Supplementary Material

A General Valence-Length Correlation for Determining Bond Orders: Application to Carbon-Carbon and Carbon-Hydrogen Chemical Bonds, by F. D. Hardcastle:

Carbon-Carbon and Carbon-Hydrogen Bonds

First Column: Bond lengths determined from Mercury Free Software

The crystallographic information files were downloaded from the Crystallography Open Database (COD)

http://www.crystallography.net/cod/index.php

Second Column: Bond order or bond valence determined from

$$s_{C-C} = \exp\left[\frac{(1.486 - R)}{0.3176}\right] \qquad \xi_{BestFit} = 1.666$$

$$s_{C-H} = \exp\left[\frac{(0.9434 - R)}{0.3970}\right] \qquad \xi_{C} = 1.666(\,fit) \qquad \xi_{H} = 1.0000(Universal)$$

Graphite_Lipson_ZPhys_181_1942

1.419	1.234832	
1.419	1.234832	
1.419	1.234832	3.704497
2.456	0.047178	
2.456	0.047178	
2.456	0.047178	
2.456	0.047178	
2.456	0.047178	
2.456	0.047178	
2.456	0.047178	3.987562
2.837	0.014217	

2.837	0.014217		
2.837	0.014217		
6.79	5.6E-08	4.030212	0.00091279

Graphite_Kukesh_Pauling_AmMiner_35_1950

1.418	1.238726		
1.418	1.238726		
1.418	1.238726	3.716178	
2.456	0.047178		
2.456	0.047178		
2.456	0.047178		
2.456	0.047178		
2.456	0.047178		
2.456	0.047178		
2.836	0.014262		
2.836	0.014262		
2.836	0.014262		
3.566	0.001432		
3.566	0.001432		
3.566	0.001432		
3.566	0.001432		
3.422	0.002254		
3.422	0.002254		
3.838	0.000608		
3.838	0.000608		
3.838	0.000608		
3.838	0.000608	4.054699	0.00299196

Graphite_Wyckoff_1963

1.418	1.238726		
1.418	1.238726		
1.418	1.238726	3.716178	
2.456	0.047178		
2.456	0.047178		
2.456	0.047178		
2.456	0.047178		
2.456	0.047178		
2.456	0.047178		
2.836	0.014262		
2.836	0.014262		
2.836	0.014262		
3.348	0.002845		
3.348	0.002845		
3.636	0.001149		
3.636	0.001149		
3.636	0.001149		
3.636	0.001149		
3.636	0.001149		
3.636	0.001149		
3.636	0.001149		
3.636	0.001149		
3.636	0.001149		
3.636	0.001149		
3.636	0.001149		
4.152	0.002716	4.064224	0.00412469

C_Diamond_Ymanaka_12oC_3oC_AC_52_B_1996

1.544	0.833101	
1.544	0.833101	
1.544	0.833101	
1.544	0.833101	3.332404
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	3.792317
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	

4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115	3.91016	0.00807125

C_Diamond_Wyckoff_CrystStruct__1_1963

1.544	0.833101		Same as previous
1.544	0.833101		
1.544	0.833101		
1.544	0.833101	3.332404	
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326	3.792317	
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		

2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115	3.91016	0.00807125

C_Diamond_Riley_Nature_153_1944

1.544	0.833101	Same as previous
1.544	0.833101	
1.544	0.833101	
1.544	0.833101	3.332404
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	

2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326	3.792317	
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115	3.91016	0.00807125

C_Diamond_Hom_JApplCryst_8_1975

1.544	0.833101	
1.544	0.833101	
1.544	0.833101	
1.544	0.833101	3.332404
2.52	0.038568	
2.52	0.038568	
2.52	0.038568	
2.52	0.038568	
2.52	0.038568	
2.52	0.038568	
2.52	0.038568	
2.52	0.038568	
2.52	0.038568	
2.52	0.038568	
2.52	0.038568	
2.52	0.038568	
2.52	0.038568	3.795222
2.953	0.009867	
2.953	0.009867	
2.953	0.009867	
2.953	0.009867	
2.953	0.009867	
2.953	0.009867	
2.953	0.009867	
2.953	0.009867	
2.953	0.009867	
2.953	0.009867	

2.953	0.009867		
2.953	0.009867		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115	3.914547	0.00730228

C_Diamond_Straumanis_JACS_73_1951

1.544	0.833101	
1.544	0.833101	
1.544	0.833101	
1.544	0.833101	3.332404
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	3.792317
2.957	0.009744	

2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115	3.91016	0.00807125

C_Diamond_Straumanis_10oC_JACS_73_1951

1.544	0.833101		
1.544	0.833101		
1.544	0.833101		
1.544	0.833101	3.332404	
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		

2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326	3.792317	
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115	3.91016	0.00807125

C_Diamond_Straumanis_20oC_JACS_73_1951

1.544	0.833101	
1.544	0.833101	
1.544	0.833101	
1.544	0.833101	3.332404
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	
2.522	0.038326	3.792317
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	
2.957	0.009744	

2.957	0.009744		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115	3.91016	0.00807125

C_Diamond_Straumanis_30oC_JACS_73_1951

1.544	0.833101		
1.544	0.833101		
1.544	0.833101		
1.544	0.833101	3.332404	
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.522	0.038326		
2.957	0.009744		
2.957	0.009744		

2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
2.957	0.009744		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115		
4.368	0.000115	3.91016	0.00807125

C_Diamond_Hexagonal_Bundy_JChemPhys_46_3437_1967

1.543	0.835728	
1.543	0.835728	
1.543	0.835728	
1.545	0.830482	3.337666
2.52	0.038568	
2.522	0.038326	
2.52	0.038568	
2.522	0.038326	
2.52	0.038568	

2.522	0.038326		
2.52	0.038568		
2.522	0.038326		
2.52	0.038568		
2.522	0.038326		
2.52	0.038568		
2.522	0.038326		
2.956	0.009774		
2.575	0.032436		
2.956	0.009774		
2.575	0.032436		
2.956	0.009774		
2.575	0.032436		
2.956	0.009774		
2.575	0.032436		
2.956	0.009774		
2.575	0.032436		
2.956	0.009774		
2.575	0.032436		
3.603	0.001275		
3.603	0.001275		
3.603	0.001275		
3.603	0.001275		
3.603	0.001275		
3.603	0.001275		
3.603	0.001275		
3.603	0.001275	4.062495	0.00390556

C21H22_Shi_ChemRev_110_5883_2010

1.327	1.649673		
1.485	1.003153		
1.485	1.003153	3.65598	
2.498	0.041334		
2.516	0.039057		
2.509	0.039927		
2.493	0.04199	3.818288	
3.781	0.000728		
3.777	0.000737		
3.779	0.000733		
3.7670	0.000761		
2.603	0.029699	3.850946	
2.636	0.014071		
2.666	0.013046		
2.671	0.012883		
2.516	0.019037		
4.494	0.000131	3.910113	0.00807962
1.276	1.936999		
1.327	1.649673	3.586672	
2.441	0.049459		
2.416	0.053509		
2.914	0.011156		
2.915	0.011121		
2.654	0.025294		
2.66	0.02482		
3.607	0.001259		
3.415	0.002304		

3.581	0.001366		
3.459	0.002006		
3.613	0.001235		
4.273	0.000155		
3.664	0.001052	3.77141	
2.638	0.014		
2.685	0.012437		
3.758	0.000833		
3.54	0.001443		
3.554	0.001393		
3.597	0.00125		
3.377	0.002176		
3.294	0.002682		
3.415	0.001977	3.809602	0.03625146
1.276	1.936999		
1.485	1.003153		
1.488	0.993723	3.933875	
2.565	0.033474		
2.54	0.036215		
2.561	0.033898		
2.589	0.031038		
3.718	0.000888		
3.763	0.00077		
2.603	0.029699		
3.605	0.001267		
3.539	0.001559	4.102682	
3.228	0.003167		

3.259	0.002929		
2.595	0.015601		
2.94	0.006542		
2.643	0.013825		
3.027	0.005255		
2.968	0.006097		
2.62	0.014649		
2.936	0.006609		
3.314	0.00255		
3.3	0.002642		
3.323	0.002493		
3.304	0.002615	4.187658	0.03521535
1.488	0.993723		
1.507	0.936024		
1.508	0.933082		
1.531	0.867905	3.730734	
2.617	0.028419		
2.644	0.026103		
2.654	0.025294		
3.929	0.000457	3.811006	
2.039	0.063303		
2.039	0.063303		
2.04	0.063144		
2.04	0.063144		
2.039	0.063303		
2.041	0.062985		
2.713	0.01159		

2.99	0.005768		
3.381	0.002154		
3.39	0.002106		
3.047	0.004997	4.216802	0.04700331
1.507	0.936024		
2.515	0.03918		
2.54	0.036215		
2.631	0.027193		
3.415	0.002304		
3.054	0.00718		
4.5	7.57E-05		
0.96	0.959047		
0.96	0.959047		
0.961	0.956634		
2.679	0.012626		
2.64	0.01393	3.949455	0.00255484
1.382	1.387386		
1.384	1.378678		
2.357	0.064431		
2.384	0.059181		
2.734	0.019662		
2.509	0.039927		
3.054	0.00718		
3.169	0.004999		
0.929	1.03694		
2.787	0.009619		

2.012	0.067758	4.075761	0.00573968
1.36	1.486886		
1.382	1.387386		
2.353	0.065248		
2.408	0.054874		
2.724	0.020291		
0.93	1.034331		
1.998	0.07019		
2.01	0.0681	4.187307	0.03508373

C36H46_Zhang_ZK_222_310_2007

1.542	0.838363	
1.522	0.892849	
1.52	0.898488	
1.548	0.822675	3.452375
2.613	0.028779	
2.407	0.055047	
2.405	0.055395	
2.615	0.028598	
2.607	0.029328	
3.715	0.000896	3.650417
2.768	0.01009	
2.792	0.009498	
2.062	0.05974	
2.062	0.05974	

2.063	0.059589		
2.064	0.059439		
2.83	0.008631	3.917145	0.00686493
1.509	0.930149		
1.509	0.930149		
2.53	0.037373		
2.596	0.030361		
3.018	0.008041		
3.604	0.001271		
3.138	0.005511		
0.97	0.93519		
0.971	0.932837		
2.727	0.011188		
2.732	0.011048		
2.036	0.063783		
2.037	0.063623		
2.031	0.064592		
2.031	0.064592	4.089708	0.00804747
1.381	1.391761		
1.381	1.391761		
2.393	0.057527		
2.386	0.058809		
2.749	0.018755		
0.93	1.034331		
2.012	0.067758		
2.019	0.066574	4.087277	0.00761726

C19H33_Mace_CM_33_7_1995

1.524	0.887244		
1.527	0.878904		
1.538	0.848987		
2.516	0.039057		
2.558	0.034219		
2.55	0.035092		
2.463	0.046149		
2.908	0.011369		
2.932	0.010542		
0.943	1.001008		
2.124	0.051102		
2.309	0.032066		
2.188	0.043493		
2.206	0.041565		
2.41	0.024863		
3.049	0.004972		
3.306	0.002602		
2.758	0.010348		
2.914	0.006985	4.010568	0.00011168
1.505	0.941937		
1.52	0.898488		
2.474	0.044578		
2.535	0.036789		
2.505	0.040433		
3.009	0.008272		

3.751	0.0008
3.884	0.000526
1.171	0.563648
0.985	0.900513
2.021	0.066239
2.158	0.046907
2.333	0.030185
2.813	0.009009
2.711	0.011648
3.416	0.001972
4.005	0.000447
2.781	0.009765
2.779	0.009815
3.63	0.00115
3.536	0.001458
3.656	0.001078
3.784	0.000781
3.806	0.000738
4.639	9.06E-05 3.627269 0.13892839

C13H10_Gerkin_AC_C_40_1892_1984

1.386	1.370024	
1.398	1.319231	
1.504	0.944907	3.634162
2.383	0.059367	
2.762	0.018003	
2.42	0.052839	
2.326	0.071037	

2.349	0.066075		
3.715	0.000896		
3.885	0.000525	3.902904	
2.07	0.058548		
2.129	0.050462		
2.102	0.054014		
2.952	0.006348		
3.892	0.000595	4.07287	0.00530998
1.387	1.365718		
1.398	1.319231		
1.471	1.048357	3.733306	
2.386	0.058809		
2.76	0.018117		
2.417	0.053341		
2.383	0.059367		
2.326	0.071037		
2.602	0.029793		
3.645	0.001117		
3.876	0.00054	4.025426	
2.051	0.061418		
3.146	0.003894		
3.063	0.004799		
2.854	0.008125		
2.679	0.012626		
3.283	0.002757		
3.316	0.002537	4.121584	0.01478259
1.385	1.374344		

1.39	1.35288		
2.386	0.058809		
2.762	0.018003		
2.41	0.054529		
4.226	0.000179		
4.147	0.00023		
3.898	0.000504		
4.096	0.00027		
3.812	0.00066		
3.836	0.000612		
0.988	0.893733		
2.062	0.05974		
2.07	0.058548		
3.143	0.003923		
3.939	0.000528		
3.162	0.00374		
3.083	0.004564		
3.628	0.001156		
3.321	0.002506		
4.316	0.000204	3.889663	0.01217416

C2H_Echigo_AM_92_1262_2007

1.407	1.282376	
1.412	1.262348	
1.413	1.25838	3.803103
2.442	0.049303	
2.818	0.015093	
2.436	0.050244	

2.428	0.051525		
2.806	0.015674		
2.424	0.052178		
2.43	0.051202		
2.804	0.015773		
2.45	0.048077		
3.737	0.000836		
3.739	0.000831		
3.726	0.000866		
3.713	0.000902	4.155607	
3.309	0.002583		
3.316	0.002537		
3.844	0.000671		
3.8	0.00075	4.162148	0.02629199
1.422	1.223224		
1.425	1.211726		
1.417	1.242632	3.677582	
2.423	0.052343		
2.831	0.014488		
2.433	0.05072		
2.45	0.048077		
2.823	0.014857		
2.418	0.053173	3.911241	
2.088	0.055952		
2.084	0.056519		
3.31	0.002576		
3.353	0.002312		
3.417	0.001967	4.030567	0.00093435

1.422	1.223224		
1.358	1.496278		
2.443	0.049149		
2.785	0.016746		
2.418	0.053173		
2.502	0.040817		
3.737	0.000836		
4.244	0.000169		
3.731	0.000852		
3.719	0.000885		
3.886	0.000523		
3.829	0.000626		
0.982	0.907344		
2.68	0.012594		
2.071	0.0584		
3.282	0.002764		
3.18	0.003574	3.867955	0.01743593

C28H10_Litvinov_CrystEngComm_4_618_2002

1.495	0.972063	
1.495	0.972063	
1.351	1.529619	3.473745
2.506	0.040306	
2.523	0.038206	
3.155	0.005224	
2.503	0.040689	
2.503	0.040689	

2.523	0.038206		
2.506	0.040306		
3.591	0.001324		
3.591	0.001324		
3.79	0.000708		
3.797	0.000692		
3.79	0.000708		
3.797	0.000692	3.722817	
2.656	0.013379		
2.656	0.013379		
2.685	0.012437		
2.685	0.012437		
3.007	0.005526		
3.007	0.005526		
3.749	0.000853		
3.749	0.000853	3.787207	0.04528083
1.398	1.319231		
1.411	1.266328		
1.441	1.1522	3.737759	
2.185	0.110731		
2.394	0.057347		
2.438	0.049928		
2.8	0.015973		
2.422	0.052508		
2.418	0.053173		
3.001	0.008483		
2.624	0.027799		
3.403	0.002393		

3.843	0.000599		
3.623	0.001197		
4.074	0.000289		
4.055	0.000307		
3.59	0.001328		
3.787	0.000714		
3.597	0.001299		
4.082	0.000282		
3.616	0.001224	4.123334	0.01521129

C34H34_Bacchi_CrystEngComm_16_8205_2014

1.482	1.012673	
1.498	0.962925	
1.35	1.534442	3.51004
2.486	0.042926	
2.526	0.037847	
2.498	0.041334	
2.502	0.040817	
2.514	0.039304	
3.728	0.00086	
3.786	0.000717	
4.277	0.000153	
3.78	0.00073	
3.778	0.000735	
4.288	0.000148	
3.781	0.000728	
4.331	0.000129	
4.541	6.65E-05	3.716532

1.986	0.072345		
2.725	0.011245		
2.653	0.013481		
2.617	0.01476		
2.581	0.016161		
2.693	0.012189	3.856713	0.02053122
1.488	0.993723		
1.49	0.987486		
2.479	0.043882		
2.858	0.013307		
2.458	0.046881		
0.969	0.937549		
0.97	0.93519		
1.985	0.072527		
1.985	0.072527		
2.026	0.06541		
2.026	0.06541		
3.294	0.002682		
2.776	0.009889		
3.254	0.002966		
2.763	0.010218		
3.266	0.002878		
3.708	0.000945	4.263472	0.06941757

C30H18_Nagarajan_CrystEngComm_16_8946_2014

1.41	1.270321
1.407	1.282376

1.5	0.956881	3.509578	
2.512	0.039552		
2.494	0.041858		
2.459	0.046734		
2.809	0.015527		
2.461	0.046441		
2.484	0.043197		
2.944	0.010151		
2.528	0.037609		
3.721	0.000879		
3.724	0.000871		
3.751	0.0008		
3.753	0.000795		
3.795	0.000697		
3.831	0.000622	3.79531	
2.609	0.015061		
2.65	0.013583		
2.665	0.013079		
2.674	0.012786	3.84982	0.02255414
1.39	1.35288		
1.389	1.357146		
2.467	0.045572		
2.433	0.05072		
2.809	0.015527		
2.44	0.049615		
2.47	0.045143		
3.697	0.000948		
3.698	0.000945		

3.716	0.000893		
3.727	0.000863		
4.187	0.000203		
4.194	0.000198		
4.309	0.000138		
0.93	1.034331		
2.65	0.013583		
2.653	0.013481	3.982186	0.00031734
1.393	1.340162		
1.424	1.215546		
1.438	1.163134	3.718842	
2.467	0.045572		
2.837	0.014217		
2.417	0.053341		
2.465	0.04586		
2.849	0.01369		
2.428	0.051525		
3.764	0.000768		
3.767	0.000761		
4.24	0.000172	3.944746	
2.018	0.066742		
2.057	0.060497		
3.263	0.0029		
3.248	0.003012	4.077896	0.00606778

C44H30_Li_CrystEngComm_14_2843_2012

1.26	2.03707

1.482	1.012673		
3.677	0.00101		
2.479	0.043882		
3.06	0.007045		
2.926	0.010743		
2.507	0.040179		
2.504	0.040561		
2.922	0.010879		
3.815	0.000654		
0.93	1.034331		
1.856	0.100375		
2.594	0.015641		
2.589	0.015839		
2.822	0.008807	4.379688	0.14416311
1.387	1.365718		
1.38	1.39615		
1.474	1.038502	3.80037	
2.414	0.053847		
2.843	0.013951		
2.407	0.055047		
2.479	0.043882		
4.328	0.00013	3.967227	
2.01	0.0681		
2.049	0.061728		
2.005	0.068964		
3.241	0.003065		
2.651	0.013549		
3.234	0.00312	4.185752	0.03450397

1.377	1.409399
1.397	1.323391
2.407	0.055047
2.722	0.020419
2.352	0.065454
2.963	0.009561
2.523	0.038206
3.781	0.000728
3.799	0.000688
0.93	1.034331
2.002	0.069487
3.628	0.001156
3.729	0.000897

2.638	0.014	4.042762	0.00182861

C20H18_Li_JMaterChem_21_17662_2011

1.516	0.909875
2.972	0.009294
2.553	0.034762
2.516	0.039057
4.323	0.000132
3.858	0.000571
3.821	0.000642
0.943	1.001008
0.947	0.990973
0.992	0.884773
2.602	0.015329

2.637	0.014035	3.900451	0.00990992
1.429	1.196562		
1.43	1.192801		
1.435	1.174171	3.563534	
2.454	0.047476		
2.789	0.016536		
2.454	0.047476		
2.459	0.046734		
2.825	0.014764		
2.484	0.043197		
2.481	0.043607		
2.826	0.014718		
2.457	0.047029		
3.766	0.000763		
4.224	0.00018		
3.767	0.000761	3.886774	0.01282017

C16H14_HungDang_Langmuir_23_11980_2007

1.512	0.921405
1.509	0.930149
2.539	0.036329
2.495	0.041726
2.854	0.013476
2.493	0.04199
3.731	0.000852
3.786	0.000717
3.797	0.000692

0.97	0.93519		
0.97	0.93519		
2.049	0.061728		
2.049	0.061728		
2.701	0.011945	3.993118	4.7361E-05
1.382	1.387386		
1.361	1.482212		
2.419	0.053006		
2.761	0.01806		
2.391	0.057891		
3.783	0.000723		
3.81	0.000664		
0.929	1.03694		
2.007	0.068617		
1.992	0.071259		
3.99	0.000465	4.177223	0.0314081
1.393	1.340162		
1.472	1.045062		
1.401	1.30683	3.692054	
2.4	0.056273		
2.754	0.018462		
2.396	0.056987		
2.469	0.045286		
2.833	0.014397		
2.499	0.041204		
2.482	0.04347		
2.848	0.013733		

2.494	0.041858	4.023723	
3.051	0.004947		
3.095	0.004428		
3.263	0.0029		
3.241	0.003065		
3.684	0.001004		
2.873	0.007745		
3.268	0.002864	4.050676	0.00256802

C3H8_Propane_Podsiadlo_JPhysChemC_117_4759_2013

1.514	0.915622		
2.515	0.03918		
0.959	0.961466		
0.96	0.959047		
0.96	0.959047		
2.046	0.062197		
2.046	0.062197		
2.713	0.01159		
2.703	0.011885		
3.332	0.002437	3.984666	0.00023512
1.498	0.962925		
1.514	0.915622		
0.97	0.93519		
0.97	0.93519		
2.03	0.064755		
2.045	0.062353		
2.046	0.062197		

2.031	0.064592		
2.045	0.062353		
2.031	0.064592	4.129768	0.01683976

C3H8_2_Propane_Podsiadlo_JPhysChemC_117_4759_2013

1.513	0.918509		
1.503	0.947886		
0.97	0.93519		
0.97	0.93519		
2.036	0.063783		
2.044	0.062511		
2.036	0.063783		
2.045	0.062353		
2.035	0.063944		
2.044	0.062511	4.11566	0.01337729
1.513	0.918509		
2.509	0.039927		
0.96	0.959047		
0.96	0.959047		
0.96	0.959047		
2.047	0.06204		
2.048	0.061884		
2.708	0.011737		
2.691	0.01225		
3.329	0.002456	3.985943	0.0001976
1.485	1.003153		

1.521	0.895664		
2.51	0.039802		
0.97	0.93519		
0.97	0.93519		
2.019	0.066574		
2.019	0.066574		
2.019	0.066574		
2.67	0.012916		
2.731	0.011076		
3.329	0.002456		
2.053	0.061109		
2.053	0.061109	4.157387	0.02477064
1.485	1.003153		
2.51	0.039802		
3.833	0.000618		
0.96	0.959047		
0.96	0.959047		
0.96	0.959047		
2.02	0.066406		
2.02	0.066406		
2.695	0.012127		
2.695	0.012127	4.077781	0.00604984

C98H126_Poly-ynes_Chalifoux_NatureChemistry_2_967_2010

1.362	1.477553	
1.201	2.452876	3.930429
2.552	0.034872	

2.563	0.033685		
3.472	0.001926		
4.169	0.000215		
4.735	3.61E-05	4.001162	
2.769	0.010065		
3.381	0.002154		
4.246	0.000244		
4.145	0.000314		
3.439	0.001861	4.015801	0.00024967
1.201	2.452876		
1.353	1.520018	3.972894	
2.563	0.033685		
2.556	0.034436		
3.219	0.004271		
4.631	5.01E-05	4.045335	
2.642	0.01386		
3.264	0.002893		
3.253	0.002974		
4.437	0.000151		
4.783	6.3E-05		
4.321	0.000202	4.065476	0.00428716
1.205	2.42218		
1.353	1.520018	3.942198	
2.568	0.033159		
2.552	0.034872		
3.441	0.002123	4.012352	
3.085	0.004541		

3.076	0.004645		
3.634	0.001139		
5.388	1.37E-05	4.02269	0.00051482
1.53	0.870642		
1.508	0.933082		
1.492	0.981288		
1.566	0.777351	3.562363	
2.53	0.037373		
2.566	0.033368		
3.811	0.000662		
3.855	0.000577		
4.308	0.000139	3.634482	
2.054	0.060956		
2.107	0.053338		
2.106	0.053472		
2.053	0.061109		
2.039	0.063303		
2.04	0.063144		
2.039	0.063303		
2.107	0.053338		
2.053	0.061109		
2.665	0.013079		
2.716	0.011503	4.192135	0.03691574

C30H16_Nobusue_OrganicLetters_16_1940_2014

1.2	2.460611	
1.436	1.17048	3.631091

2.476	0.044299		
2.442	0.049303		
3.248	0.003898		
3.39	0.002493		
3.486	0.001843		
2.994	0.008672		
3.292	0.003394		
3.016	0.008092		
3.071	0.006805		
3.248	0.003898		
2.626	0.027625		
3.716	0.000893		
3.732	0.000849		
4.015	0.000348		
4.241	0.000171	3.793675	
2.603	0.01529		
5.39	1.37E-05		
3.74	0.000872		
4.322	0.000201		
3.244	0.003042	3.813094	0.03493375
1.2	2.460611		
1.437	1.166801	3.627412	
2.635	0.026853		
2.399	0.056451		
2.518	0.038812		
3.533	0.001589		
3.032	0.007695		
3.023	0.007916		

3.138	0.005511		
3.297	0.003341		
3.57	0.001414		
3.755	0.00079		
3.717	0.00089		
3.695	0.000954		
4.217	0.000184		
3.391	0.002485	3.782297	
3.279	0.002785		
3.642	0.001116		
3.482	0.00167		
3.427	0.001919		
2.53	0.018377	3.808165	0.03680076

Shi_ChemRev_110_5883_2010

1.36	1.486886		
1.368	1.449904		
2.384	0.059181		
2.79	0.016484		
2.379	0.06012		
4.275	0.000154		
0.93	1.034331		
1.991	0.071439		
2.001	0.069662		
3.215	0.003273		
3.212	0.003297	4.25473	0.06488747
1.504	0.944907		

2.518	0.038812		
2.626	0.027625		
2.56	0.034005		
3.045	0.007386		
3.524	0.001635		
3.931	0.000454		
0.96	0.959047		
0.96	0.959047		
0.96	0.959047		
2.709	0.011707		
2.645	0.013755		
2.785	0.009667		
3.327	0.002468	3.96956	0.00092657
1.331	1.629029		
1.481	1.015866		
1.489	0.9906	3.635495	
2.602	0.029793		
2.489	0.042522		
2.52	0.038568		
2.521	0.038447		
2.498	0.041334		
3.765	0.000766		
3.781	0.000728		
3.783	0.000723		
3.773	0.000746		
4.279	0.000152		
4.282	0.00015	3.829425	
2.631	0.014249		

2.642	0.01386		
2.679	0.012626		
2.683	0.0125	3.882659	0.013769

Gagnon_OrganicLetters_12_380_2010

1.394	1.335949		
1.404	1.294545		
1.501	0.953873	3.584368	
2.437	0.050086		
2.431	0.051041		
2.518	0.038812		
3.24	0.003997		
2.508	0.040053		
2.506	0.040306		
3.279	0.003536		
2.53	0.037373		
3.506	0.00173		
2.803	0.015823		
3.778	0.000735		
3.833	0.000618		
3.796	0.000694	3.869172	
2.661	0.013212		
2.663	0.013145		
3.209	0.003322		
3.574	0.001325		
3.16	0.003759		
3.618	0.001186	3.905121	0.00900199

1.374	1.422773		
1.384	1.378678		
2.401	0.056097		
2.403	0.055744		
2.781	0.016958		
0.95	0.983512		
2.023	0.065906		
2.032	0.064429		
3.255	0.002959		
3.259	0.002929	4.049986	0.00249857

C30H34_Modjewski_OrganicLetters_11_4656_2009

1.535	0.857044	
1.561	0.789685	
1.553	0.809827	
1.544	0.833101	3.289656
2.548	0.035314	
2.589	0.031038	
3.061	0.007023	
3.131	0.005634	
2.642	0.026268	
3.854	0.000578	
3.846	0.000593	
4.381	0.00011	
4.244	0.000169	
4.332	0.000128	3.396512
2.091	0.055531	
2.092	0.055391	

2.685	0.012437		
2.086	0.056235		
2.087	0.056094		
2.086	0.056235		
2.093	0.055252		
2.094	0.055113		
2.093	0.055252	3.854052	0.02130073
1.393	1.340162		
1.392	1.344388		
2.477	0.044159		
2.526	0.037847		
3.033	0.00767		
2.375	0.060882		
2.741	0.019234		
2.431	0.051041		
3.619	0.001212		
3.846	0.000593		
0.95	0.983512		
2.694	0.012158		
2.823	0.008785		
2.864	0.007923		
3.306	0.002602		
3.239	0.003081		
3.619	0.001183	3.926431	0.00541243
1.544	0.833101		
2.473	0.044719		
2.489	0.042522		

2.55	0.035092		
2.837	0.014217		
0.98	0.911927		
0.98	0.911927		
0.98	0.911927		
2.397	0.025691		
2.899	0.007254		
2.422	0.024123		
3.934	0.000535		
2.625	0.014466		
2.703	0.011885		
3.343	0.002371	3.791756	0.04336565

C33H24_Wu_OrganicLetters_7_4353_2005

1.401	1.30683	
1.411	1.266328	
1.413	1.25838	3.831537
2.395	0.057166	
2.728	0.020037	
2.393	0.057527	
2.334	0.06927	
2.333	0.069488	
2.388	0.05844	
2.725	0.020227	
2.391	0.057891	4.241584
3.261	0.002915	
3.677	0.001022	
3.258	0.002937	

3.674	0.00103		
3.257	0.002944		
3.26	0.002922	4.255353	0.06520525
1.368	1.449904		
1.37	1.440804		
2.372	0.061459		
2.765	0.017834		
2.383	0.059367		
0.951	0.981038		
2.02	0.066406		
2.02	0.066406		
3.238	0.003088		
3.226	0.003183	4.14949	0.02234741

C2H2_acetylene_McMullan_ACB_48_726_1992

1.186	2.57149	
3.916	0.000476	
3.855	0.000577	
4.818	2.78E-05	
3.916	0.000476	
3.855	0.000577	
3.855	0.000577	
3.916	0.000476	
3.855	0.000577	
3.916	0.000476	
3.916	0.000476	
3.916	0.000476	
3.855	0.000577	2.577256

4.239	0.000248		
4.086	0.000365		
3.091	0.004472		
4.086	0.000365		
3.29	0.002709		
1.015	0.834969		
3.29	0.002709		
4.086	0.000365		
3.091	0.004472		
2.202	0.041986		
4.239	0.000248		
3.091	0.004472	3.474637	0.27600579

C2H2_2_acetylene_McMullan_ACB_48_726_1992

3.867	0.000555
3.926	0.000461
3.867	0.000555
3.867	0.000555
3.926	0.000461
3.926	0.000461
4.821	2.75E-05
3.867	0.000555
4.868	2.38E-05
3.926	0.000461
3.867	0.000555
4.868	2.38E-05
4.821	2.75E-05
3.926	0.000461
1.176	2.653736

3.867	0.000555		
4.821	2.75E-05		
3.926	0.000461		
4.868	2.38E-05		
4.821	2.75E-05		
4.821	2.75E-05		
4.868	2.38E-05		
4.868	2.38E-05		
4.821	2.75E-05	2.660118	
3.293	0.002689		
3.095	0.004428		
4.251	0.000241		
2.2	0.042198		
3.293	0.002689		
1.025	0.814199		
4.099	0.000353		
3.293	0.002689		
4.099	0.000353		
4.251	0.000241		
3.095	0.004428		
4.251	0.000241		
4.099	0.000353	3.535218	0.21602253

C5H10_Torrisi_JPhysChem_B_112_1184_2008

4.269	0.000157
4.668	4.46E-05
4.164	0.000218
1.533	0.862458
2.438	0.049928

3.794	0.000699	
1.542	0.838363	
4.139	0.000236	
3.894	0.00051	
2.436	0.050244	
4.168	0.000215	
4.084	0.00028	
3.973	0.000398	
4.694	4.11E-05	1.803791
4.647	8.88E-05	
4.166	0.000298	
4.615	9.62E-05	
3.366	0.002237	
3.51	0.001557	
2.071	0.0584	
2.824	0.008763	
1.032	0.799968	
4.518	0.000123	
2.12	0.051619	
3.36	0.002271	
3.055	0.004897	
3.08	0.004598	
2.073	0.058107	
4.203	0.000272	
3.482	0.00167	
0.973	0.928149	
3.293	0.002689	
2.124	0.051102	

4.61	9.74E-05		
2.776	0.009889		
4.966	3.97E-05		
3.881	0.000611		
3.438	0.001866		
4.686	8.05E-05		
4.078	0.000372		
3.232	0.003135		
4.346	0.000189		
4.307	0.000209		
4.74	7.02E-05	3.797256	0.04110495

C6H6_Benzene_Budzianowski_AC_B_62_94_2006

4.184	0.000205
4.221	0.000182
4.859	2.44E-05
4.087	0.000278
4.753	3.41E-05
4.77	3.23E-05
3.627	0.001182
4.957	1.8E-05
4.77	3.23E-05
3.885	0.000525
1.396	1.327564
2.379	0.06012
3.885	0.000525
3.776	0.000739
2.739	0.019355
1.353	1.520018

2.384	0.059181		
4.49	7.81E-05		
3.726	0.000866		
4.184	0.000205		
3.572	0.001406		
3.794	0.000699		
4.859	2.44E-05	2.993291	
4.518	0.000123		
3.578	0.001312		
4.935	4.3E-05		
3.035	0.00515		
4.678	8.21E-05		
3.758	0.000833		
3.14	0.003953		
3.726	0.000903		
1.992	0.071259		
0.993	0.882547		
4.862	5.17E-05		
1.96	0.077241		
3.28	0.002778		
3.661	0.001064		
3.414	0.001982		
3.252	0.002981		
4.502	0.000128		
2.879	0.007629		
4.016	0.000435	4.053788	0.00289316

C8H6_Dziubek_JACS_129_12620_2007

4.64	4.87E-05

4.64	4.87E-05	
3.687	0.000979	
3.66	0.001065	
4.784	3.1E-05	
2.432	0.05088	
4.205	0.000192	
1.456	1.099053	
4.165	0.000217	
3.66	0.001065	
4.957	1.8E-05	
2.396	0.056987	
3.65	0.0011	
1.179	2.62879	
3.987	0.000381	
4.538	6.72E-05	
3.999	0.000366	
4.868	2.38E-05	
3.445	0.002096	
4.728	3.69E-05	
4.636	4.93E-05	
4.958	1.79E-05	
3.766	0.000763	
4.927	1.97E-05	
4.453	8.78E-05	3.844383
4.891	4.8E-05	
4.53	0.000119	
2.974	0.006005	
4.393	0.000168	

4.04	0.00041		
2.588	0.015879		
3.912	0.000565		
3.632	0.001145		
3.138	0.003973		
3.814	0.000724		
2.102	0.054014		
4.205	0.00027		
4.404	0.000164		
4.772	6.48E-05		
3.317	0.002531		
2.571	0.016574		
3.914	0.000563		
4.912	4.55E-05	3.947644	0.00274111
4.998	1.58E-05		
4.926	1.98E-05		
4.045	0.000317		
4.025	0.000338		
4.779	3.14E-05		
2.347	0.066492		
1.391	1.348627		
2.751	0.018637		
3.955	0.000421		
4.703	3.99E-05		
4.549	6.49E-05		
2.317	0.073078		
1.456	1.099053		
1.344	1.563703		

2.633	0.027023		
4.823	2.74E-05		
3.446	0.00209		
4.728	3.69E-05		
3.44	0.00213		
4.051	0.000311		
4.029	0.000333		
4.493	7.74E-05		
4.433	9.35E-05	4.202959	
4.558	0.000111		
4.21	0.000267		
4.45	0.000146		
3.276	0.002806		
2.033	0.064267		
3.119	0.004168		
3.679	0.001017		
3.563	0.001362		
3.495	0.001616		
3.517	0.001529		
3.303	0.002622		
4.711	7.56E-05		
2.004	0.069138		
3.156	0.003797		
4.481	0.000135		
4.49	0.000132	4.356148	0.12684133

C10H8_fabbiani_AC_B_62_826_2006

4.366	0.000115	naphthalene
4.671	4.42E-05	

4.93	1.95E-05	
4.692	4.14E-05	
2.431	0.051041	
3.52	0.001656	
1.424	1.215546	
4.671	4.42E-05	
2.816	0.015188	
3.987	0.000381	
4.702	4.01E-05	
1.423	1.219379	
4.757	3.37E-05	
2.438	0.049928	
1.4	1.310951	
4.684	4.24E-05	
2.424	0.052178	
4.366	0.000115	
3.458	0.002012	
2.431	0.051041	
2.796	0.016176	
3.792	0.000703	
4.906	2.11E-05	3.986697
4.49	0.000132	
4.972	3.92E-05	
4.344	0.00019	
3.45	0.001811	
4.622	9.45E-05	
2.052	0.061264	
3.27	0.002849	

2.047	0.06204		
2.835	0.008523		
3.316	0.002537		
4.612	9.7E-05		
4.143	0.000316		
3.265	0.002885		
3.746	0.000859		
4.442	0.000149		
3.008	0.005512		
3.273	0.002828		
3.726	0.000903		
3.271	0.002842		
3.621	0.001177	4.143746	0.02066292
4.963	1.76E-05		
3.937	0.000445		
4.854	2.48E-05		
4.549	6.49E-05		
3.683	0.000991		
4.697	4.07E-05		
4.655	4.65E-05		
4.012	0.000352		
1.376	1.413843		
3.814	0.000656		
3.739	0.000831		
4.099	0.000267		
4.854	2.48E-05		
4.578	5.92E-05		
3.937	0.000445		

2.431	0.051041	
3.843	0.000599	
3.844	0.000597	
4.239	0.000172	
1.414	1.254424	
3.893	0.000512	
2.796	0.016176	
2.399	0.056451	
4.22	0.000183	
4.764	3.3E-05	
4.879	2.3E-05	2.798319
4.774	6.45E-05	
4.62	9.5E-05	
3.299	0.002648	
3.748	0.000855	
3.357	0.002288	
4.271	0.000229	
4.021	0.00043	
2.008	0.068444	
3.101	0.004361	
3.349	0.002335	
4.182	0.000286	
0.93	1.034331	
3.529	0.001484	
4.093	0.000358	
2.047	0.06204	
3.199	0.003407	
4.759	6.7E-05	

3.24	0.003073		
4.988	3.76E-05		
3.193	0.003459		
3.257	0.002944		
4.95	4.14E-05	3.991598	7.0597E-05

C16H10_fabbiani_AC_B_62_826_2006

4.185	0.000204
2.793	0.016329
2.429	0.051363
3.618	0.001216
2.429	0.051363
3.592	0.00132
1.421	1.227081
4.638	4.9E-05
3.97	0.000401
1.426	1.207917
2.454	0.047476
4.084	0.00028
4.895	2.18E-05
3.771	0.000751
2.46	0.046587
4.028	0.000334
3.522	0.001645
2.85	0.013647
4.545	6.57E-05
3.556	0.001478
1.444	1.141368
3.852	0.000582

2.8	0.015973		
2.5	0.041075		
4.86	2.44E-05		
2.466	0.045715		
3.901	0.000499		
4.143	0.000233		
3.761	0.000775		
4.189	0.000201		
3.743	0.00082		
4.237	0.000173	3.916971	
4.361	0.000182		
3.806	0.000738		
4.285	0.000221		
3.779	0.00079		
4.514	0.000124		
4.196	0.000276		
3.288	0.002723		
3.272	0.002835		
4.487	0.000133		
3.723	0.00091		
3.731	0.000892		
3.3	0.002642		
3.271	0.002842		
4.166	0.000298		
4.442	0.000149		
3.922	0.000551		
4.679	8.19E-05	3.933361	0.00444079
4.962	1.77E-05		

4.545	6.57E-05
4.705	3.97E-05
3.852	0.000582
4.166	0.000217
4.005	0.00036
3.566	0.001432
4.277	0.000153
3.766	0.000763
4.928	1.97E-05
3.805	0.000675
2.467	0.045572
2.5	0.041075
2.812	0.015381
1.426	1.207917
2.42	0.052839
2.865	0.013017
1.398	1.319231
2.425	0.052014
1.443	1.144968
4.648	4.75E-05
4.126	0.000246
4.69	4.16E-05
3.562	0.001451
3.74	0.000828
4.189	0.000201
3.618	0.001216
4.895	2.18E-05
3.973	0.000398

3.852	0.000582		
4.028	0.000334		
4.596	5.59E-05	3.901761	
4.113	0.000341		
3.542	0.001436		
4.224	0.000258		
4.522	0.000122		
4.474	0.000137		
3.503	0.001584		
4.689	7.99E-05		
4.966	3.97E-05		
3.254	0.002966		
4.506	0.000127		
2.026	0.06541		
2.067	0.058992		
3.259	0.002929		
4.799	6.05E-05		
4.941	4.23E-05		
4.491	0.000132		
4.494	0.000131		
4.578	0.000106	4.036653	0.00134344

C18H24_Ioannou_AC_E_68_o2150_2012

4.907	2.1E-05
4.504	7.47E-05
2.498	0.041334
4.183	0.000205
4.912	2.07E-05
4.425	9.58E-05

2.576	0.032334	
1.543	0.835728	
3.583	0.001358	
2.926	0.010743	
3.774	0.000744	
3.091	0.00639	
2.497	0.041465	
4.387	0.000108	
3.693	0.00096	
1.515	0.912744	
3.988	0.000379	
4.033	0.000329	
4.701	4.02E-05	
3.83	0.000624	
4.849	2.52E-05	
2.526	0.037847	
4.425	9.58E-05	
4.103	0.000264	
3.043	0.007433	
3.938	0.000444	
4.893	2.2E-05	1.931828
4.662	8.55E-05	
4.759	6.7E-05	
4.973	3.91E-05	
3.947	0.000518	
4.912	4.55E-05	
3.856	0.000651	
3.416	0.001972	

3.344	0.002365
2.094	0.055113
2.834	0.008545
4.259	0.000236
2.671	0.012883
4.267	0.000231
3.055	0.004897
3.427	0.001919
3.834	0.000688
4.388	0.00017
3.732	0.00089
4.246	0.000244
4.214	0.000264
0.985	0.900513
1.012	0.841303
2.741	0.0108
3.443	0.001843
3.869	0.00063
4.895	4.75E-05
2.627	0.014393
3.371	0.002209
3.969	0.00049
3.066	0.004763
4.723	7.33E-05
3.76	0.000829
4.154	0.000307
3.798	0.000754
4.878	4.96E-05

3.91	0.000568		
4.525	0.000121		
4.512	0.000125	3.80347	0.03862414