

Bond valence calculation for CdTeMoO₆

	bond distances	bond valence
Cd—O1	2.221	0.42
Cd—O1 ⁱ	2.221	0.42
Cd—O1 ⁱⁱ	2.221	0.42
Cd—O1 ⁱⁱⁱ	2.221	0.42
Cd		1.70

Mo—O2	1.709	1.71
Mo—O2 ^{viii}	1.709	1.71
Mo—O3	1.869	1.11
Mo—O3 ^{viii}	1.869	1.11
Mo		5.63

Te—O1 ⁱ	1.877	1.31
Te—O1 ^{iv}	1.877	1.31
Te—O3	2.148	0.63
Te—O3 ^v	2.148	0.63
Te		3.88

Symmetry code: (i) 1-x, 1-y, z; (ii) 1-y, x, 1-z; (iii) y, 1-x, 1-z; (iv) 1+x, y, z;
(v) 2-x, 1-y, z; (vi) -1+x, y, z; (vii) -0.5+x, 0.5-y, 1-z; (viii) 1-x, -y, z.

TeO ₄ in CdTeMoO ₆			Cart. Coord.			distance	unit vector			dipole moment for each			
Z	atom	charges	x	y	z	Å	x	y	z	unitized Vec	C_grav	C_charge	u_debye
52	Te	3.88	5.286	2.643	2.19787								
8	O1 ⁱ	-1.31	4.27637	3.652626	3.41698	1.877	-0.53789	0.53789	0.6495	1	0.13333	0.16212	14.9
8	O1 ^{iv}	-1.31	6.29563	1.633374	3.41698	1.877	0.53789	-0.53789	0.6495	1	0.13333	0.16212	14.9
8	O3	-0.63	3.79482	1.1518194	2.60376	2.148	-0.69422	-0.69422	0.18896	1	0.13333	0.15207	11.0
8	O3 ^v	-0.63	6.77718	4.1341806	2.60376	2.148	0.69422	0.69422	0.18896	1	0.13333	0.15207	11.0
2	Lp	-2	0	0	-1.25	1.25	0	0	-1	1	0.03704	0.07675	12.4
			Cell Volume			252.95				Dipole Moment			Magnitude
			Z			2				x	y	z	
			Total Dipole Moment =			0.0875	esu*cm/Å ³	0	0	11.07	11.07	esu*cm	

MoO ₄ in CdTeMoO ₆			Cart. Coord.			distance	unit vector				dipole moment for each			
Z	atom	charges	x	y	z	Å	x	y	z	unitized Vec	C_grav	C_charge	u_debye	
42	Mo	5.63	2.643	0	1.68619									
8	O2	-1.71	1.68993	0.95307	0.63553	1.709	-0.55767	0.55767	-0.61478	0.99995605	0.16	0.21069	19.2	
8	O2 ^{viii}	-1.71	3.59607	-0.95307	0.63553	1.709	0.55767	-0.55767	-0.61478	0.99995605	0.16	0.21069	19.2	
8	O3	-1.11	3.79482	1.15182	2.60376	1.869	0.61628	0.61628	0.49094	1.00061529	0.16	0.20028	16.4	
8	O3 ^{viii}	-1.11	1.49118	-1.15182	2.60376	1.869	-0.61628	-0.61628	0.49094	1.00061529	0.16	0.20028	16.4	
						Cell Volume	252.95					Dipole Moment		Magnitude
						Z	2	x	y	z				
						Total Dipole Moment =	0.0587	esu*cm/Å ³	0	0	-7.42	7.42	debye	

CdO ₄ in CdTeMoO ₆			Cart. Coord.			distance	unit vector				dipole moment for each			
Z	atom	charges	x	y	z	Å	x	y	z	unitized Vec	C_grav	C_charge	u_debye	
48	Cd	1.70	2.643	2.643	4.533									
8	O1	-0.42	1.00963	1.63337	3.41698	2.221	-0.73543	-0.45459	-0.50249	1	0.14286	0.15394	6.5	
8	O1 ⁱ	-0.42	4.27637	3.65263	3.41698	2.221	0.73543	0.45459	-0.50249	1	0.14286	0.15394	6.5	
8	O1 ⁱⁱ	-0.42	3.65263	1.00963	5.64902	2.221	0.45459	-0.73543	0.50249	1	0.14286	0.15394	6.5	
8	O1 ⁱⁱⁱ	-0.42	1.63337	4.27637	5.64902	2.221	-0.45459	0.73543	0.50249	1	0.14286	0.15394	6.5	
						Cell Volume	252.95				Dipole Moment			Magnitude
						Z	2				x	y	z	
						Total Dipole Moment =	0	esu*cm/A ³	0	0	0	0	debye	