

Supplementary Material

Table S1: The electron charge density, $\rho(r)$, its $\nabla^2\rho(r)$, ellipticity, ϵ of structures **2a,b**, **4a,b** and **6a,c** for the different BCPs at the B3LYP/6-311+G** level

	$\rho(r)$ (e/a_o^3)	$\nabla^2\rho(r)$ (e/a_o^5)	ϵ	$\rho(r)$ (e/a_o^3)	$\nabla^2\rho(r)$ (e/a_o^5)	ϵ
	2a			2b		
N ₁ -C ₂	-0.808	0.091	-0.412	-0.994	0.321	-0.575
C ₂ -N ₃	-1.117	0.230	-0.582	-0.788	0.140	-0.421
N ₃ -C _{3a}	-0.913	0.102	-0.367	-0.873	0.179	-0.408
C _{3a} -N ₄	-1.187	0.225	-0.565	-1.204	0.215	-0.549
N ₄ -C ₅	-0.857	0.055	-0.358	-0.839	0.063	-0.355
C ₅ -C ₆	-0.661	0.121	-0.234	-0.658	0.124	-0.233
C ₆ -C ₇	-0.976	0.327	-0.379	-0.976	0.327	-0.378
C ₇ -N ₈	-0.602	0.066	-0.408	-0.618	0.053	-0.415
N ₈ -N ₁	-0.575	0.157	-0.297	-0.585	0.093	-0.318
C _{3a} -N ₈	-0.753	0.134	-0.396	-0.884	0.187	-0.427
C ₅ -O ₅	-0.257	0.099	-0.688	-0.270	0.098	-0.687
	4a			4b		
N ₁ -C ₂	0.313	-0.663	0.140	0.377	-1.020	0.316
C ₂ -N ₃	0.369	-1.130	0.218	0.304	-0.761	0.135
N ₃ -C _{3a}	0.327	-0.983	0.141	0.312	-0.881	0.191
C _{3a} -N ₄	0.368	-1.181	0.194	0.375	-1.197	0.205
N ₄ -C ₅	0.327	-0.965	0.074	0.318	-0.931	0.063
C ₅ -C ₆	0.315	-0.873	0.263	0.322	-0.911	0.287
C ₆ -C ₇	0.292	-0.788	0.207	0.285	-0.753	0.183
C ₇ -N ₈	0.268	-0.609	0.046	0.262	-0.641	0.054
N ₈ -N ₁	0.359	-0.686	0.201	0.343	-0.591	0.080
C _{3a} -N ₈	0.303	-0.712	0.153	0.319	-0.906	0.205
C ₇ -O ₇	0.404	-0.376	0.101	0.415	-0.264	0.101
	6a			6b		
N ₁ -C ₂	0.300	-0.820	0.087	0.372	-0.978	0.319
C ₂ -N ₃	0.384	-1.106	0.235	0.308	-0.798	0.144
N ₃ -C _{3a}	0.310	-0.901	0.098	0.304	-0.862	0.177
C _{3a} -N ₄	0.388	-1.189	0.239	0.389	-1.217	0.231
N ₄ -C ₅	0.292	-0.830	0.048	0.288	-0.803	0.055
C ₅ -C ₆	0.271	-0.670	0.149	0.272	-0.673	0.166
C ₆ -C ₇	0.327	-0.931	0.368	0.323	-0.911	0.367
C ₇ -N ₈	0.296	-0.747	0.126	0.297	-0.758	0.114
N ₈ -N ₁	0.328	-0.556	0.142	0.340	-0.574	0.094
C _{3a} -N ₈	0.293	-0.747	0.127	0.310	-0.857	0.179
C ₅ -O ₅	0.408	-0.270	0.099	0.407	-0.290	0.097
C ₇ -N ₇	0.308	-0.933	0.126	0.318	-0.974	0.162

Table S2: Electron charge density, $\rho(r)$, Laplacian of the charge density, $\nabla^2\rho(r)$, and distance, Δr , from the nucleus for $-\nabla^2\rho(r)$ in the VSCC, at the B3LYP/6-311+G** level

maxima	$\rho(r)$ (e/a_o^3)	$\nabla^2\rho(r)$ (e/a_o^5)	Δr (\AA)	$\rho(r)$ (e/a_o^3)	$\nabla^2\rho(r)$ (e/a_o^5)	Δr (\AA)	$\rho(r)$ (e/a_o^3)	$\nabla^2\rho(r)$ (e/a_o^5)	Δr (\AA)
	1			2c			2d		
@N ₁	0.391	-1.015	0.467	0.390	-0.999	0.468	0.396	-1.026	0.468
	0.514	-1.989	0.431	0.525	-2.081	0.429	0.578	-2.728	0.389
	0.563	-2.565	0.392	0.581	-2.759	0.388	0.519	-2.047	0.429
@N ₃	0.558	-2.490	0.393	0.566	-2.570	0.392	0.570	-2.613	0.391
	0.478	-1.641	0.441	0.483	-1.624	0.445	0.479	-1.671	0.439
	0.471	-1.590	0.442	0.473	-1.626	0.439	0.483	-1.657	0.443
@N ₄	0.561	-2.495	0.393	0.496	-2.076	0.434	0.568	-2.568	0.392
	0.474	-1.643	0.438	0.481	-1.564	0.411	0.475	-1.650	0.442
	0.473	-1.567	0.446	0.476	-1.662	0.440	0.498	-1.745	0.440
				0.489	-1.772	0.430			
@N ₈	0.469	-1.467	0.412	0.474	-1.694	0.436	0.482	-1.764	0.434
	0.507	-1.943	0.427	0.505	-1.900	0.431	0.507	-1.970	0.429
	0.466	-1.629	0.438	0.499	-1.921	0.430	0.509	-1.984	0.426
	0.500	-1.909	0.430	0.469	-1.461	0.412			
@O ₅	0.926	-4.784	0.344	0.933	-4.883	0.343	0.938	-4.865	0.342
	0.931	-4.832	0.343	0.937	-4.917	0.342	0.938	-4.865	0.342
	0.735	-2.457	0.386	0.751	-2.582	0.386	0.757	-3.156	0.377
							0.728	-2.591	0.380
	3			4c			4d		
@N ₁	0.577	-2.711	0.389	0.589	-2.849	0.387	0.399	-1.033	0.468
	0.401	-1.088	0.464	0.397	-1.050	0.466	0.514	-1.997	0.430
	0.517	-2.019	0.431	0.525	-2.088	0.429	0.568	-2.614	0.391
@N ₃	0.558	-2.500	0.393	0.564	-2.555	0.392	0.571	-2.635	0.390
	0.478	-1.634	0.442	0.485	-1.637	0.445	0.480	-1.646	0.443
	0.480	-1.670	0.440	0.476	-1.654	0.438	0.483	-1.691	0.439
@N ₄	0.562	-2.517	0.393	0.495	-2.061	0.435	0.584	-2.754	0.389
	0.470	-1.601	0.444	0.480	-1.535	0.411	0.477	-1.676	0.442
	0.482	-1.683	0.440	0.483	-1.727	0.438	0.495	-1.786	0.437
				0.488	-1.763	0.434			
@N ₈	0.500	-1.879	0.428	0.496	-1.817	0.432	0.506	-1.942	0.431
	0.466	-1.634	0.438	0.499	-1.947	0.424	0.514	-2.010	0.424
	0.464	-1.453	0.413	0.467	-1.476	0.412	0.482	-1.749	0.435
	0.500	-1.955	0.424	0.473	-1.683	0.436			
@O ₇	0.735	-2.430	0.387	0.761	-2.673	0.385	0.939	-4.860	0.342
	0.926	-4.770	0.343	0.944	-5.021	0.342	0.939	-4.860	0.342
	0.920	-4.684	0.344	0.938	-4.945	0.342	0.764	-3.228	0.376
							0.715	-2.450	0.383

Table S2: Cont.

maxima	$\rho(r)$ (e/a_o^3)	$\nabla^2\rho(r)$ (e/a_o^5)	Δr (\AA)	$\rho(r)$ (e/a_o^3)	$\nabla^2\rho(r)$ (e/a_o^5)	Δr (\AA)	$\rho(r)$ (e/a_o^3)	$\nabla^2\rho(r)$ (e/a_o^5)	Δr (\AA)
	5			6c			6d		
@N ₁	0.512	-1.968	0.431	0.523	-2.057	0.429	0.571	-2.648	0.391
	0.559	-2.514	0.393	0.575	-2.693	0.390	0.394	-1.011	0.468
	0.389	-0.997	0.467	0.389	-0.994	0.468	0.518	-2.023	0.430
@N ₃	0.468	-1.577	0.443	0.474	-1.631	0.440	0.479	-1.668	0.440
	0.479	-1.648	0.441	0.480	-1.605	0.445	0.481	-1.641	0.443
	0.558	-2.491	0.393	0.565	-2.567	0.392	0.569	-2.605	0.391
@N ₄	0.471	-1.622	0.438	0.484	-1.583	0.410	0.560	-2.481	0.393
	0.558	-2.465	0.393	0.485	-1.596	0.410	0.489	-1.682	0.442
	0.475	-1.570	0.446	0.476	-1.645	0.441	0.472	-1.612	0.444
				0.494	-2.058	0.434			
				0.487	-1.765	0.430			
@N ₈	0.478	-1.531	0.411	0.479	-1.555	0.410	0.476	-1.703	0.436
	0.479	-1.564	0.410	0.479	-1.548	0.410	0.509	-1.954	0.426
	0.507	-1.926	0.427	0.506	-1.889	0.431	0.496	-1.869	0.432
	0.494	-1.849	0.432	0.491	-1.848	0.432	0.469	-1.458	0.412
	0.462	-1.590	0.439	0.470	-1.652	0.437	0.470	-1.459	0.412
@O ₅	0.925	-4.768	0.344	0.946	-5.042	0.342	0.756	-3.144	0.377
	0.929	-4.811	0.343	0.942	-5.007	0.342	0.938	-4.868	0.342
	0.734	-2.446	0.386	0.758	-2.671	0.384	0.938	-4.867	0.342
							0.726	-2.582	0.380
	6b								
@N ₁	0.401	-1.119	0.461	@N ₄ 0.562	-2.512	0.393	@O ₅ 0.929	-4.809	0.343
	0.594	-2.899	0.386	0.472	-1.641	0.439	0.932	-4.864	0.343
	0.525	-2.051	0.432	0.481	-1.603	0.448	0.753	-2.593	0.386
@N ₃	0.489	-1.760	0.435	@N ₈ 0.498	-1.836	0.432			
	0.495	-2.075	0.434	0.455	-1.552	0.441			
	0.475	-1.490	0.412	0.507	-2.015	0.421			
	0.490	-1.762	0.433	0.472	-1.520	0.411			