Supplementary data

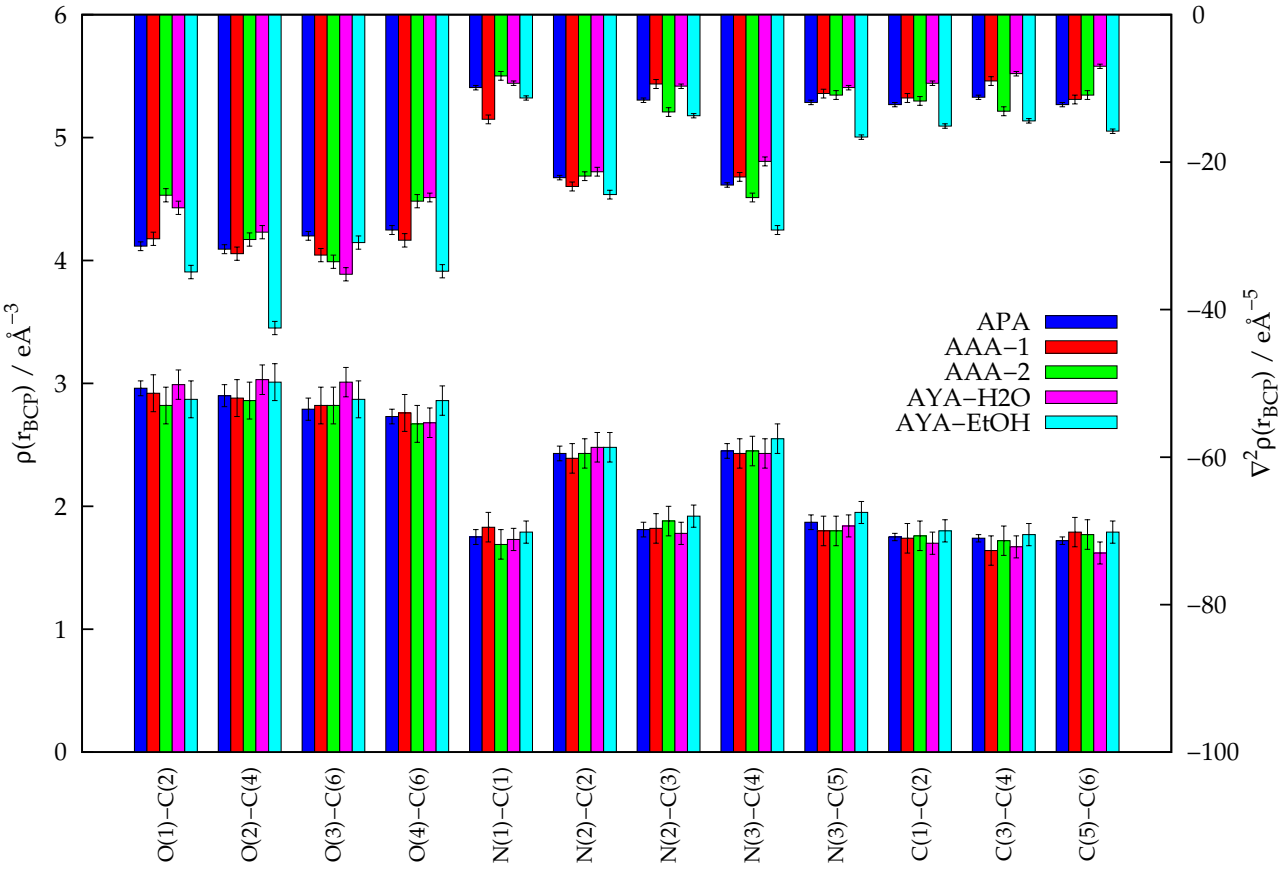

Figure 1: Comparison of bond topological parameters for several tripeptides, error bars 3× esd: Visualization of Table 4 of the paper.

Table 1: Comparison of refined multipole model with invariom approach: Data of Figure 3 of the paper.

	ref		*inv*		*inv083*	
Bond	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$
O(1)–C(2)	2.96(2)	−31.4(2)	2.88	−33.8	2.88	−34.1
O(2)–C(4)	2.90(2)	−31.8(2)	2.60	−30.1	2.61	−29.9
O(3)–C(6)	2.79(3)	−30.0(2)	2.66	−31.3	2.67	−31.5
O(4)–C(6)	2.73(2)	−29.2(2)	2.66	−31.0	2.66	−31.0
N(1)–C(1)	1.75(2)	−9.9(1)	1.75	−9.6	1.74	−9.5
N(2)–C(2)	2.43(2)	−22.1(1)	2.23	−22.4	2.24	−22.6
N(2)–C(3)	1.81(2)	−11.6(1)	1.74	−8.4	1.74	−8.3
N(2)–C(22)	1.74(2)	−9.1(1)	1.72	−9.6	1.72	−9.7
N(3)–C(4)	2.45(2)	−23.1(1)	2.29	−22.6	2.30	−23.0
N(3)–C(5)	1.87(2)	−11.9(1)	1.80	−10.1	1.79	−10.0
C(1)–C(7)	1.66(2)	−9.4(1)	1.66	−10.8	1.66	−10.9
C(2)–C(1)	1.75(1)	−12.1(1)	1.71	−12.1	1.71	−12.1
C(3)–C(20)	1.65(2)	−10.6(1)	1.62	−10.3	1.62	−10.3
C(4)–C(3)	1.74(1)	−11.2(1)	1.77	−11.4	1.76	−11.2
C(5)–C(8)	1.63(1)	−9.4(1)	1.63	−10.2	1.62	−10.2
C(6)–C(5)	1.72(1)	−12.2(1)	1.69	−12.8	1.69	−12.8
C(20)–C(21)	1.62(2)	−8.8(1)	1.60	−9.9	1.61	−9.9
C(21)–C(22)	1.64(2)	−9.2(1)	1.65	−11.1	1.65	−11.1
N(1)–H(11A)	2.22(5)	−33.7(3)	2.22	−33.8	2.22	−33.7
N(1)–H(11B)	2.28(5)	−33.7(3)	2.22	−33.8	2.22	−33.8
N(1)–H(11C)	2.22(5)	−33.1(3)	2.22	−33.7	2.22	−33.7
N(3)–H(13)	2.30(6)	−30.0(4)	2.29	−33.2	2.29	−33.1
C(1)–H(1)	1.97(4)	−19.7(2)	1.88	−20.7	1.88	−20.7
C(3)–H(3)	1.94(4)	−18.7(2)	1.88	−20.7	1.88	−20.7
C(5)–H(5)	1.93(5)	−18.2(2)	1.88	−20.7	1.88	−20.7
C(7)–H(7A)	1.91(0)	−15.7(1)	1.95	−22.4	1.95	−22.4
C(7)–H(7B)	1.90(0)	−15.7(1)	1.95	−22.4	1.96	−22.4
C(7)–H(7C)	1.90(0)	−15.7(1)	1.95	−22.3	1.95	−22.3
C(8)–H(8A)	1.90(3)	−15.7(1)	1.96	−22.4	1.96	−22.4
C(8)–H(8B)	1.90(1)	−15.6(1)	1.95	−22.2	1.95	−22.3
C(8)–H(8C)	1.90(1)	−15.7(1)	1.95	−22.3	1.95	−22.3
C(20)–H(20A)	1.89(4)	−17.4(1)	1.88	−20.6	1.87	−20.5
C(20)–H(20B)	1.88(2)	−17.2(1)	1.87	−20.6	1.87	−20.6
C(21)–H(21A)	1.94(4)	−18.5(1)	1.87	−20.6	1.88	−20.7
C(21)–H(21B)	1.94(2)	−18.4(1)	1.88	−20.7	1.88	−20.7
C(22)–H(22A)	1.90(4)	−16.8(1)	1.90	−21.6	1.89	−21.6
C(22)–H(22B)	1.90(2)	−16.7(1)	1.92	−22.3	1.92	−22.4
O(100)–H(101)	2.37(7)	−38.0(5)	2.48	−48.4	2.48	−48.3
O(100)–H(102)	2.50(8)	−41.0(6)	2.48	−48.3	2.48	−48.4

Table 2: Topological Parameters of Bonds Formed by Non-Hydrogen-Atoms

Bindung	$\rho(r)$	$\nabla^2\rho(r)$	R_{ij}	d_1	d_2	ϵ
O(1)–C(2)	2.96	−31.4	1.240	0.740	0.500	0.09
	2.74	−17.4		0.809	0.431	0.12
	2.80	−28.4		0.740	0.500	0.12
O(2)–C(4)	2.90	−31.8	1.243	0.756	0.487	0.07
	2.70	−16.5		0.813	0.430	0.09
	2.74	−27.8		0.756	0.487	0.10
O(3)–C(6)	2.79	−30.0	1.266	0.768	0.498	0.08
	2.57	−18.2		0.826	0.440	0.09
	2.61	−26.8		0.767	0.499	0.11
O(4)–C(6)	2.73	−29.2	1.271	0.766	0.505	0.09
	2.56	−20.0		0.826	0.445	0.11
	2.60	−26.8		0.765	0.506	0.12
N(1)–C(1)	1.75	−9.9	1.495	0.821	0.674	0.05
	1.59	−13.6		0.939	0.556	0.01
	1.65	−11.6		0.821	0.674	0.00
N(2)–C(2)	2.43	−22.1	1.354	0.772	0.582	0.30
	2.26	−25.4		0.832	0.522	0.25
	2.28	−23.2		0.772	0.582	0.28
N(2)–C(3)	1.81	−11.6	1.475	0.820	0.655	0.10
	1.70	−15.5		0.899	0.577	0.03
	1.73	−13.1		0.820	0.655	0.05
N(2)–C(22)	1.74	−9.1	1.485	0.831	0.654	0.03
	1.68	−15.0		0.891	0.594	0.04
	1.70	−13.0		0.830	0.655	0.06
N(3)–C(4)	2.45	−23.1	1.346	0.757	0.590	0.23
	2.32	−26.6		0.826	0.520	0.25
	2.34	−23.9		0.757	0.590	0.28
N(3)–C(5)	1.87	−11.9	1.462	0.818	0.644	0.07
	1.72	−15.8		0.912	0.550	0.01
	1.75	−13.8		0.817	0.645	0.04
C(1)–C(7)	1.66	−9.4	1.534	0.779	0.755	0.03
	1.63	−13.2		0.810	0.724	0.01
	1.63	−13.0		0.779	0.755	0.02
C(2)–C(1)	1.75	−12.1	1.537	0.783	0.754	0.10
	1.70	−14.5		0.753	0.784	0.09
	1.70	−14.5		0.782	0.755	0.09
C(3)–C(20)	1.65	−10.6	1.547	0.793	0.754	0.05
	1.61	−12.8		0.791	0.757	0.02
	1.61	−12.8		0.794	0.753	0.02
C(4)–C(3)	1.74	−11.2	1.539	0.775	0.764	0.11
	1.69	−14.4		0.762	0.776	0.07
	1.69	−14.4		0.775	0.763	0.07
C(5)–C(8)	1.63	−9.4	1.546	0.783	0.763	0.07
	1.60	−12.7		0.784	0.762	0.04
	1.60	−12.7		0.782	0.764	0.04
C(6)–C(5)	1.72	−12.2	1.544	0.779	0.764	0.07
	1.68	−14.1		0.750	0.794	0.08
	1.68	−14.1		0.779	0.764	0.09
C(20)–C(21)	1.62	−8.8	1.540	0.771	0.769	0.07
	1.62	−12.8		0.763	0.777	0.00
	1.62	−12.8		0.772	0.769	0.00
C(21)–C(22)	1.64	−9.2	1.538	0.765	0.772	0.02
	1.64	−13.5		0.744	0.794	0.02
	1.64	−13.4		0.766	0.772	0.02

ρ in eÅ^{-3}, $\nabla^2\rho$ in eÅ^{-5}, d und R-l in Å

The first entry for each bond refers to multipole model,

second to results of analyzing the theoretic density,

third to topological parameters of the theoretical density, obtained at the experimental location of the BCP

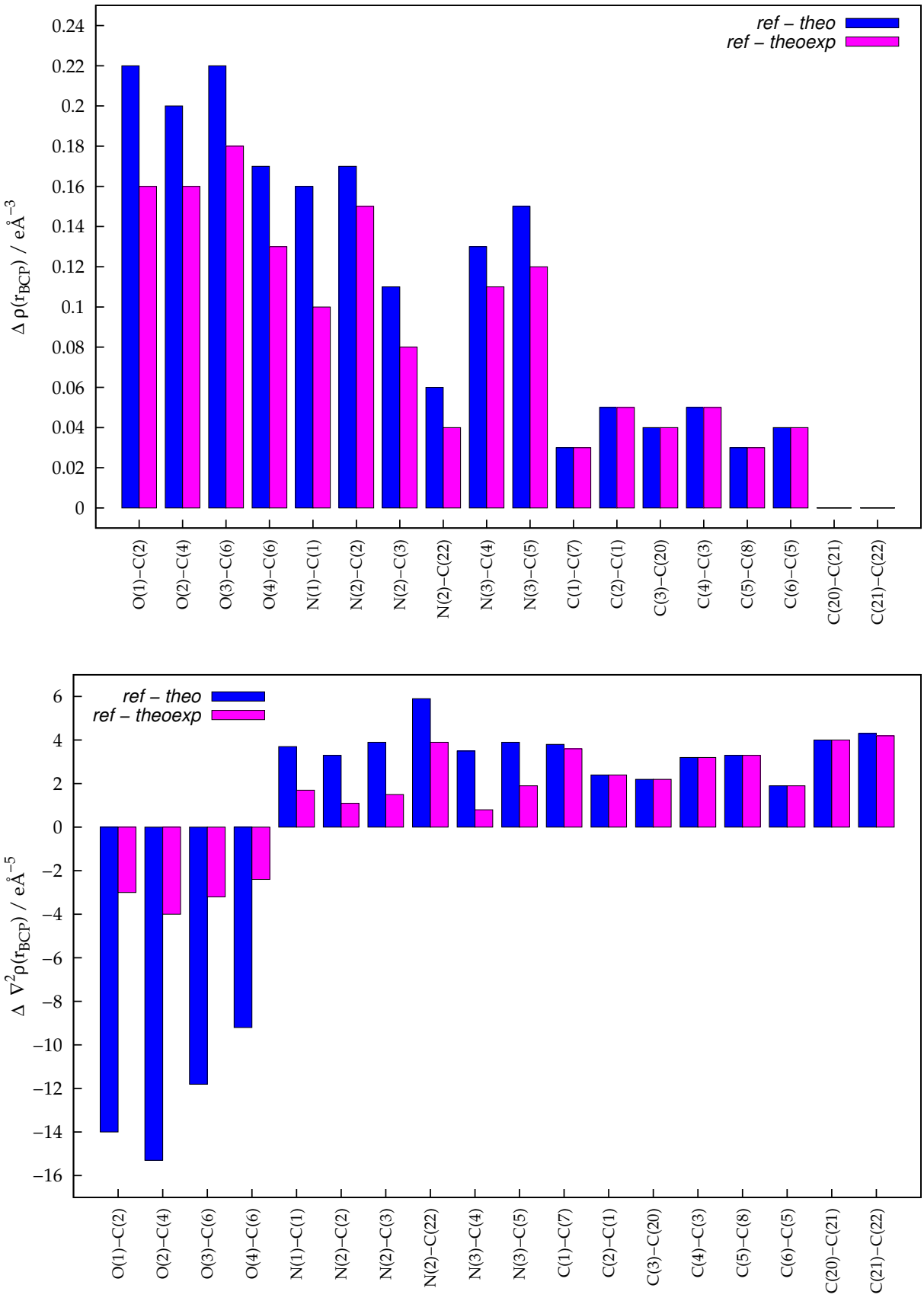

Figure 2: Differences between model *ref* and theory for topological properties of bonds formed by non-hydrogen-atoms (*theoexp*: theoretical density, obtained at the experimental location of the bcp); mean deviations in ρ: 0.10 eÅ^{-3} for *theo*, 0.08 eÅ^{-3} for *theoexp*, in $\nabla^2\rho$: 5.53 eÅ^{-5} for *theo*, 2.68 eÅ^{-5} for *theoexp*.

Table 3: Atomic Properties *ref* (every first row), *inv* (every second row), *sam* (every third row) and *theo* (every fourth row): Complete integration data. Units are Å^3, e, au.

Atom	V_{tot}	V_{001}	N	Q	VNEO	DM	Atom	V_{tot}	V_{001}	N	Q	VNEO	DM
O(1)	19.486	17.905	9.005	-1.005	-185.700	0.185	H(1)	6.384	5.242	0.935	0.065	-1.302	0.031
	18.090	17.824	8.854	-0.854	-184.167	0.199		7.096	6.671	1.006	-0.006	-1.301	0.138
	15.602	15.602	8.547	-0.547	-181.578	0.163		6.426	6.348	0.871	0.129	-1.027	0.323
	74.876	19.771	9.135	-1.135	-151.429	0.408		35.089	6.325	0.968	0.032	-1.255	0.124
O(2)	18.657	17.224	9.052	-1.052	-185.886	0.278	H(3)	7.269	6.383	1.042	-0.042	-1.421	0.021
	17.036	16.764	8.808	-0.808	-183.834	0.182		7.610	7.475	1.009	-0.009	-1.302	0.145
	14.492	14.492	8.567	-0.567	-181.661	0.151		6.943	6.943	0.874	0.126	-1.025	0.334
	49.812	19.094	9.206	-1.206	-151.485	0.333		38.284	6.953	0.986	0.014	-1.262	0.132
O(3)	16.857	15.410	9.055	-1.055	-185.910	0.221	H(5)	8.039	7.816	1.009	-0.009	-1.363	0.031
	15.600	15.330	8.950	-0.950	-184.472	0.208		7.599	6.155	0.996	0.004	-1.300	0.151
	12.615	12.615	8.560	-0.560	-181.599	0.107		7.462	7.462	0.872	0.128	-1.022	0.337
	173.363	21.588	9.248	-1.248	-151.385	0.227		44.390	6.972	0.982	0.018	-1.253	0.136
O(4)	18.318	16.142	9.114	-1.114	-186.302	0.208	H(7A)	7.564	6.478	1.052	-0.052	-1.431	0.044
	16.799	16.038	8.918	-0.918	-184.335	0.214		7.260	7.016	0.961	0.039	-1.265	0.147
	13.753	13.684	8.557	-0.557	-181.568	0.109		6.625	6.625	0.868	0.132	-1.026	0.340
	195.595	22.294	9.213	-1.213	-151.288	0.246		42.947	7.417	0.996	0.004	-1.290	0.131
N(1)	13.244	11.783	7.967	-0.967	-135.322	0.165	H(7B)	6.754	6.026	1.056	-0.056	-1.433	0.042
	12.408	12.047	7.875	-0.875	-134.380	0.071		6.490	6.275	0.961	0.039	-1.267	0.143
	12.949	12.925	7.931	-0.932	-133.465	0.292		6.044	6.044	0.864	0.136	-1.026	0.330
	40.031	12.532	7.925	-0.925	-110.180	0.032		13.403	5.932	0.928	0.072	-1.232	0.106
N(2)	10.762	10.720	7.933	-0.933	-135.254	0.147	H(7C)	6.850	6.035	1.053	-0.053	-1.432	0.041
	10.514	10.514	7.868	-0.868	-134.106	0.064		6.482	6.242	0.962	0.038	-1.267	0.145
	9.192	9.192	7.578	-0.578	-132.315	0.050		6.083	6.040	0.863	0.137	-1.025	0.330
	15.985	11.034	8.083	-1.083	-110.500	0.186		66.213	7.298	1.035	-0.035	-1.323	0.137
N(3)	13.012	12.651	7.951	-0.951	-135.368	0.115	H(8A)	7.497	6.160	1.050	-0.050	-1.429	0.038
	12.479	12.476	7.870	-0.870	-134.546	0.068		7.209	6.776	0.956	0.044	-1.263	0.142
	11.607	11.607	7.699	-0.699	-132.682	0.237		6.474	6.474	0.863	0.137	-1.024	0.333
	21.616	13.517	8.115	-1.115	-110.562	0.178		65.369	7.319	1.019	-0.019	-1.303	0.143
C(1)	6.933	6.908	5.848	0.152	-90.503	0.366	H(8B)	7.318	6.227	1.055	-0.055	-1.432	0.045
	6.720	6.719	5.758	0.242	-89.721	0.306		6.946	6.710	0.960	0.040	-1.265	0.150
	7.887	7.886	5.969	0.031	-89.657	0.346		6.642	6.642	0.869	0.131	-1.027	0.344
	12.308	7.689	5.757	0.243	-75.574	0.394		44.177	7.820	1.060	-0.060	-1.347	0.147
C(2)	6.147	6.092	5.035	0.965	-87.322	0.570	H(8C)	7.145	6.456	1.056	-0.056	-1.433	0.044
	6.311	6.311	4.963	1.037	-86.475	0.588		6.867	6.662	0.959	0.041	-1.264	0.144
	7.259	7.259	5.248	0.752	-87.009	0.501		6.411	6.366	0.867	0.133	-1.026	0.334
	11.081	6.276	4.632	1.368	-74.260	0.616		64.291	7.553	1.041	-0.041	-1.325	0.147
C(3)	6.626	6.580	5.716	0.284	-89.871	0.325	H(11A)	2.142	1.982	0.453	0.547	-0.791	0.063
	6.698	6.698	5.725	0.275	-89.603	0.317		2.835	2.804	0.536	0.464	-0.865	0.097
	7.949	7.949	5.949	0.051	-89.605	0.387		3.936	3.936	0.698	0.302	-0.897	0.277
	7.083	6.673	5.657	0.343	-75.526	0.479		37.787	4.111	0.559	0.441	-0.886	0.140
C(4)	6.119	5.974	4.983	1.017	-87.005	0.582	H(11B)	2.110	2.085	0.499	0.501	-0.858	0.070
	6.535	6.517	5.060	0.940	-86.817	0.779		2.798	2.768	0.538	0.462	-0.868	0.094
	7.361	7.361	5.248	0.752	-87.018	0.488		3.928	3.928	0.692	0.308	-0.893	0.258
	7.307	5.481	4.603	1.397	-74.244	0.641		30.587	4.031	0.539	0.461	-0.858	0.138
C(5)	6.952	6.945	5.760	0.240	-90.085	0.350	H(11C)	2.019	1.933	0.474	0.526	-0.819	0.069
	6.922	6.922	5.764	0.236	-89.738	0.338		2.768	2.669	0.537	0.463	-0.867	0.094
	8.263	8.263	5.946	0.054	-89.575	0.371		3.697	3.697	0.691	0.309	-0.894	0.253
	18.794	10.345	6.071	-0.071	-75.767	1.536		41.742	4.278	0.583	0.417	-0.914	0.143
C(6)	5.797	5.610	4.731	1.269	-85.893	0.588	H(13)	4.341	3.210	0.564	0.436	-0.916	0.112
	6.212	6.127	4.788	1.212	-85.707	0.598		4.580	4.106	0.606	0.394	-0.936	0.146
	7.395	7.374	5.096	0.904	-86.381	0.494		5.371	5.371	0.708	0.292	-0.892	0.352
	8.364	5.181	4.362	1.638	-73.885	0.632		13.061	3.845	0.576	0.424	-0.910	0.167
C(7)	9.388	8.645	5.721	0.279	-89.857	0.015	H(20A)	6.334	5.660	0.954	0.046	-1.323	0.014
	10.225	9.980	6.087	-0.087	-91.036	0.042		6.763	6.755	0.982	0.018	-1.280	0.129
	12.626	12.624	6.366	-0.366	-90.807	0.283		6.137	6.137	0.871	0.129	-1.026	0.324
	19.276	9.602	5.872	0.128	-75.890	0.076		27.137	6.993	1.007	-0.007	-1.276	0.129
C(8)	9.417	8.902	5.727	0.273	-89.870	0.033	H(20B)	6.515	5.902	0.955	0.045	-1.320	0.017
	10.416	10.256	6.093	-0.093	-91.035	0.023		7.172	7.060	0.980	0.020	-1.277	0.128
	13.073	13.043	6.363	-0.364	-90.781	0.274		6.772	6.772	0.874	0.126	-1.026	0.326
	25.337	9.522	5.867	0.133	-75.876	0.033		56.571	7.310	0.978	0.022	-1.236	0.126
C(20)	8.415	8.274	5.881	0.119	-90.538	0.072	H(21A)	7.192	5.852	1.014	-0.014	-1.402	0.033
	8.565	8.538	6.001	-0.001	-90.595	0.101		7.794	7.342	0.981	0.019	-1.277	0.131
	10.347	10.347	6.228	-0.228	-90.406	0.349		7.197	7.179	0.877	0.123	-1.026	0.335
	13.802	8.638	5.918	0.082	-75.803	0.086		69.736	7.371	1.004	-0.004	-1.259	0.133
C(21)	8.161	7.990	5.811	0.189	-90.264	0.016	H(21B)	6.889	5.894	1.017	-0.017	-1.405	0.027
	8.678	8.672	6.006	-0.006	-90.621	0.082		7.514	7.415	0.985	0.015	-1.280	0.137
	10.402	10.402	6.231	-0.231	-90.412	0.346		7.094	7.094	0.872	0.128	-1.024	0.335
	16.382	8.776	5.911	0.089	-75.781	0.088		62.642	7.393	1.019	-0.019	-1.281	0.136
C(22)	8.059	7.802	5.668	0.332	-89.663	0.406	H(22A)	6.237	5.735	0.992	0.008	-1.361	0.036
	7.995	7.978	5.765	0.235	-89.624	0.371		6.480	6.328	0.986	0.014	-1.283	0.135
	9.931	9.931	6.082	-0.082	-89.924	0.481		5.847	5.847	0.873	0.127	-1.028	0.318
	11.081	7.704	5.639	0.361	-75.478	0.443		26.112	6.774	0.992	0.008	-1.270	0.125
O(100)	23.193	19.318	9.037	-1.037	-185.565	0.190	H(22B)	6.277	5.861	0.990	0.010	-1.359	0.037
	21.046	19.632	8.975	-0.975	-184.583	0.229		6.612	6.505	0.985	0.015	-1.283	0.142
	18.756	18.619	8.743	-0.744	-182.209	0.336		6.152	6.152	0.870	0.130	-1.026	0.318
	140.168	22.188	9.195	-1.195	-151.198	0.279		47.569	7.051	1.030	-0.030	-1.300	0.132
H(101)	2.666	2.651	0.473	0.527	-0.707	0.076							
	1.829	1.769	0.382	0.618	-0.782	0.131							
	3.753	3.753	0.606	0.394	-0.800	0.279							
	2.417	2.009	0.368	0.632	-0.679	0.127							
H(102)	1.890	1.777	0.396	0.604	-0.738	0.071	$\sum$	334.975	306.240	148.084	-0.084	-2341.853	5.794
	2.734	2.715	0.475	0.525	-0.782	0.139		332.687	323.561	147.871	0.129	-2329.669	7.588
	3.733	3.733	0.613	0.387	-0.803	0.294		334.186	333.718	147.964	0.033	-2309.210	12.439
	30.725	3.828	0.458	0.542	-0.782	0.179		1722.510	356.488	148.537	-0.537	-1940.350	9.791

Table 4: Bond topological properties: Additional data to Table 10 of the paper.

D–H$\cdots$A	$\mathbf{R_{ij}}$	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	$\lambda\mathbf{1}$	$\lambda\mathbf{2}$	$\lambda\mathbf{3}$	ϵ
O(100)–H(101)$\cdots$O(2)	1.921	0.13(2)	2.12(4)	-0.83	-0.81	3.76	0.02
	1.921	0.16	2.29	-0.72	-0.70	3.71	0.02
	1.920	0.22(1)	2.34(1)	-1.03	-1.02	4.39	0.01
O(100)–H(102)$\cdots$O(3)	1.972	0.10(1)	1.98(3)	-0.62	-0.57	3.16	0.09
	1.975	0.14	1.91	-0.63	-0.60	3.14	0.05
	1.972	0.19(1)	2.11(1)	-0.86	-0.84	3.80	0.03
N(1)–H(11A)$\cdots$O(3)	1.874	0.16(1)	2.46(2)	-1.00	-0.81	4.27	0.24
	1.878	0.17	2.79	-0.88	-0.83	4.50	0.06
	1.873	0.25(1)	2.62(1)	-1.17	-1.11	4.90	0.05
N(1)–H(11B)$\cdots$O(4)	1.818	0.23(1)	2.06(3)	-1.55	-1.49	5.09	0.04
	1.817	0.19	3.12	-1.06	-1.04	5.22	0.02
	1.816	0.28(1)	2.85(1)	-1.41	-1.39	5.65	0.01
N(1)–H(11C)$\cdots$O(4)	1.816	0.22(2)	2.27(3)	-1.53	-1.45	5.25	0.06
	1.824	0.19	3.17	-1.10	-1.07	5.35	0.03
	1.814	0.29(1)	2.85(1)	-1.54	-1.47	5.86	0.05
C(7)–H(7B)$\cdots$O(100)	2.579	0.04(1)	0.68(1)	-0.13	-0.12	0.92	0.09
	2.582	0.04	0.67	-0.16	-0.14	0.96	0.13
	2.578	0.06(1)	0.73(1)	-0.18	-0.17	1.07	0.06
C(7)–H(7C)$\cdots$O(3)	2.485	0.04(1)	0.84(1)	-0.17	-0.15	1.16	0.10
	2.479	0.05	0.81	-0.20	-0.17	1.17	0.16
	2.481	0.07(1)	0.85(1)	-0.23	-0.21	1.29	0.10
C(8)–H(8A)$\cdots$O(1)	2.594	0.03(2)	0.66(1)	-0.13	-0.12	0.91	0.07
	2.583	0.04	0.65	-0.14	-0.12	0.91	0.18
	2.589	0.06(1)	0.71(1)	-0.18	-0.18	1.07	0.04

Table 5: Mutual Penetration: Additional data to Table 10 of the paper.

D–H$\cdots$A	R_{ij}	$r_b(H)$	$\Delta r(H)$	$r_b(O)$	$\Delta r(O)$	$\Delta r(H)+\Delta r(O)$	$\frac{\Delta r(H)}{\Delta r(H)+\Delta r(O)}$
H(101)-O(2)	1.921	0.664	-0.536	1.256	-0.264	-0.799	0.6700
H(102)-O(3)	1.972	0.692	-0.508	1.280	-0.239	-0.748	0.6797
H(11A)-O(3)	1.874	0.658	-0.542	1.216	-0.304	-0.846	0.6403
H(11B)-O(4)	1.818	0.641	-0.559	1.176	-0.344	-0.902	0.6191
H(11C)-O(4)	1.816	0.628	-0.572	1.188	-0.332	-0.904	0.6329
H(7B)-O(100)	2.579	1.059	-0.141	1.520	0.000	-0.141	1.0000
H(7C)-O(3)	2.485	1.021	-0.179	1.464	-0.057	-0.235	0.7599
H(8A)-O(1)	2.594	1.077	-0.123	1.517	-0.003	-0.126	0.9785
H(101)-O(2)	1.921	0.693	-0.507	1.228	-0.292	-0.799	0.6349
H(102)-O(3)	1.975	0.729	-0.471	1.246	-0.274	-0.745	0.6327
H(11A)-O(3)	1.877	0.684	-0.516	1.194	-0.326	-0.843	0.6129
H(11B)-O(4)	1.817	0.643	-0.557	1.175	-0.345	-0.903	0.6173
H(11C)-O(4)	1.824	0.641	-0.558	1.182	-0.338	-0.896	0.6230
H(7B)-O(100)	2.582	1.078	-0.122	1.504	-0.016	-0.138	0.8832
H(7C)-O(3)	2.479	1.039	-0.161	1.440	-0.080	-0.241	0.6682
H(8A)-O(1)	2.583	1.099	-0.101	1.484	-0.036	-0.137	0.7385
H(101)-O(2)	1.920	0.762	-0.438	1.159	-0.361	-0.800	0.5481
H(102)-O(3)	1.972	0.800	-0.400	1.172	-0.348	-0.748	0.5350
H(11A)-O(3)	1.873	0.740	-0.460	1.133	-0.387	-0.847	0.5433
H(11B)-O(4)	1.816	0.700	-0.500	1.116	-0.404	-0.904	0.5532
H(11C)-O(4)	1.814	0.691	-0.509	1.124	-0.396	-0.906	0.5623
H(7B)-O(100)	2.578	1.136	-0.064	1.442	-0.078	-0.142	0.4531
H(7C)-O(3)	2.481	1.096	-0.104	1.385	-0.135	-0.239	0.4351
H(8A)-O(1)	2.589	1.149	-0.051	1.440	-0.080	-0.131	0.3876

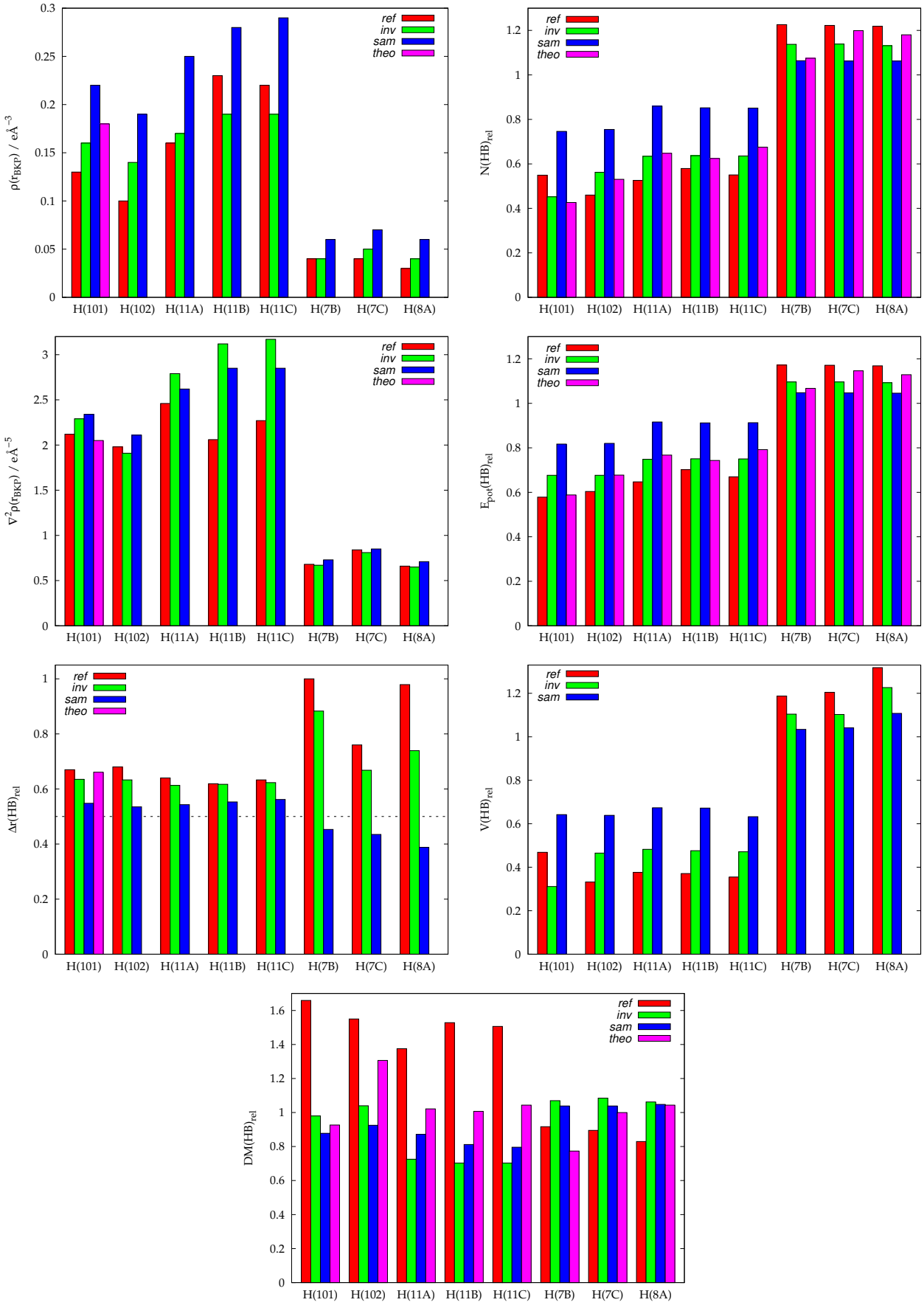

Figure 3: Visualization of the Koch and Popelier paramter from Table 10 of the paper.