

Supplementary Material

A Bond Length – Bond Valence Relationship for Carbon – Nitrogen Bonds, by C. Harris and F. D. Hardcastle

4.061	0.00011721	3.651	0.000481095	4.301	0.000140748
4.031	0.000129968	4.433	3.2549E-05	N 3.943	0.000175981
1.333	1.410676779		4.037922604	3.848	0.000244098
3.614	0.00054648			1.43	1.010038052
2.581	0.019173676	Drueck 1984		4.647	1.55755E-05
3.75	0.000342097	C2	Valence	3.27	0.001786978
4.657	1.50482E-05	C 4.151	0.000225738	3.685	0.000427931
3.852	0.000240758	4.261	0.000159644		3.952096163
	4.245652012	4.245	0.000167895	Marsh 1988	
		4.109	0.000257661	C39	Valence
Kroke 1999		4.109	0.000257661	C 4.28	0.000150372
C11	Valence	2.827	0.014604697	4.031	0.000329407
C 4.389	0.00010668	4.151	0.000225738	4.482	7.95944E-05
4.712	3.85747E-05	2.446	0.048484352	4.232	0.000174911
4.481	7.98454E-05	1.429	1.192870931	4.03	0.000330446
4.141	0.00023296	3.727	0.000858077	1.374	1.418466785
4.368	0.000113974	2.451	0.047726863	2.402	0.055690634
3.558	0.001461081	4.225	0.00017881	2.775	0.01720343
3.542	0.001536591	2.827	0.014604697	1.41	1.266428049
4.705	3.94345E-05	3.73	0.000850008	2.432	0.050669889
1.452	1.109520751	N 4.55	2.17537E-05	3.839	0.000603031
4.311	0.000136385	4.415	3.46307E-05	4.259	0.000160653
4.596	5.55853E-05	4.352	4.30224E-05	4.284	0.000148489
4.382	0.000109058	3.557	0.000665017	N 2.389	0.037144404
4.061	0.00029971	1.157	2.586325635	3.952	0.00017061
4.246	0.000167367	4.496	2.62002E-05	4.608	1.78147E-05
4.345	0.000122536	3.22	0.002122793	3.958	0.00016712
4.074	0.000287687	3.222	0.002108221	3.327	0.001468454
3.705	0.000919637	3.543	0.000697869	2.444	0.030734489
4.225	0.00017881	4.611	1.76315E-05	4.455	3.01738E-05
N 4.258	5.94699E-05		3.913535547		2.880168757
3.565	0.000646944			Nitrogen Environments	
4.1	0.000102478	Marsh 1988		Liu 2013	
2.376	0.038845295	C410	Valence	N1	Valence
4.613	1.75105E-05	C 4.505	7.40328E-05	C 2.417	0.033729648
4.575	1.9959E-05	4.252	0.000164234	1.361	1.280990565
4.337	4.53035E-05	4.311	0.000136385	2.415	0.033962789
4.145	8.77646E-05	4.509	7.31061E-05	1.463	0.901524003
2.349	0.042630874	1.374	1.418466785	1.47	0.880049089
4.523	2.38736E-05	3.923	0.00046286	2.852	0.007539655
1.13	2.838370079	1.381	1.387538329	2.477	0.02743251
4.214	6.92008E-05	2.4	0.056042519	2.489	0.026321843
3.455	0.000944934	3.906	0.000488316		
4.085	0.000107911	2.384	0.058938827		
4.45	3.0698E-05	2.781	0.016881405		

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	2.851	0.007565667		2.367	0.025914678		4.645	5.18234E-06	
		3.199115771		3.896	8.52615E-05		2.493	0.016178819	
	Vo 2014			4.005	5.67229E-05		1.11	2.848816348	
	N1	Valence		4.674	4.64981E-06		3.386	0.000573974	
N	3.519	0.000349081		4.674	4.64981E-06		1.261	1.61983362	
	3.48	0.000403882		2.367	0.025914678		4.011	5.54646E-05	
	3.519	0.000349081		3.896	8.52615E-05		3.482	0.000400873	
	3.48	0.000403882		4.645	5.18234E-06		4.172	3.03797E-05	
	4.652	5.04846E-06		2.35	0.027615343		4.011	5.54646E-05	
	3.392	0.000561241		4.447	1.08652E-05		3.694	0.000181452	
	4.652	5.04846E-06		4.448	1.08247E-05		3.244	0.000976049	
	3.392	0.000561241		3.897	8.49433E-05		4.295	1.91803E-05	
	4.52	8.26991E-06		3.896	8.52615E-05	C	4.604	1.80618E-05	
	3.341	0.000679146		2.35	0.027615343		3.566	0.00064472	
	3.341	0.000679146		2.368	0.025817966		3.888	0.000212683	
	3.103	0.00165359		4.447	1.08652E-05		3.819	0.000269737	
	3.103	0.00165359		4.448	1.08247E-05		4.455	3.01738E-05	
	3.183	0.001226094		3.897	8.49433E-05		2.206	0.06976209	
	3.902	8.33701E-05		4.675	4.63246E-06		4.604	1.80618E-05	
	3.183	0.001226094		4.005	5.67229E-05		3.566	0.00064472	
	3.902	8.33701E-05		4.646	5.163E-06		3.888	0.000212683	
C	4.436	3.22144E-05	C	4.65	1.54154E-05			4.5606635	
	4.436	3.22144E-05		4.65	1.54154E-05				
	2.585	0.018911339		2.604	0.017713429		Rosokha 2004		
	1.139	2.751738002		1.399	1.123845563		N1	Valence	
	3.731	0.000365232		4.65	1.54154E-05	N	3.372	0.000604819	
	3.561	0.000655918		2.604	0.017713429		4.192	2.81908E-05	
	3.008	0.004405662		4.65	1.54154E-05		3.927	7.59303E-05	
	4.282	5.47519E-05		1.4	1.119981539		2.822	0.00472842	
	3.17	0.002521717		1.4	1.119981539		3.417	0.000511157	
	3.561	0.000655918		2.605	0.017652527		3.426	0.000494242	
	4.282	5.47519E-05		4.65	1.54154E-05		3.532	0.000332519	
	4.072	0.000112852		4.65	1.54154E-05		4.091	4.11256E-05	
		2.789471748			3.578362499		3.448	0.000455215	
							3.755	0.000144447	
							3.694	0.000181452	
	Miller 2004			Miller 2004			C	3.707	0.000396705
	N1	Valence		N7	Valence		4.355	4.25802E-05	
N	4.447	1.08652E-05	N	4.011	5.54646E-05		2.395	0.036384698	
	4.645	5.18234E-06		3.482	0.000400873		2.369	0.039793196	
	3.896	8.52615E-05		4.172	3.03797E-05		1.333	1.410676779	
	4.674	4.64981E-06		4.011	5.54646E-05		4.573	2.00969E-05	
	4.674	4.64981E-06		3.694	0.000181452		2.394	0.036510228	
	4.004	5.69354E-05		3.244	0.000976049		4.194	7.41356E-05	
	4.447	1.08652E-05		4.295	1.91803E-05		3.707	0.000396705	
	2.349	0.027718789		4.66	4.89969E-06				

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	3.149	0.0013923
	4.278	2.04391E-05
C	4.271	5.6866E-05
	3.839	0.000251782
	4.598	1.84389E-05
	3.943	0.000175981
	4.032	0.000129521
	3.96	0.000165973
	4.658	1.49965E-05
	3.685	0.000427931
	2.444	0.030734489
	4.176	7.88771E-05
	1.397	1.131613649
	3.672	0.000447527
	2.399	0.035886879
	2.859	0.007360055
	3.304	0.001589509
	3.762	0.000328246
	4.45	3.0698E-05
		1.212933809

Kroll 2003

	N1	Valence
C	3.844	0.000247484
	4.473	2.836E-05
	2.96	0.005197664
	3.844	0.000247484
	3.844	0.000247484
	3.774	0.000314957
	2.824	0.008302962
	3.774	0.000314957
	2.824	0.008302962
	1.537	0.698699197
	3.844	0.000247484
	1.657	0.462165721
	2.96	0.005197664
	4.353	4.28745E-05
	3.651	0.000481095
	2.96	0.005197664
	3.774	0.000314957
	3.651	0.000481095
	1.657	0.462165721
	1.657	0.462165721
	3.774	0.000314957
	2.824	0.008302962

	2.869	0.00711088
	3.774	0.000314957
	3.774	0.000314957
	4.353	4.28745E-05
	3.651	0.000481095
N	4.155	3.23734E-05
	4.218	2.55793E-05
	3.472	0.000416145
	4.218	2.55793E-05
	4.218	2.55793E-05
	2.509	0.015239334
	2.399	0.022992393
	3.314	0.000751287
	2.399	0.022992393
	3.472	0.000416145
	4.155	3.23734E-05
	2.399	0.022992393
	2.509	0.015239334
	4.218	2.55793E-05
	4.218	2.55793E-05
	4.155	3.23734E-05
	2.287	0.034950223
	2.509	0.015239334
	4.089	4.14342E-05
	4.155	3.23734E-05
	4.155	3.23734E-05
	2.399	0.022992393
	2.287	0.034950223
	4.089	4.14342E-05
	3.314	0.000751287
	2.399	0.022992393
	3.472	0.000416145
	4.155	3.23734E-05
	4.155	3.23734E-05
	2.399	0.022992393
	2.287	0.034950223
	4.089	4.14342E-05
	3.314	0.000751287
	4.089	4.14342E-05
		2.429791754

Parrish 2015

	N3	Valence
C	4.527	2.3547E-05
	3.609	0.000555972

	3.983	0.000153333
	1.333	1.410676779
	2.257	0.058524156
	3.648	0.000486091
	1.351	1.325878232
	2.434	0.031811468
	3.186	0.002386514
	3.444	0.00098142
	4.56	2.10172E-05
	4.33	4.6409E-05
N	3.973	6.39323E-05
	3.641	0.000221219
	3.365	0.000620857
	3.348	0.000661601
	2.356	0.027002728
	2.321	0.030778021
	3.164	0.001316364
	3.195	0.001172298
	3.488	0.00039198
	3.447	0.00045692
	3.3	0.00079166
		2.89502252

Parrish 2015

	N6	Valence
C	3.942	0.000176588
	4.071	0.000113242
	3.993	0.000148142
	4.171	8.02471E-05
	3.393	0.001169875
	1.393	1.147311273
	3.395	0.001161844
	3.683	0.000430889
	4.366	4.09972E-05
	4.463	2.93538E-05
	3.661	0.000464807
N	4.479	9.63999E-06
	3.164	0.001316364
	2.885	0.003736084
	4.403	1.28081E-05
	1.095	3.01315503
	3.806	0.00011937
	4.471	9.9327E-06
	2.356	0.027002728
	2.353	0.027307318

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	3.26	0.000919371		1.479	0.853188434		4.214	6.92008E-05
		4.224715903		2.563	0.020399957		2.897	0.006457163
				1.54	0.691517112		1.275	1.722591233
				2.884	0.006752845		2.469	0.028198871
				4.352	4.30224E-05		2.837	0.007939406
Parkes 1963				3.053	0.003773128		1.435	0.992793399
N1 Valence				3.724	0.000374144		2.392	0.036762589
C 3.259	0.001855977			4.387	3.81367E-05		2.932	0.00572387
3.293	0.001650884			4.432	3.26613E-05		2.449	0.030209751
3.753	0.00033858			4.484	2.73057E-05		3.778	0.000310647
4.339	4.49925E-05				2.782643891		3.783	0.000305344
3.183	0.0024113						4.26	5.90617E-05
3.251	0.001907826						1.5	0.793658678
1.127	2.867849344							3.669272254
2.498	0.025518454		Iglesias 2008					
4.401	3.63414E-05		N19 Valence					
4.246	6.19793E-05		N 2.331	0.029648497				
3.853	0.00023993		C 4.332	4.60904E-05				
4.502	2.56643E-05		4.472	2.84579E-05				
4.278	5.55114E-05		3.582	0.000610153				
N 3.725	0.000161593		4.441	3.16644E-05				
3.635	0.000226238		2.85	0.007591769				
3.603	0.000254992		2.961	0.005179793				
3.858	9.82783E-05		1.284	1.670014701				
3.543	0.000319121		4.289	5.34476E-05				
3.712	0.000169642		3.212	0.002182096				
3.725	0.000161593		2.41	0.034552717				
3.543	0.000319121		1.543	0.684408853				
3.624	0.000235737		3.875	0.000222422				
3.635	0.000226238		1.49	0.821469567				
3.712	0.000169642		2.473	0.027813051				
3.603	0.000254992		4.289	5.34476E-05				
	2.904593972		2.476	0.027527155				
			3.813	0.000275369				
Iglesias 2008			2.919	0.005985974				
N14 Valence				3.317695225				
N 2.331	0.029648497		Iglesias 2008					
C 4.113	9.79906E-05		N68 Valence					
3.627	0.000522551		N 2.272	0.036966384				
3.641	0.000497953		C 4.372	4.01587E-05				
2.447	0.030418562		4.318	4.83672E-05				
2.832	0.008077312		4.379	3.92021E-05				
2.493	0.025961705		3.513	0.000773832				
1.404	1.104657843		2.903	0.006325096				
2.89	0.00661473							