

Bond Valence Ro parameters and M-O bond distances (bond valence and ionic), crystal and ionic radii

Bond Valence Parameter Radii									Crystal and Ionic Radii								
Element	Ox.	Anion	Ox.	Ro	M-O (VI)	M-O (IX)	M-O (XII)	r (VI)	Ox.	CN	cr	ir	M-O (VI)	CN	cr	ir	M-O (XII)
Ag	1	O	-2	1.842	2.505	2.655	2.761	1.295	1	6	1.29	1.15	2.50				
Au	1	O							1	6	1.51	1.37	2.72				
Cs	1	O	-2	2.417	3.080	3.230	3.336	1.870	1	6	1.81	1.67	3.02	12	2.02	1.88	3.23
Cu	1	O	-2	1.61	2.273	2.423	2.529	1.063	1	6	0.91	0.77	2.12				
Fr	1	O							1	6	1.94	1.80	3.15				
Hg	1	O	-2	1.9	2.563	2.713	2.819	1.353	1	6	1.33	1.19	2.54				
K	1	O	-2	2.132	2.795	2.945	3.051	1.585	1	6	1.52	1.38	2.73	12	1.78	1.64	2.99
Li	1	O	-2	1.466	2.129	2.279	2.385	0.919	1	6	0.90	0.76	2.11				
Na	1	O	-2	1.803	2.466	2.616	2.722	1.256	1	6	1.16	1.02	2.37	12	1.53	1.39	2.74
Rb	1	O	-2	2.263	2.926	3.076	3.182	1.716	1	6	1.66	1.52	2.87	12	1.86	1.72	3.07
Tl	1	O	-2	2.124	2.787	2.937	3.043	1.577	1	6	1.64	1.50	2.85	12	1.84	1.70	3.05
V	1	O	-2	1.88	2.543	2.693	2.799	1.333									
Ag	2	O							2	6	1.08	0.94	2.29				
Ba	2	O	-2	2.285	2.691	2.842	2.948	1.481	2	6	1.49	1.35	2.70	12	1.75	1.61	2.96
Be	2	O	-2	1.381	1.787	1.938	2.044	0.577	2	6	0.59	0.45	1.80				
C	2	O	-2	1.366	1.772	1.923	2.029	0.562									
Ca	2	O	-2	1.967	2.373	2.524	2.630	1.163	2	6	1.14	1.00	2.35	12	1.48	1.34	2.69
Cd	2	O	-2	1.904	2.310	2.461	2.567	1.100	2	6	1.09	0.95	2.30	12	1.45	1.31	2.66
Co	2	O	-2	1.692	2.098	2.249	2.355	0.888	2	6	0.89	0.75	2.10				
Cr	2	O	-2	1.73	2.136	2.287	2.393	0.926	2	6	0.94	0.80	2.15				
Cu	2	O	-2	1.679	2.085	2.236	2.342	0.875	2	6	0.87	0.73	2.08				
Dy	2	O	-2	1.9	2.306	2.457	2.563	1.096	2	6	1.21	1.07	2.42				
Er	2	O	-2	1.88	2.286	2.437	2.543	1.076									
Eu	2	O	-2	2.13	2.536	2.687	2.793	1.326	2	6	1.31	1.17	2.52				
Fe	2	O	-2	1.734	2.140	2.291	2.397	0.930	2	6	0.92	0.78	2.13				
Gd	2	O	-2	2.01	2.416	2.567	2.673	1.206									
Ge	2	O							2	6	0.87	0.73	2.08				
Hg	2	O	-2	1.972	2.378	2.529	2.635	1.168	2	6	1.16	1.02	2.37				
Mg	2	O	-2	1.693	2.099	2.250	2.356	0.889	2	6	0.86	0.72	2.07				
Mn	2	O	-2	1.79	2.196	2.347	2.453	0.986	2	6	0.97	0.83	2.18				
Nd	2	O	-2	1.95	2.356	2.507	2.613	1.146									
Ni	2	O	-2	1.654	2.060	2.211	2.317	0.850	2	6	0.83	0.69	2.04				
No	2	O							2	6	1.24	1.10	2.45				
Np	2	O							2	6	1.15	1.01	2.36				
Pb	2	O	-2	2.112	2.518	2.669	2.775	1.308	2	6	1.33	1.19	2.54	12	1.63	1.49	2.84
Pd	2	O	-2	1.792	2.198	2.349	2.455	0.988	2	6	1.00	0.86	2.21				
Pt	2	O	-2	1.768	2.174	2.325	2.431	0.964	2	6	0.94	0.80	2.15				
Ra	2	O												12	1.84	1.70	3.05
S	2	O	-2	1.74	2.146	2.297	2.403	0.936	2	6	1.70	1.56	2.91				
Sn	2	O	-2	1.94	2.346	2.497	2.603	1.136									
Sr	2	O	-2	2.118	2.524	2.675	2.781	1.314	2	6	1.32	1.18	2.53	12	1.58	1.44	2.79
Ti	2	O							2	6	1.00	0.86	2.21				
Tm	2	O							2	6	1.17	1.03	2.38				
V	2	O	-2	1.70	2.106	2.257	2.363	0.896	2	6	0.93	0.79	2.14				
Zn	2	O	-2	1.704	2.110	2.261	2.367	0.900	2	6	0.88	0.74	2.09				
Zr	2	O	-2	2.34	2.746	2.897	3.003	1.536									

Metal-Oxygen Bond Valence Parameters and Distances Sorted by Oxidation State

M-O = Ro - b*LN(Oxidation State B/CN(B-site)) with b = 0.37 in majority of examples

Ro values obtained from Accumulated Table of Bond Valence Parameters Version 2.2

http://www.ccp14.ac.uk/ccp/web-mirrors/i_d_brown/

High Spin unless otherwise noted.

Crystal Radius of Oxygen = 1.21 Å, Ionic Radius of Oxygen = 1.35 Å (2-coordinate)

R.D.Shannon, Acta Cryst. (1976) A32, 751

For comments and questions on this file, please contact

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Bond Valence Ro parameters and M-O bond distances (bond valence and ionic), crystal and ionic radii

Bond Valence Parameter Radii								Crystal and Ionic Radii								
Element	Ox.	Anion	Ox.	Ro	M-O (VI)	M-O (XII)	r (VI)	Ox.	CN	cr	ir	M-O (VI)	CN	cr	ir	M-O (XII)
Ac	3	O	-2	2.24	2.496	2.753	1.286	3	6	1.26	1.12	2.47				
Ag								3	6	0.89	0.75	2.10				
Al	3	O	-2	1.62	1.876	2.133	0.666	3	6	0.68	0.54	1.89				
Am	3	O	-2	2.11	2.366	2.623	1.156									
As	3	O	-2	1.789	2.045	2.302	0.835	3	6	0.72	0.58	1.93				
Au	3	O	-2	1.89	2.146	2.403	0.936	3	6	0.99	0.85	2.20				
B	3	O	-2	1.371	1.627	1.884	0.417	3	6	0.41	0.27	1.62				
Bi	3	O	-2	2.094	2.350	2.607	1.140	3	6	1.17	1.03	2.38				
Bk	3	O	-2	2.08	2.336	2.593	1.126									
Ce	3	O	-2	2.151	2.407	2.664	1.197	3	6	1.15	1.01	2.36	12	1.48	1.34	2.69
Cf	3	O	-2	2.07	2.326	2.583	1.116									
Cl	3	O	-2	1.71	1.966	2.223	0.756									
Cm	3	O	-2	2.23	2.486	2.743	1.276	3	6	1.11	0.97	2.32				
Co	3	O	-2	1.637	1.893	2.150	0.683	3	6	0.75	0.61	1.96				
Cr	3	O	-2	1.724	1.980	2.237	0.770	3	6	0.76	0.62	1.97				
Cu	3	O	-2	1.753	2.009	2.266	0.799	3	6	0.68	0.54	1.89				
Dy	3	O	-2	2.001	2.257	2.514	1.047	3	6	1.05	0.91	2.26				
Er	3	O	-2	1.988	2.244	2.501	1.034	3	6	1.03	0.89	2.24				
Es	3	O	-2	2.08	2.323	2.565	1.113									
Eu	3	O	-2	2.074	2.330	2.587	1.120	3	6	1.09	0.95	2.30				
Fe	3	O	-2	1.759	2.015	2.272	0.805	3	6	0.79	0.65	2.00				
Ga	3	O	-2	1.73	1.986	2.243	0.776	3	6	0.76	0.62	1.97				
Gd	3	O	-2	2.065	2.321	2.578	1.111	3	6	1.08	0.94	2.29				
Ho	3	O	-2	2.025	2.281	2.538	1.071	3	6	1.04	0.90	2.25				
In	3	O	-2	1.902	2.158	2.415	0.948	3	6	0.94	0.80	2.15				
Ir								3	6	0.82	0.68	2.03				
La	3	O	-2	2.172	2.428	2.685	1.218	3	6	1.17	1.03	2.38	12	1.50	1.36	2.71
Lu	3	O	-2	1.971	2.227	2.484	1.017	3	6	1.00	0.86	2.21				
Mn	3	O	-2	1.76	2.016	2.273	0.806	3	6	0.79	0.65	1.995				
Mo	3	O	-2	2.2	2.443	2.685	1.233	3	6	0.83	0.69	2.04				
Nb	3	O	-2	1.91	2.153	2.395	0.943	3	6	0.86	0.72	2.07				
Nd	3	O	-2	2.105	2.361	2.618	1.151	3	6	1.12	0.98	2.33	12	1.41	1.27	2.62
Ni	3	O	-2	1.74	1.996	2.253	0.786	3	6	0.70	0.56	1.91				
P	3	O	-2	1.63	1.886	2.143	0.676	3	6	0.58	0.44	1.79				
Pd								3	6	0.90	0.76	2.11				
Pr	3	O	-2	2.138	2.394	2.651	1.184	3	6	1.13	0.99	2.34				
Pt	3	O	-2	1.87	2.126	2.383	0.916									
Pu	3	O	-2	2.11	2.366	2.623	1.156	3	6	1.14	1.00	2.35				
Re	3	O	-2	1.9	2.143	2.385	0.933									
Rh	3	O	-2	1.793	2.049	2.306	0.839	3	6	0.81	0.67	2.02				
Ru	3	O	-2	1.77	2.026	2.283	0.816	3	6	0.82	0.68	2.03				
Sb	3	O	-2	1.973	2.229	2.486	1.019	3	6	0.90	0.76	2.11				
Sc	3	O	-2	1.849	2.105	2.362	0.895	3	6	0.89	0.75	2.10				
Sm	3	O	-2	2.088	2.344	2.601	1.134	3	6	1.10	0.96	2.31				
Ta								3	6	0.86	0.72	2.07				
Tb	3	O	-2	2.032	2.288	2.545	1.078	3	6	1.06	0.92	2.27				
Ti	3	O	-2	1.791	2.047	2.304	0.837	3	6	0.81	0.67	2.02				
Tl	3	O	-2	2.003	2.259	2.516	1.049	3	6	1.03	0.89	2.24				
Tm	3	O	-2	2.000	2.256	2.513	1.046	3	6	1.02	0.88	2.23				
U								3	6	1.17	1.03	2.38				
V	3	O	-2	1.743	1.999	2.256	0.789	3	6	0.78	0.64	1.99				
Y	3	O	-2	2.019	2.275	2.532	1.065	3	6	1.04	0.90	2.25				
Yb	3	O	-2	1.965	2.221	2.478	1.011	3	6	1.01	0.87	2.22				

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Bond Valence Parameter Radii								Crystal Radii								
Element	Ox.	Anion	Ox.	Ro	M-O (VI)	M-O (XII)	r (VI)	Ox.	CN	cr	ir	M-O (VI)	CN	cr	ir	M-O (XII)
Am	4	O	-2	2.08	2.230	2.486	1.020	4	6							
Am	4	O	-2	2.12	2.270	2.526	1.060									
Bk	4	O	-2	2.07	2.212	2.455	1.002	4	6							
C	4	O	-2	1.39	1.540	1.796	0.330	4	6	0.3	0.16	1.51				
Ce	4	O	-2	2.028	2.178	2.434	0.968	4	6	1.01	0.87	2.22	12	1.28	1.14	2.49
Cf	4	O	-2	2.06	2.202	2.445	0.992	4	6	0.961	0.82	2.17				
Cm	4	O	-2	2.08	2.222	2.465	1.012	4	6	0.99	0.85	2.20				
Co	4	O	-2	1.72	1.870	2.126	0.660	4	6	0.67	0.53	1.88				
Cr	4	O	-2	1.81	1.960	2.216	0.750	4	6	0.69	0.55	1.90				
Fe	4	O						4	6	0.725	0.59	1.94				
Ge	4	O	-2	1.748	1.898	2.154	0.688	4	6	0.67	0.53	1.88				
Hf	4	O	-2	1.923	2.073	2.329	0.863	4	6	0.85	0.71	2.06				
Ir	4	O	-2	1.87	2.020	2.276	0.810	4	6	0.765	0.63	1.98				
Mn	4	O	-2	1.753	1.903	2.159	0.693	4	6	0.67	0.53	1.88				
Mo	4	O	-2	2.24	2.390	2.646	1.180	4	6	0.79	0.65	2.00				
Nb	4	O	-2	1.88	2.030	2.286	0.820	4	6	0.82	0.68	2.03				
Ni (L.S.)	4	O	-2	1.78	1.922	2.186	0.712	4	6	0.62	0.48	1.83				
Np	4	O	-2	2.18	2.330	2.586	1.120	4	6	1.01	0.87	2.22				
Os	4	O	-2	1.811	1.961	2.217	0.751	4	6	0.77	0.63	1.98				
P	4	O	-2	1.64	1.790	2.046	0.580									
Pa	4	O	-2	2.15	2.292	2.535	1.082	4	6	1.04	0.90	2.25				
Pb	4	O	-2	2.042	2.192	2.448	0.982	4	6	0.915	0.78	2.13				
Pd	4	O						4	6	0.755	0.62	1.97				
Po	4	O	-2	2.19	2.340	2.596	1.130	4	6	1.08	0.94	2.29				
Pr	4	O						4	6	0.99	0.85	2.20				
Pt	4	O	-2	1.879	2.029	2.285	0.819	4	6	0.765	0.63	1.98				
Pu	4	O	-2	2.09	2.232	2.475	1.022	4	6							
Pu	4	O						4	6	1.00	0.86	2.21				
Re	4	O						4	6	0.77	0.63	1.98				
Rh	4	O						4	6	0.74	0.60	1.95				
Ru	4	O	-2	1.834	1.984	2.240	0.774	4	6	0.76	0.62	1.97				
S	4	O	-2	1.644	1.794	2.050	0.584									
Se	4	O	-2	1.811	1.961	2.217	0.751	4	6	0.64	0.50	1.85				
Si	4	O	-2	1.624	1.774	2.030	0.564	4	6	0.54	0.40	1.75				
Sn	4	O	-2	1.905	2.055	2.311	0.845	4	6	0.83	0.69	2.04				
Ta	4	O	-2	2.29	2.440	2.696	1.230	4	6	0.82	0.68	2.03				
Tb	4	O						4	6	0.9	0.76	2.11				
Tc	4	O						4	6	0.785	0.65	2.00				
Te	4	O	-2	1.977	2.127	2.383	0.917	4	6	1.11	0.97	2.32				
Th	4	O	-2	2.167	2.317	2.573	1.107	4	6	1.08	0.94	2.29	12	1.35	1.21	2.56
Ti	4	O	-2	1.815	1.965	2.221	0.755	4	6	0.745	0.61	1.96				
U	4	O	-2	2.112	2.262	2.518	1.052	4	6	1.03	0.89	2.24	12	1.31	1.17	2.52
V	4	O	-2	1.784	1.934	2.190	0.724	4	6	0.72	0.58	1.93				
W	4	O						4	6	0.8	0.66	2.01				
Zr	4	O	-2	1.928	2.078	2.334	0.868	4	6	0.86	0.72	2.07				

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Bond Valence Parameter Radii								Crystal and Ionic Radii				
Element	Ox.	Anion	Ox.	Ro	M-O (VI)	M-O (XII)	r (VI)	Ox.	C.N.	cr	ir	M-O (VI)
Am	5	O	-2	2.07	2.134	2.376	0.924					
As	5	O	-2	1.767	1.834	2.091	0.624	5	6	0.6	0.46	1.81
Au								5	6	0.71	0.57	1.92
Bi	5	O	-2	2.06	2.127	2.384	0.917	5	6	0.9	0.76	2.11
Br	5	O	-2	1.84	1.907	2.164	0.697					
Cl	5	O	-2	1.67	1.737	1.994	0.527					
Cr	5	O	-2	1.78	1.847	2.104	0.637	5	6	0.63	0.49	1.84
I	5	O	-2	2.003	2.070	2.327	0.860					
Ir	5	O	-2	1.916	1.983	2.240	0.773	5	6	0.71	0.57	1.92
Mo	5	O	-2	1.85	1.917	2.174	0.707	5	6	0.75	0.61	1.96
N	5	O	-2	1.432	1.499	1.756	0.289	5	6	0.27	0.13	1.48
Nb	5	O	-2	1.911	1.978	2.235	0.768	5	6	0.78	0.64	1.99
Np	5	O	-2	2.09	2.154	2.396	0.944	5	6	0.89	0.75	2.10
Os								5	6	0.715	0.58	1.93
P	5	O	-2	1.617	1.684	1.941	0.474	5	6	0.52	0.38	1.73
Pa	5	O	-2	2.09	2.154	2.396	0.944	5	6	0.92	0.78	2.13
Pt								5	6	0.71	0.57	1.92
Pu	5	O	-2	2.11	2.177	2.434	0.967	5	6	0.88	0.74	2.09
Re	5	O	-2	1.86	1.927	2.184	0.717	5	6	0.72	0.58	1.93
Rh								5	6	0.69	0.55	1.90
Ru	5	O	-2	1.9	1.967	2.224	0.757	5	6	0.705	0.57	1.92
Sb	5	O	-2	1.942	2.009	2.266	0.799	5	6	0.74	0.60	1.95
Ta	5	O	-2	1.92	1.987	2.244	0.777	5	6	0.78	0.64	1.99
Tc								5	6	0.74	0.60	1.95
U	5	O	-2	2.075	2.142	2.399	0.932	5	6	0.9	0.76	2.11
V	5	O	-2	1.803	1.870	2.127	0.660	5	6	0.68	0.54	1.89
W	5	O	-2	1.89	1.957	2.214	0.747	5	6	0.76	0.62	1.97
Am	6	O	-2	2.05	2.050	2.293	0.84					
Cr	6	O	-2	1.794	1.794	2.050	0.58	6	6	0.58	0.44	1.79
Fe	6	O	-2	1.76	1.760	2.003	0.55					
Mn	6	O	-2	1.79	1.790	2.046	0.58	7	6	0.6	0.46	1.81
Mo	6	O	-2	1.907	1.907	2.163	0.70	6	6	0.73	0.59	1.94
Np	6	O	-2	2.07	2.070	2.313	0.86	6	6	0.86	0.72	2.07
Os	6	O	-2	2.03	2.030	2.286	0.82	6	6	0.685	0.55	1.90
Po	6		-2					6	6	0.81	0.67	2.02
Pu	6	O	-2	2.06	2.060	2.303	0.85	6	6	0.85	0.71	2.06
Re	6	O	-2	1.86	1.860	2.116	0.65	6	6	0.69	0.55	1.90
Ru	6	O	-2	1.87	1.870	2.113	0.66					
Se	6	O	-2	1.788	1.788	2.044	0.58	6	6	0.56	0.42	1.77
Te	6	O	-2	1.917	1.917	2.173	0.71	6	6	0.7	0.56	1.91
U	6	O	-2	2.051	2.051	2.411	0.84	6	6	0.87	0.73	2.08
W	6	O	-2	1.917	1.917	2.173	0.71	6	6	0.74	0.60	1.95
Np	7	O	-2	2.06	2.003	2.259	0.79					
Os	7	O	-2					7	6	0.665	0.53	1.88
Pu	7	O	-2	2.05	1.993	2.249	0.78					
Re	7	O	-2	1.97	1.913	2.169	0.70	7	6	0.67	0.53	1.88
Ru	7	O	-2	1.99	1.933	2.189	0.72					
Tc	7	O	-2	1.9	1.843	2.099	0.63	7	6	0.7	0.56	1.91