	3.45098	0.203383

Nazar, L.F.; Rowsell, J.L.C.

Synthesis, structure, and solid-state electrochemical properties of Ce₃B₂O₆: a new chromium(III) borate with the norbergite structure

Journal of Materials Chemistry, 2001, 11, 3228-3233

COD: 7209462

BCr3O6

4.403	0.000341546
4.361	0.000387886
3.693	0.002934342
3.523	0.004910878
4.652	0.000160646
1.893	0.684782491
1.907	0.65634857
4.445	0.000300743
3.531	0.004793299
1.961	0.557305446
5.231	2.78068E-05
3.761	0.002388094
3.482	0.005560296
3.262	0.010827426

2.03	0.452187287		
3.805	0.002090095		
2.016	0.471776661		
4.501	0.000253818		
4.551	0.000218144		
3.815	0.00202773		
4.704	0.000137234		
4.367	0.0003809		
3.377	0.007642469	2.867784	0.017481

Daturi, M; Busca, G; Borel, M M; Leclaire, A; Piaggio, P

Vibrational and XRD study of the system Cd W O4 - Cd Mo O4

Journal of Physical Chemistry, 1997, 101, 4358-4369

COD: 1001800
CdMoO4

1.751	1.550631		
1.751	1.550631		
1.751	1.550631		
1.751	1.550631		
2.85	0.048335		
2.85	0.048335		
2.856	0.047428		
4.045	0.001113		
4.045	0.001113		
4.045	0.001113		
4.071	0.001025		
4.071	0.001025		
4.071	0.001025		
4.11	0.000906		
4.11	0.000906		
4.11	0.000906		
4.11	0.000906		
4.604	0.000191		
4.604	0.000191		
4.685	0.000148		
4.685	0.000148		
5.167	3.23E-05	6.357371	0.127714

MoCaO4 Crichton W. Zeitschrift, 2004, 219

Mo-O	5.761	4.95E-06	
	5.225	2.69E-05	
	4.047	0.001106	
	4.08	0.000996	
	4.494	0.00027	
	5.604	8.12E-06	
	4.494	0.00027	
	5.361	1.75E-05	
	5.518	1.07E-05	
	4.047	0.001106	
	2.692	0.079581	
	1.872	1.05845	
	4.215	0.000651	
	4.003	0.001271	
	4.497	0.000267	
	5.225	2.69E-05	
	4.676	0.000152	
	5.361	1.75E-05	
	4.003	0.001271	
	1.872	1.05845	
	2.671	0.085033	
	4.494	0.00027	
	3.855	0.002027	
	1.872	1.05845	
	3.853	0.00204	
	4.827	9.43E-05	
	2.671	0.085033	
	3.964	0.001437	
	3.964	0.001437	
	4.676	0.000152	
	5.342	1.86E-05	
	4.827	9.43E-05	
	4.215	0.000651	3.440687

Sitepu, H.; O'Connor B H; Li, D.

Comparative evaluation of the March and generalized spherical harmonic preferred orientation models using X-ray diffraction data for powders

Journal of Applied Crystallography, 2005, 38, 158-167

COD: 9009669

4.892 7.68E-05

MoO3	5.489	1.17E-05		
	4.448	0.000312		
	4.081	0.000993		
	4.992	5.6E-05		
	4.998	5.5E-05		
	3.497	0.006273		
	4.219	0.000643		
	2.471	0.159846		
	4.566	0.000215		
	4.081	0.000993		
	4.185	0.000715		
	4.317	0.000472		
	1.899	0.971997		
	2.029	0.644899		
	4.448	0.000312		
	4.075	0.001012		
	4.566	0.000215		
	4.215	0.000651		
	1.958	0.806866		
	1.899	0.971997		
	4.456	0.000304		
	3.774	0.002617		
	4.219	0.000643		
	1.71	1.764825		
	4.215	0.000651		
	3.493	0.006353		
	4.072	0.001022		
	3.774	0.002617		
	4.702	0.00014		
	4.075	0.001012		
	3.493	0.006353		
	4.998	5.5E-05		
	4.832	9.29E-05		
	4.702	0.00014	5.355437	0.415462

Yip, Thomas W. S.; Cussen, Edmund J.; Wilson, Claire

Spontaneous formation of crystalline lithium molybdate from solid reagents at room temperature.

Dalton transactions (Cambridge, England : 2003), 2010, 39, 411-417

COD: 7024042	4.816	9.77E-05		
Li2MoO4	4.577	0.000208		
	3.723	0.003074		
	4.626	0.000178		
	3.946	0.001521		
	3.316	0.011106		

4.926	6.9E-05		
1.759	1.511973		
4.32	0.000467		
3.87	0.001933		
4.528	0.000242		
3.853	0.00204		
1.766	1.478938		
3.7	0.003306		
3.887	0.001832		
4.694	0.000144		
4.887	7.81E-05		
1.769	1.465003		
1.77	1.460386		
4.76	0.000117		
3.712	0.003183		
3.869	0.001939		
4.94	6.6E-05		
4.916	7.12E-05		
4.561	0.000218		
5.435	1.38E-05		
4.567	0.000214	5.948419	0.002661

Begue, P.; Enjalbert, R.; Galy, J.; Castro, A.

Single-crystal X-ray investigations of the structures of gamma(H)Bi₂MoO₆ and its partially substituted As(3+) and Sb(3+) homologues

Solid State Sciences, **2000**, 2, 637-653

COD: 1525625

Bi₂MoO₆

4.199	0.000684		
5.709	5.83E-06		
4.191	0.000702		
4.206	0.00067		
2.885	0.04328		
1.748	1.565382		
3.223	0.014895		
4.778	0.00011		
4.145	0.000812		
4.804	0.000101		
1.789	1.375394		
3.731	0.002998		
1.81	1.287198		
5.049	4.68E-05		
4.605	0.00019		
1.742	1.595305		
4.191	0.000702		

4.592	0.000198		
2.841	0.049727		
4.031	0.001163		
5.333	1.91E-05		
5.495	1.15E-05	5.939593	0.003649

Seisenbaeva, G.A.; Sundberg, M.; Nygren, M.; Dubrovinsky, L.; Kessler, V.G.

Thermal decomposition of the methoxide complexes Mo O (O Me)₄, Re₄ O₆ (O Me)₁₂ and (Re_{1-x} Mo_x) O₆ (O Me)₁₂ (0.24 < x < 0.55)

MoO₂

COD: 1533435

Materials Chemistry and Physics, 2004, 87, 142-148

4.244	0.000594		
3.492	0.006373		
2.069	0.568419		
3.492	0.006373		
4.638	0.000171		
3.687	0.003444		
5.674	6.51E-06		
4.434	0.000326		
4.638	0.000171		
1.956	0.811975		
1.956	0.811975		
1.956	0.811975		
5.674	6.51E-06		
5.674	6.51E-06		
4.638	0.000171		
3.687	0.003444		
4.683	0.000149		
3.687	0.003444		
3.492	0.006373		
2.069	0.568419		
4.638	0.000171		
4.244	0.000594		
4.244	0.000594		
4.244	0.000594		
4.244	0.000594	3.606365	0.154949

Azad, A.K.; Eriksson, S.G.; Ivanov, S.A.; Svedlindh, P.; Mathieu, R.; Eriksen, J.; Rundlof, H.

Synthesis, structural and magnetic characterisation of the double perovskite A₂ Mn Mo O₆ (A = Ba, Sr)

Journal of Alloys Compd., 2004, 364, 77-82

COD: 1533564

MoO₄Sr

4.294	0.000507		
4.294	0.000507		
3.097	0.022168		
4.931	6.79E-05		

4.298	0.000501		
4.178	0.000731		
5.677	6.45E-06		
4.178	0.000731		
1.77	1.460386		
3.097	0.022168		
1.77	1.460386		
4.298	0.000501		
4.985	5.73E-05		
1.77	1.460386		
4.178	0.000731		
4.289	0.000515		
4.931	6.79E-05		
1.77	1.460386		
3.097	0.022168		
4.289	0.000515		
3.097	0.022168		
4.294	0.000507		
4.178	0.000731		
4.985	5.73E-05		
4.294	0.000507	5.937462	0.003911

CuMoO4 Ehrenberg H, Journal of Physical Sciences. 1997, 58

Mo-O	3.91	0.001704
	5.223	2.7E-05
	4.387	0.000378
	4.386	0.000379
	1.683	1.921795
	4.035	0.001149
	4.14	0.000825
	1.781	1.41056
	4.072	0.001022
	4.536	0.000236
	5.641	7.23E-06
	3.732	0.002988
	1.926	0.892606
	3.884	0.00185
	3.942	0.00154
	2.105	0.507374
	4.557	0.000221
	2.471	0.159846

4.472	0.000289	
4.708	0.000137	
3.978	0.001375	
4.205	0.000672	
4.938	6.65E-05	4.907047

Mo4O11 Hoong-Kun Fun, Acta Crystallographica sec. c. 1999, 55

Mo-O

5.253	2.46E-05	
4.085	0.000981	
4.272	0.000544	
5.517	1.07E-05	
4.001	0.001279	
4.1	0.000936	
4.299	0.000499	
5.331	1.92E-05	
5.539	9.97E-06	
4.315	0.000475	
1.795	1.349596	
4.075	0.001012	
3.922	0.001641	
4.027	0.001178	
1.771	1.455785	
2.043	0.617026	
4.284	0.000523	
4.675	0.000152	
4.162	0.000769	
4.26	0.000565	
2.042	0.618976	
4.17	0.00075	
4.407	0.000355	
5.542	9.88E-06	
4.078	0.001003	
2.066	0.573826	
4.245	0.000592	
4.494	0.00027	
4.308	0.000485	
4.336	0.000444	4.629736

CaMo5O8 Gougeon, P Acta Crystallographica, sec E. 2002, 58

Mo-O	4.382	0.000384	
	4.339	0.00044	
	4.491	0.000272	
	4.572	0.000211	
	4.384	0.000382	
	4.301	0.000496	
	3.428	0.0078	
	2.057	0.590358	
	4.438	0.000322	
	3.35	0.009976	
	2.041	0.620933	
	5.373	1.68E-05	
	3.457	0.007117	
	4.38	0.000387	
	3.665	0.003692	
	2.068	0.570216	
	2.087	0.53703	
	3.744	0.002877	
	2.144	0.448618	
	4.755	0.000118	
	4.527	0.000243	2.80189

Livage, Carine; Hynaux, Amélie; Marrot, Jérôme; Nogues, Marc; Férey, Gérard

Solution process for the synthesis of the "high-pressure" phase CoMoO4 and X-ray single crystal resolution

COD: 7205001

Journal of Materials Chemistry, 2002, 12, 1423

CoMoO4

5.309	2.06E-05
4.252	0.000579
5.558	9.39E-06
4.252	0.000579
3.251	0.013635
4.222	0.000637
4.621	0.000181
5.5	1.13E-05
3.705	0.003254
4.222	0.000637
3.251	0.013635
1.775	1.437524
1.775	1.437524
3.555	0.005224
1.895	0.984345
5.309	2.06E-05
3.996	0.001299

3.705	0.003254		
4.1	0.000936		
3.996	0.001299		
4.479	0.000283		
1.895	0.984345		
3.555	0.005224		
2.154	0.434681		
2.154	0.434681		
3.82	0.002264		
4.1	0.000936		
5.037	4.86E-05		
3.82	0.002264		
4.674	0.000153	5.76948	0.05314

Christiansen, A.F.; Fjellvag, H.; Kjekshus, A.; Klewe, B.

Synthesis and characterization of molybdenum(VI) oxide sulfates and crystal structures of two polymorphs of Mo O₂ (S O₄)

COD: 7037802

Journal of the Chemical Society, Dalton Transactions, **2001**, 2001, 806-815

MoO₆S

4.632	0.000175		
4.293	0.000509		
3.989	0.001328		
3.798	0.002426		
4.324	0.000461		
4.655	0.000162		
4.947	6.46E-05		
2.212	0.361975		
4.202	0.000678		
4.126	0.000862		
1.679	1.946208		
4.065	0.001045		
4.678	0.000151		
4.125	0.000865		
2.24	0.331362		
2.019	0.665575		
1.675	1.970931		
4.565	0.000216		
4.732	0.000127		
4.361	0.000411		
4.678	0.000151		
3.682	0.003499		
4.252	0.000579		
4.949	6.42E-05	5.289823	0.504351

Fortes, A. Dominic

Crystal structures of spinel-type Na₂MoO₄ and Na₂WO₄ revisited using neutron powder diffraction

COD: 2240655

Acta Crystallographica Section E, 2015, 71, 592-596

MoNa2O4

3.747	0.00285		
3.747	0.00285		
5.098	4.01E-05		
5.098	4.01E-05		
3.747	0.00285		
5.098	4.01E-05		
1.772	1.451198		
3.747	0.00285		
3.747	0.00285		
1.772	1.451198		
3.747	0.00285		
3.747	0.00285		
3.747	0.00285		
1.772	1.451198		
1.772	1.451198		
3.747	0.00285		
5.098	4.01E-05		
3.747	0.00285		
3.747	0.00285		
3.747	0.00285	5.839154	0.025872

Nogueira, I. C.; Cavalcante, L. S.; Pereira, P. F. S.; de Jesus, M. M.

Rietveld refinement, morphology and optical properties of (Ba_{1-x}Sr_x)MoO₄ crystals

COD: 2300459

Journal of Applied Crystallography, 2013, 46, 1434-1446

4.483	0.000279		
4.295	0.000506		
4.483	0.000279		
3.361	0.009636		
3.361	0.009636		
1.721	1.704612		
1.721	1.704612		
4.462	0.000298		
1.721	1.704612		
1.721	1.704612		
3.361	0.009636		
3.361	0.009636		
4.295	0.000506		
4.463	0.000298		
4.483	0.000279		
4.483	0.000279	6.859716	0.739112

Mtioui-Sghaier, Olfa; Mendoza-Meroño, Rafael; Ktari, Lilia;

Redetermination of the crystal structure of β -zinc molybdate from single-crystal X-ray diffraction data

COD: 2240887

Acta Crystallographica Section E, 2015, 71, i6-i7

MoO₄Zn

4.282	0.000527		
4.003	0.001271		
4.219	0.000643		
3.256	0.013422		
4.157	0.000782		
1.769	1.465003		
4.282	0.000527		
4.461	0.000299		
5.063	4.48E-05		
3.553	0.005257		
1.894	0.987456		
3.256	0.013422		
4.219	0.000643		
2.171	0.411975		
4.461	0.000299		
1.769	1.465003		
3.853	0.00204		
1.894	0.987456		
3.553	0.005257		
4.864	8.39E-05		
3.746	0.002859		
2.171	0.411975		
3.746	0.002859		
3.853	0.00204		
4.695	0.000143		
5.031	4.96E-05		
4.003	0.001271		
4.157	0.000782	5.783386	0.046922

Nogueira, I. C.; Cavalcante, L. S.; Pereira, P. F. S.; de Jesus, M. M.; Rivas Mercury,

Rietveld refinement, morphology and optical properties of (Ba_{1-x})Sr_xMoO₄ crystals

COD: 2300460

Journal of Applied Crystallography, 2013, 46, 1434-1446

MoO₄Sr

4.923	6.97E-05		
5.034	4.91E-05		
3.112	0.021143		
4.32	0.000467		
4.279	0.000532		
1.735	1.630939		
4.201	0.00068		
3.112	0.021143		

1.735	1.630939		
4.279	0.000532		
4.279	0.000532		
1.735	1.630939		
1.735	1.630939		
4.32	0.000467		
5.034	4.91E-05		
4.279	0.000532		
3.112	0.021143		
4.201	0.00068		
5.034	4.91E-05	6.591822	0.350254

Gemmi, Mauro; La Placa, Maria G. I.; Galanis, Athanassios S.;

Fast electron diffraction tomography

COD: 2300504
MgMoO4

Journal of Applied Crystallography, 2015, 48

4.707	0.000138		
3.528	0.005689		
4.221	0.000639		
4.874	8.13E-05		
1.715	1.737196		
3.788	0.002504		
3.528	0.005689		
4.362	0.000409		
4.633	0.000174		
4.874	8.13E-05		
3.941	0.001545		
4.211	0.000659		
1.715	1.737196		
1.835	1.189546		
4.362	0.000409		
1.855	1.116786		
4.211	0.000659		
4.221	0.000639		
4.463	0.000298		
4.297	0.000502		
4.707	0.000138		
3.389	0.008821		
3.941	0.001545		
4.463	0.000298	5.81164	0.035479

Bernuy-Lopez, Carlos; Allix, Mathieu; Bridges, Craig A.; Claridge, John B.; Rosseinsky, Matthew J.

Sr₂MgMoO_{6-δ}: Structure, Phase Stability, and Cation Site Order Control of Reduction

Chemistry of Materials, 2007, 19, 1035

COD: 4001303

MoO4Sr	4.296	0.000504		
	4.182	0.000722		
	4.936	6.69E-05		
	4.296	0.000504		
	3.099	0.022029		
	4.293	0.000509		
	4.936	6.69E-05		
	4.293	0.000509		
	1.772	1.451198		
	3.099	0.022029		
	2.954	0.034811		
	1.772	1.451198		
	4.99	5.64E-05		
	4.293	0.000509		
	1.772	1.451198		
	4.182	0.000722		
	1.772	1.451198		
	4.182	0.000722		
	3.099	0.022029	5.91058	0.007996

Barinova, A.V.; Rastsvetaeva, R.K.; Nekrasov, Yu.V.; Pushcharovskii, D.Yu.

Crystal structure of Li₂ Mo O₄

COD: 1525609

Doklady Akad. Nauk, 2001, 376, 343-346

Li₂MoO₄

3.904	0.001737		
4.526	0.000244		
3.872	0.001921		
4.791	0.000106		
4.026	0.001182		
1.734	1.636094		
4.546	0.000229		
3.437	0.007581		
1.754	1.53602		
1.827	1.21996		
4.616	0.000184		
4.25	0.000583		
1.712	1.753721		
4.609	0.000188		
3.594	0.004619	6.164367	0.027016

Seisenbaeva, G.A.; Sundberg, M.; Nygren, M.; Dubrovinsky, L.; Kessler, V.G.

COD: 1533435

Thermal decomposition of the methoxide complexes Mo O (O Me)₄, Re₄ O₆ (O Me)₁₂ and (Re_{1-x} Mo_x)

O6 (O Me)12 (0.24 < x < 0.55)

MoO2

Materials Chemistry and Physics, 2004, 87, 142-148

1.956	0.811975		
1.956	0.811975		
1.956	0.811975		
1.956	0.811975		
2.069	0.568419		
2.069	0.568419		
3.492	0.006373		
3.492	0.006373		
3.492	0.006373		
3.492	0.006373		
3.687	0.003444		
4.244	0.000594		
4.244	0.000594		
4.244	0.000594		
4.244	0.000594		
4.244	0.000594		
4.434	0.000326		
4.434	0.000326		
4.434	0.000326		
4.434	0.000326		
4.638	0.000171		
4.638	0.000171		
4.638	0.000171		
4.638	0.000171		
4.786	0.000107	4.418742	0.175345

MoO4Zn

Mtioui 2015

1.769	1.465003
1.894	0.987456
1.894	0.987456
2.171	0.411975
2.171	0.411975
3.256	0.013422
3.256	0.013422
3.553	0.005257
3.553	0.005257
3.746	0.002859
3.746	0.002859

3.853	0.00204	
4.003	0.001271	
4.003	0.001271	
4.157	0.000782	
4.157	0.000782	
4.219	0.000643	
4.282	0.000527	
4.282	0.000527	
4.432	0.000328	
4.461	0.000299	
4.624	0.000179	
4.624	0.000179	
4.695	0.000143	4.31591
4.695	0.000143	
3.853	0.00204	