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Bond Length – Bond Valence Relationships for Carbon – Carbon and Carbon – Oxygen Bonds

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Running Title: Bond Length – Bond Valence Relationships for C-C and C-O Bonds

Abstract

In the present study, relationships are developed for determining bond orders (also referred to as bond valences or bond numbers) from published bond lengths for carbon-carbon (C-C) and carbon-oxygen (C-O) bonds. The relationships are based on Pauling's empirical formula $s = exp((R_o\text{-}R)/b))$, where s is the bond order, R is the corresponding bond length, R_o is the unit valence bond length, and b is a fitting parameter. We use a recently derived relationship for the b parameter in terms of the bonding atoms' published atomic orbital exponents. The resulting equations were checked against published x-ray diffraction (XRD) data for 176 carbon systems with 540 published C-C bond lengths, and 50 oxygen systems having 72 published C-O bond lengths. The C-C and C-O bond length-valence relationships are shown to have sufficient applicability and accuracy for use in any bonding environment, regardless of physical state or oxidation number.

Introduction

In 1929, Linus Pauling published his five rules of chemical bonding which could be used for predicting crystal structures (Pauling 1929). Pauling's second rule is that of local charge neutrality, commonly known as the valence sum rule, which states that the charge of an anion is neutralized by the sum of the adjacent cationic charges, while any cationic charge is neutralized by adjacent anionic charges. In terms of bond valence, the total valence at any one atom is equal to the sum of that atom's individual bond valences. In 1947, Pauling published the following empirical bond length-valence relationship:

$$s = \exp\left(\frac{R_o - R}{b}\right) \tag{1}$$

where s is the bond valence, which corresponds to the number of lone pairs of electrons contributing to the bond, R_o is the length of a chemical bond with unit valence, R is an observed bond length, and b is an empirical fitting parameter (Pauling 1947). A wide range of determined values for the b parameter, anywhere from 0.25 to 0.65 Å (Hardcastle 2013), led to many inconsistencies in valence values, an issue that hindered the ability of chemists to compare findings. As a result, it was proposed that a universal value of 0.37 Å for b be established as the average from the crystallographic data (Brown and Altermatt 1985). This resulted in consistent relationships having only one fitting parameter, R_o; however, when applied to shorter and longer bonds, the calculated valence was shown to be less reliable owing to the inaccuracy of b.

Theory

In 2013, Hardcastle derived Pauling's bond length-valence, including a new definition for the b fitting parameter (Hardcastle 2013). Since then, a slight modification has been made (Hardcastle *unpublished data*), resulting in the following equation:

$$b = \frac{2a_o}{(\xi_1 + \xi_2)} \tag{2}$$

where b is dependent upon the Bohr radius of a hydrogen atom, a_o (0.529 Å), and the sum of the orbital exponent values for each of the atoms contributing to the bond. This definition results in values for b that are specific to the type of chemical bond, a much more accurate alternative to the average universal value of 0.37 Å assumed for any type of bond. Using published values for atomic orbital exponents to determine the value of the b parameter for any bond, and substituting this value into Equation (1), results in a bond length-valence relationship specific to that bond type.

Uncertainty in R_o

With a definition for the *b* parameter, R_o is left as the only fitting parameter in Equation (1). The precise length of a C-O bond having a bond order of exactly one (a true C-O single bond) is a matter of debate, but has been estimated between 1.33 and 1.43 Å by Allen (Allen et al 1987) and at 1.39 Å by Brese and O'Keeffe, which they refer to as the "bond-valence parameter" because they were using b = 0.37 Å as a universal constant (Brese and O'Keeffe 1991). For the C-C bond length of unit valence, however, most investigators agree on the published C-C length found for crystalline diamond at R_o = 1.542 Å (Brown 2002) as representing the C-C bond length of unit valence.

Results and Discussion

The atomic orbital exponents for carbon and oxygen are from data published by Clementi and Raimondi (1963), with values of 1.5679 and 2.2266 respectively. Substituting these values into Equation (2), results in *b* parameters of 0.337 Å for C-C bonds and 0.279 Å for C-O bonds. Note that both of these values are much lower than the previously assumed universal constant of 0.37 Å. This leaves R_o, the bond length of unit valence, as the only remaining fitting parameter. In the case of C-C bonds, our initial guess would be the C-C bond length in diamond at R_o = 1.542 Å. But for C-O bonds, this value could be anywhere from 1.33 (Allen et al 1987) to 1.43 Å (Schomaker and Stevenson 1941).

The total atom valence for a carbon-centered environment was predicted to be 4.00, carbon having four electrons available for bonding, while the atom valence for an oxygen-centered environment was predicted to be 2.00. These predictions were based upon the number of bonding electrons available (oxidation state) in each atom, 4 for carbon and 2 for oxygen. Comparing the calculated atomic valences to the predicted valences, the total error for the C-O bonding was minimized by manipulating R_o. Clementi's orbital exponents were not changed to minimize error, but were held constant.

X-ray diffraction data, limited to results published in the year 2000 or later, was collected for C-C and C-O bond lengths, totaling 612 bonds (176 carbon environments and 50 oxygen environments). Each environment is represented by an individual table within Table 1. Bond lengths were recorded and converted to bond valence values, which were then totaled for the atom valence. Data analysis and error minimization led to two specific relationships, one for C-C bonds:

$$s = \exp\left(\frac{1.5420-\mathrm{R}}{0.337}\right) \tag{3}$$

and one for C-O bonds:

$$s = \exp\left(\frac{1.3669-\mathrm{R}}{0.279}\right) \tag{4}$$

Each equation was shown to produce accurate valence values from published bond length data. The error in the data (XRD data and valence sum rule) was minimized at R_o = 1.5420 Å for C-C bonds, consistent with the C-C bond length of diamond, and R_o = 1.3669 Å for C-O bonds, consistent with the estimated 1.33-1.44 Å range for a C-O bond of unit valence.

Conclusion

Bond length – bond valence relationships, based on Pauling's formula, provide useful tools for the prediction and evaluation of crystal structures when used with the valence sum rule. In the present study, atomic orbital exponents were used to independently determine the value of the *b* parameter (previously either a floating fitting parameter, or set as a universal constant at 0.37 Å) for C-C and C-O bonds at 0.337 and 0.279 Å, respectively. This approach resulted in bond length – valence relationships for C-C and C-O bonds by using published crystallographically determined bond lengths for 612 bonds and the valence sum rule. The optimized bond lengths of unit valence are minimized at R_o = 1.5420 Å for C-C bonds, consistent with the C-C bond length of diamond, and R_o = 1.3669 Å for C-O bonds, consistent with the estimated 1.33-1.44 Å range for a C-O bond of unit valence.

Acknowledgments

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Table 1. Bond valence calculations from published XRD data.

Carbon Environments		
Alonso et al. 2009		
	C11	Valence
C10	1.474	1.223
O2	1.210	1.755
O3	1.304	1.253
		4.232
	C11	Valence
C10	1.475	1.220
O2	1.213	1.737
O3	1.349	1.066
		4.023
	C11	Valence
C10	1.460	1.275
O2	1.225	1.663
O3	1.331	1.137
		4.076
	C11	Valence
C10	1.468	1.245
O1	1.230	1.634
O2	1.318	1.192
		4.071
	C8	Valence
C7	1.483	1.191
C9	1.514	1.087
C10	1.336	1.841
		4.119
	C8	Valence
C7	1.465	1.256
C9	1.521	1.064
C10	1.347	1.782
		4.103
	C8	Valence
C7	1.476	1.216
C9	1.511	1.096
C10	1.339	1.825
		4.137
	C8	Valence
C7	1.481	1.198
C9	1.468	1.245
C10	1.352	1.756
		4.200
Andreu et al. 2009		
	C4	Valence
C3	1.442	1.345
O2	1.380	0.954
O3	1.215	1.724
		4.023
	C21	Valence
C16	1.504	1.119
C22	1.537	1.015
C23	1.536	1.018
C24	1.527	1.045
		4.198
	C17	Valence
C14	1.508	1.106
C18	1.516	1.080
C19	1.535	1.021
C20	1.530	1.036
		4.243
	C14	Valence
C13	1.338	1.831
C17	1.508	1.106
O1	1.360	1.025
		3.962
	C16	Valence
C15	1.341	1.814
C21	1.504	1.119
O1	1.361	1.021
		3.955
	C12	Valence
C1	1.393	1.555
C13	1.425	1.414
C15	1.427	1.406
		4.376
	C3	Valence
C2	1.381	1.612
C4	1.442	1.345
C5	1.430	1.394
		4.350
	C6	Valence
C5	1.474	1.223
C7	1.387	1.583
C11	1.383	1.602
		4.408
	C26	Valence
C25	1.502	1.126
C27	1.540	1.006
C28	1.526	1.049
C29	1.531	1.033
		4.214
	C20	Valence
C19	1.515	1.083
C21	1.490	1.167
C22	1.529	1.039
C23	1.513	1.090
		4.379
	C25	Valence
C24	1.338	1.831
C26	1.502	1.126
O1	1.365	1.007
		3.963
	C19	Valence
C18	1.338	1.831
C20	1.515	1.083
O1	1.357	1.036
		3.950
	C17	Valence
C1	1.391	1.564
C18	1.420	1.436
C24	1.424	1.419
		4.419
	C8	Valence
C7	1.498	1.139
C9	1.374	1.645
C13	1.377	1.631
		4.415
Basuli et al. 2003		
	C5	Valence
C4	1.421	1.431
C6	1.391	1.564
C13	1.518	1.074
		4.070
	C9	Valence
C4	1.429	1.398
C8	1.390	1.569
C10	1.525	1.052
		4.019
	C40	Valence
C35	1.410	1.479
C39	1.397	1.537
C41	1.517	1.077
		4.093
	C36	Valence
C35	1.413	1.466
C37	1.395	1.546
C44	1.522	1.061
		4.073
	C4	Valence
C3	1.426	1.410
C5	1.390	1.569
C9	1.518	1.074
		4.053
	C8	Valence
C3	1.416	1.453
C7	1.394	1.551
C12	1.519	1.071
		4.074
	C21	Valence
C20	1.408	1.488
C22	1.400	1.523
C26	1.520	1.067
		4.078
	C25	Valence
C20	1.406	1.496
C24	1.392	1.560
C29	1.520	1.067
		4.124
	C35	Valence
C34	1.408	1.488
C36	1.394	1.551
C40	1.517	1.077
		4.115
	C39	Valence
C34	1.408	1.488
C38	1.396	1.541
C43	1.518	1.074
		4.103
	C4	Valence
C3	1.419	1.440
C5	1.397	1.537
C9	1.517	1.077
		4.054
	C8	Valence
C3	1.422	1.427
C7	1.392	1.560
C12	1.512	1.093
		4.080
	C21	Valence
C20	1.419	1.440
C22	1.398	1.532
C29	1.520	1.067
		4.040
	C35	Valence
C34	1.417	1.448
C36	1.403	1.510
C43	1.517	1.077
		4.035
	C39	Valence
C34	1.398	1.532
C38	1.398	1.532
C40	1.520	1.067
		4.132
Borbulevych et al. 2002		
	C8	Valence
C7	1.500	1.133
C9	1.540	1.006
O5	1.432	0.792
O6	1.430	0.797
		3.728
	C4	Valence
C3	1.410	1.479
C5	1.462	1.268
C9	1.420	1.436
		4.182
Burlakov et al. 2015		
	C7	Valence
C6	1.430	1.394
C8	1.203	2.731
		4.125
	C2	Valence
C1	1.205	2.715
C3	1.424	1.419
		4.134
Chen et al. 2009		
	C2	Valence
C1	1.431	1.390
C3	1.190	2.839
		4.228
	C3	Valence
C2	1.190	2.839
C4	1.440	1.353
		4.192
	C6	Valence
C5	1.430	1.394
C7	1.201	2.747
		4.141
	C7	Valence
C6	1.201	2.747
C8	1.436	1.369
		4.117
	C9	Valence
C8	1.430	1.394
C10	1.190	2.839
		4.232
	C10	Valence
C9	1.190	2.839
C11	1.440	1.353
		4.192
	C13	Valence
C12	1.430	1.394
C14	1.201	2.747
		4.141
	C14	Valence
C13	1.201	2.747
C1	1.436	1.369
		4.117
	C2	Valence
C1	1.423	1.423
C3	1.204	2.723
		4.146
	C3	Valence
C2	1.204	2.723
C4	1.431	1.390
		4.113
	C6	Valence
C5	1.423	1.423
C7	1.200	2.756
		4.179
	C7	Valence
C6	1.200	2.756
C8	1.423	1.423
		4.179
	C9	Valence
C8	1.423	1.423
C10	1.205	2.715
		4.138
	C10	Valence
C9	1.205	2.715
C11	1.430	1.394
		4.109
	C13	Valence
C12	1.425	1.414
C14	1.199	2.764
		4.178
	C14	Valence
C13	1.199	2.764
C1	1.419	1.440
		4.204
Chiang et al. 2001		
	C1	Valence
C1a	1.568	0.926
O4	1.254	1.499
O3	1.251	1.515
		3.940
DiPasquale et al. 2006		
	C11	Valence
C12	1.522	1.061
C13	1.520	1.067
C14	1.525	1.052
O2	1.458	0.721
		3.901
Draskovic et al. 2010		
	C2	Valence
C3	1.436	1.369
C7	1.380	1.616
O1	1.364	1.010
		3.996
	C3	Valence
C2	1.436	1.369
C4	1.429	1.398
O2	1.287	1.332
		4.099
	C4	Valence
C3	1.429	1.398
C5	1.419	1.440
C8	1.419	1.440
		4.278
	C10	Valence

C9	1.537	1.015
O3	1.246	1.543
O4	1.265	1.441
		3.999

Gavenonis and Tilley 2004

	C2	Valence
C1	1.412	1.470
C3	1.397	1.537
C5	1.518	1.074
		4.081

	C9	Valence
C8	1.428	1.402
C10	1.405	1.501
C14	1.502	1.126
		4.029

	C13	Valence
C8	1.404	1.505
C12	1.399	1.528
C17	1.520	1.067
		4.101

	C6	Valence
C5	1.407	1.492
C7	1.396	1.541
C11	1.522	1.061
		4.095

	C10	Valence
C5	1.411	1.474
C9	1.409	1.483
C14	1.517	1.077
		4.035

	C18	Valence
C17	1.421	1.431
C19	1.392	1.560
C23	1.507	1.109
		4.101

	C22	Valence
C17	1.416	1.453
C21	1.380	1.616
C26	1.530	1.036
		4.105

	C30	Valence
C29	1.419	1.440
C31	1.393	1.555
C35	1.516	1.080
		4.075

	C34	Valence
C29	1.410	1.479
C33	1.386	1.588
C38	1.526	1.049
		4.115

Hill et al. 2007

	C11	Valence
C10	1.383	1.602
C12	1.226	2.551
		4.153

	C12	Valence
C11	1.226	2.551
C13	1.415	1.457
		4.008

	C3	Valence
C4	1.190	2.839
C31	1.420	1.436
		4.274

	C4	Valence
C3	1.190	2.839
C5	1.430	1.394
		4.232

	C9	Valence
C8	1.420	1.436
C10	1.140	3.292
		4.728

	C3	Valence
C2	1.192	2.822
C4	1.475	1.220
		4.041

	C11	Valence
C10	1.186	2.872
C12	1.459	1.279
		4.151

Krawczuk and Stadnicka 2012

	C2	Valence
C3	1.356	1.738
C9	1.490	1.168
O1	1.347	1.074
		3.981

	C5	Valence
C4	1.458	1.284
C6	1.356	1.737
O8	1.351	1.061
		4.081

Lee et al. 2006

	C9	Valence
C8	1.522	1.062
C13	1.516	1.080
C14	1.521	1.065
O2	1.457	0.725
		3.933

Leon et al. 2002

	C	Valence
C1	1.386	1.588
C	1.387	1.583
O	1.378	0.961
		4.132

	C	Valence
C4	1.387	1.583
C	1.387	1.583
O	1.387	0.930
		4.097

	C	Valence
C1	1.378	1.626
C	1.390	1.569
O	1.369	0.992
		4.188

	C	Valence
C4	1.369	1.670
C	1.390	1.569
O	1.359	1.029
		4.268

	C	Valence
C6	1.358	1.725
C	1.377	1.631
O	1.391	0.917
		4.273

	C	Valence
C9	1.355	1.741
C	1.377	1.631
O	1.384	0.941
		4.312

	C	Valence
C1	1.376	1.636
C	1.386	1.588
O	1.378	0.961
		4.184

	C	Valence
C4	1.374	1.645
C	1.386	1.588
O	1.379	0.958
		4.191

	C	Valence
C6	1.376	1.636
C	1.388	1.578
O	1.377	0.964
		4.178

	C	Valence
C9	1.379	1.621
C	1.388	1.578
O	1.378	0.961
		4.161

	C	Valence
C1	1.430	1.394
C	1.400	1.523
O	1.350	1.062
		3.979

	C	Valence
C4	1.320	1.931
C	1.400	1.523
O	1.400	0.888
		4.342

	C	Valence
C6	1.400	1.523
C	1.380	1.616
O	1.340	1.101
		4.241

	C	Valence
C9	1.420	1.436
C	1.380	1.616
O	1.360	1.025
		4.077

Liu et al. 2002

	C3	Valence
C1	1.508	1.106
C4	1.211	2.667
		3.773

	C4	Valence
C3	1.211	2.667
C5	1.453	1.302
		3.969

	C3	Valence
C2	1.339	1.825
C4	1.506	1.113
C9	1.495	1.149
		4.087

	C5	Valence
C4	1.453	1.302
C6	1.401	1.519
C10	1.399	1.528
		4.348

	C1	Valence
C2	1.573	0.912
C3	1.508	1.106
C11	1.529	1.039
O1	1.445	0.756
		3.813

Liu et al. 2013

	C10	Valence
C4	1.398	1.532
C5	1.419	1.440
C9	1.415	1.457
		4.429

	C9	Valence
C8	1.371	1.660
C10	1.415	1.457
O1	1.386	0.934
		4.051

	C2	Valence
C3	1.437	1.365
O1	1.373	0.978
O2	1.237	1.593
		3.937

	C10	Valence
C4	1.408	1.487
C5	1.411	1.474
C9	1.405	1.500
		4.461

	C9	Valence
C8	1.392	1.561
C10	1.405	1.500
O1	1.372	0.980
		4.042

	C2	Valence
C3	1.453	1.303
O1	1.395	0.906
O2	1.211	1.748
		3.957

	C10	Valence
C4	1.438	1.361
C5	1.408	1.488
C9	1.409	1.483
		4.332

	C9	Valence
C8	1.370	1.665
C10	1.409	1.483
O1	1.379	0.958
		4.106

	C2	Valence
C3	1.442	1.345
O1	1.382	0.947
O2	1.206	1.781
		4.073

	C10	Valence
C4	1.435	1.373
C5	1.408	1.488
C9	1.398	1.532
		4.393

	C9	Valence
C8	1.378	1.626
C10	1.398	1.532
O1	1.381	0.951
		4.109

	C2	Valence
C3	1.448	1.321
O1	1.375	0.971
O2	1.211	1.749
		4.042

	C10	Valence
C4	1.430	1.394
C5	1.406	1.496
C9	1.401	1.519
		4.409

	C9	Valence
C8	1.378	1.626
C10	1.401	1.519
O1	1.377	0.964
		4.109

	C2	Valence
C3	1.452	1.306
O1	1.380	0.954
O2	1.203	1.800
		4.060

Liu et al. 2014

	C17	Valence
O2	1.198	1.833
O3	1.304	1.253
O3A	1.304	1.253
		4.339

	C7	Valence
O5	1.228	1.646
O6	1.289	1.322
C4	1.519	1.071
		4.039

	C6	Valence
O3	1.242	1.565
O4	1.272	1.405
C2	1.505	1.116
		4.086

	C1	Valence
O5	1.245	1.548
O6	1.254	1.499
C2	1.513	1.090
		4.137

	C18	Valence
O3	1.290	1.318
O4	1.232	1.622
C16	1.496	1.146
		4.086

Lu and Peters 2006

	C29	Valence
C28	1.484	1.188
C30	1.397	1.537
C34	1.399	1.528
		4.252

	C33	Valence
C28	1.431	1.390
C32	1.389	1.574
C38	1.517	1.077
		4.040

	C29	Valence
C28	1.419	1.440
C30	1.394	1.551
C35	1.508	1.106
		4.097

	C29	Valence
C28	1.537	1.015
C30	1.376	1.636
C34	1.400	1.523
		4.174

	C34	Valence
C29	1.400	1.523
C33	1.376	1.636
C35	1.537	1.015
		4.174

	C36	Valence
C35	1.526	1.049

C37	1.377	1.631
C41	1.405	1.501
		4.180
	C41	Valence
C28	1.529	1.039
C36	1.405	1.501
C40	1.372	1.655
		4.195
	C29	Valence
C28	1.390	1.569
C30	1.428	1.402
C34	1.435	1.373
		4.344
	C34	Valence
C29	1.435	1.373
C33	1.418	1.444
C35	1.422	1.427
		4.244
	C36	Valence
C35	1.453	1.302
C37	1.405	1.501
C41	1.408	1.488
		4.290
	C2	Valence
C1	1.521	1.064
C3	1.414	1.461
C7	1.366	1.685
		4.210
	C7	Valence
C2	1.366	1.685
C6	1.374	1.645
C8	1.539	1.009
		4.339
	C14	Valence
C1	1.530	1.036
C9	1.382	1.607
C13	1.390	1.569
		4.212
	C21	Valence
C16	1.317	1.948
C20	1.425	1.414
C22	1.552	0.971
		4.333
	C16	Valence
C15	1.623	0.787
C17	1.371	1.660
C21	1.317	1.948
		4.395
	C23	Valence
C22	1.543	0.997
C24	1.346	1.788
C28	1.401	1.519
		4.304
	C28	Valence
C15	1.524	1.055
C23	1.401	1.519
C27	1.367	1.680
		4.253
Maher et al. 2010		
	C10	Valence
C1	1.473	1.227
O1	1.348	1.070
O2	1.211	1.749
		4.046
	C1	Valence
C2	1.407	1.492
C9	1.415	1.457
C10	1.473	1.227
		4.176
	C6	Valence
C7	1.393	1.555
C7#1	1.393	1.555
C6#2	1.512	1.093
		4.203
Manbeck et al. 2012		
	C2	Valence
C1	1.504	1.119
C3	1.396	1.541
C7	1.395	1.546
		4.207
	C9	Valence
C8	1.514	1.087
C10	1.389	1.574
C14	1.393	1.555
		4.216
	C1	Valence
C2	1.393	1.555
C6	1.361	1.710
C7	1.511	1.096
		4.361
	C6	Valence
C1	1.414	1.461
C5	1.391	1.564
C7	1.497	1.143
		4.169
	C3	Valence
C4	1.530	1.036
O3	1.281	1.361
O4	1.227	1.652
		4.049
	C1	Valence
C2	1.517	1.077
O1	1.261	1.462
O2	1.237	1.593
		4.132
	C8	Valence
C9	1.514	1.087
O3	1.291	1.313
O4	1.225	1.663
		4.063
	C1	Valence
C2	1.504	1.119
O1	1.278	1.376
O2	1.242	1.565
		4.060
	C1	Valence
C2	1.501	1.129
O1	1.291	1.313
O2	1.228	1.646
		4.088
	C3	Valence
C4	1.506	1.113
O1	1.336	1.117
O2	1.203	1.800
		4.030
	C7	Valence
C1	1.511	1.096
O1	1.280	1.366
O2	1.221	1.688
		4.149
	C7	Valence
C6	1.497	1.143
O1	1.314	1.209
O2	1.227	1.652
		4.003
Mattar et al. 2004		
	C13	Valence
C5	1.394	1.550
C9	1.490	1.166
C14	1.392	1.559
		4.276
	C14	Valence
C8	1.396	1.543
C10	1.489	1.170
C13	1.392	1.559
		4.272
Mehn et al. 2003		
	C1	Valence
C2	1.569	0.923
O1	1.278	1.376
O3	1.194	1.859
		4.158
	C1	Valence
C2	1.493	1.156
O1	1.285	1.341
O2	1.240	1.576
		4.074
	C1	Valence
C2	1.505	1.116
O1	1.263	1.452
O2	1.237	1.593
		4.161
	C1	Valence
C2	1.528	1.042
O1	1.201	1.813
O2	1.251	1.515
		4.371
Munshi et al. 2010		
	C3	Valence
C2	1.454	1.299
C4	1.379	1.620
C19	1.480	1.204
		4.122
	C8	Valence
C7	1.437	1.364
C9	1.505	1.116
C18	1.423	1.423
		3.903
	C3	Valence
C2	1.458	1.284
C4	1.382	1.607
C19	1.473	1.228
		4.119
	C8	Valence
C7	1.438	1.361
C9	1.506	1.112
C18	1.419	1.438
		3.911
	C2	Valence
C3	1.454	1.299
O1	1.392	0.915
O11	1.211	1.747
		3.960
	C19	Valence
C3	1.480	1.204
O20	1.220	1.694
O21	1.336	1.117
		4.014
	C2	Valence
C3	1.458	1.284
O1	1.389	0.923
O11	1.214	1.733
		3.941
	C19	Valence
C3	1.473	1.228
O20A	1.223	1.676
O21	1.340	1.100
		4.005
Pandey et al. 2014		
	C6	Valence
C7	1.491	1.163
O3	1.339	1.105
O4	1.200	1.820
		4.088
	C5	Valence
C1	1.520	1.067
O1	1.261	1.462
O2	1.231	1.628
		4.157
	C18	Valence
C19	1.489	1.170
O9	1.341	1.097
O10	1.205	1.787
		4.055
	C17	Valence
C13	1.524	1.055
O7	1.264	1.446
O8	1.237	1.593
		4.095
Reddy et al. 2014		
	C1	Valence
C2	1.487	1.177
O1	1.297	1.285
O2	1.203	1.800
		4.262
Saeed et al. 2012		
	C11	Valence
C1	1.455	1.293
C15	1.355	1.742
O12	1.362	1.017
		4.052
	C31	Valence
C2	1.459	1.280
C35	1.357	1.730
O32	1.371	0.985
		3.994
Schumann et al. 2003		
	C14	Valence
C9	1.376	1.636
C13	1.381	1.612
O	1.435	0.783
		4.030
	C8	Valence
C3	1.391	1.564
C7	1.378	1.626
O	1.404	0.875
		4.066
	C3	Valence
C2	1.502	1.126
C4	1.396	1.541
C8	1.391	1.564
		4.232
	C7	Valence
C2	1.398	1.532
C6	1.382	1.607
O	1.407	0.866
		4.005
	C2	Valence
C1	1.503	1.123
C3	1.396	1.541
C7	1.398	1.532
		4.196
	C10	Valence
C9	1.365	1.690
C11	1.415	1.457
O1	1.382	0.947
		4.094
	C11	Valence
C2	1.419	1.440
C6	1.421	1.431
C10	1.415	1.457
		4.328
	C6	Valence
C5	1.411	1.474
C7	1.423	1.423
C11	1.421	1.431
		4.329
	C21	Valence
C20	1.348	1.777
C22	1.421	1.431
O2	1.404	0.875
		4.084
	C22	Valence
C13	1.426	1.410
C17	1.411	1.474
C21	1.421	1.431
		4.316
	C17	Valence
C16	1.406	1.496
C18	1.425	1.414
C22	1.411	1.474
		4.385
	C11	Valence
C10	1.361	1.710
C12	1.425	1.414
O1	1.391	0.917
		4.042
	C12	Valence
C3	1.420	1.436
C7	1.417	1.448
C11	1.425	1.414
		4.299
	C7	Valence
C6	1.406	1.496
C8	1.418	1.444
C12	1.417	1.448
		4.389
	C22	Valence
C21	1.361	1.710
C23	1.420	1.436
O2	1.390	0.920
		4.066
	C23	Valence
C14	1.429	1.398
C18	1.412	1.470

C22	1.420	1.436
		4.304
	C18	Valence
C17	1.438	1.361
C19	1.424	1.419
C23	1.412	1.470
		4.250
	C9	Valence
C8	1.327	1.891
C10	1.435	1.373
O	1.389	0.924
		4.188
	C10	Valence
C1	1.435	1.373
C5	1.413	1.466
C9	1.435	1.373
		4.212
	C5	Valence
C4	1.416	1.453
C6	1.406	1.496
C10	1.413	1.466
		4.415
Song et al. 2007		
	C5	Valence
C4	1.340	1.820
C6	1.406	1.496
C13	1.479	1.205
		4.522
	C1	Valence
O1	1.172	2.012
O2	1.362	1.018
O3	1.303	1.258
		4.287
	C2	Valence
O2	1.341	1.097
O4	1.337	1.113
C6	1.319	1.937
		4.147
Varga et al. 2009		
	C29	Valence
C30	1.515	1.083
C31	1.521	1.064
C32	1.521	1.064
O4	1.440	0.769
		3.981
	C21	Valence
C22	1.526	1.049
C23	1.524	1.055
C24	1.525	1.052
O2	1.441	0.766
		3.921
	C25	Valence
C26	1.522	1.061
C27	1.523	1.058
C28	1.515	1.083
O3	1.444	0.758
		3.961
	C21	Valence
C22	1.531	1.033
C23	1.526	1.049
C24	1.527	1.045
O1	1.414	0.845
		3.972

Oxygen Environments

Bleeke et al. 2010		
	O1	Valence
C4	1.385	0.937
C5	1.428	0.802
		1.740
	O1	Valence
C1	1.148	2.197
		2.197
	O2	Valence
C2	1.149	2.189
		2.189
Bleeke and Anutrasakda 2012		
	O1	Valence
C9	1.156	2.133
		2.133
	O5	Valence
C59	1.156	2.131
		2.131
	O1	Valence
C9	1.116	2.459
		2.459
Draskovic et al 2010		
	O1	Valence
C1	1.427	0.806
C2	1.364	1.010
		1.817
Esteruelas et al. 2000		
	O3	Valence
C9	1.156	2.131
		2.131
Huynh et al. 2005		
	O1	Valence
C1	1.162	2.085
		2.085
	O2	Valence
C2	1.145	2.216
		2.216
	O3	Valence
C3	1.170	2.026
		2.026
Krawczuk and Stadnicka 2012		
	O1	Valence
C2	1.347	1.074
C6	1.360	1.026
		2.100
	O7	Valence
C4	1.248	1.532
		1.532
Liu et al. 2013		
	O1	Valence
C2	1.373	0.978
C9	1.386	0.934
		1.912
	O1	Valence
C2	1.395	0.906
C9	1.372	0.980
		1.886
	O1	Valence
C2	1.382	0.946
C9	1.379	0.956
		1.902
	O1	Valence
C2	1.375	0.971
C9	1.377	0.964
		1.936
	O1	Valence
C2	1.380	0.954
C9	1.377	0.964
		1.919
Lu and Peters 2006		
	O1	Valence
C28	1.073	2.869
		2.869
	O2	Valence
C29	1.146	2.208
		2.208
	O3	Valence
C30	1.147	2.200
		2.200
	O4	Valence
C31	1.139	2.265
		2.265
Munshi et al. 2010		
	O11	Valence
C2	1.211	1.747
		1.747
	O20	Valence
C19	1.220	1.694
		1.694
	O11	Valence
C2	1.214	1.733
		1.733
	O20A	Valence
C19	1.223	1.676
		1.676
	O1	Valence
C2	1.392	0.915
C9	1.369	0.992
		1.907
	O21	Valence
C19	1.336	1.117
C22	1.445	0.757
		1.874
	O1	Valence
C2	1.389	0.923
C9	1.372	0.982
		1.905
	O21	Valence
C19	1.340	1.100
C22	1.443	0.762
		1.862
Pandian et al. 2010		
	O1	Valence
C9	1.361	1.021
C25	1.436	0.780
		1.802
	O2	Valence
C16	1.381	0.951
C29	1.455	0.729
		1.680
	O3	Valence
C17	1.331	1.137
C33	1.444	0.758
		1.896
	O4	Valence
C24	1.369	0.992
C37	1.467	0.698
		1.691
Pierce et al. 2009		
	O1	Valence
C1	1.151	2.169
		2.169
	O2	Valence
C2	1.151	2.169
		2.169
	O1	Valence
C1	1.115	2.468
		2.468
	O2	Valence
C2	1.145	2.216
		2.216
	O1	Valence
C1	1.146	2.208
		2.208
	O2	Valence
C2	1.144	2.224
		2.224
	O1	Valence
C1	1.140	2.256
		2.256
	O2	Valence
C2	1.160	2.100
		2.100
Reddy et al. 2014		
	O2	Valence
C1	1.203	1.800
		1.800
	O3	Valence
C3	1.229	1.640
		1.640
Saeed et al. 2012		
	O12	Valence
C11	1.362	1.017
C13	1.359	1.030
		2.047
	O11	Valence
C1	1.210	1.754
		1.754
	O21	Valence
C2	1.218	1.708
		1.708
Schumann et al. 2003		
	O	Valence
C14	1.435	0.783
C15	1.446	0.753
		1.536
Song et al. 2007		
	O1	Valence
C1	1.325	1.162
C5	1.414	0.845
		2.007

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