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SUPORTING INFORMATION FILE FOR

Boron triel bonding: A weak electrostatic interaction lacking of electron-density descriptors

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1. Theoretical AIM analysis of compounds 2–3

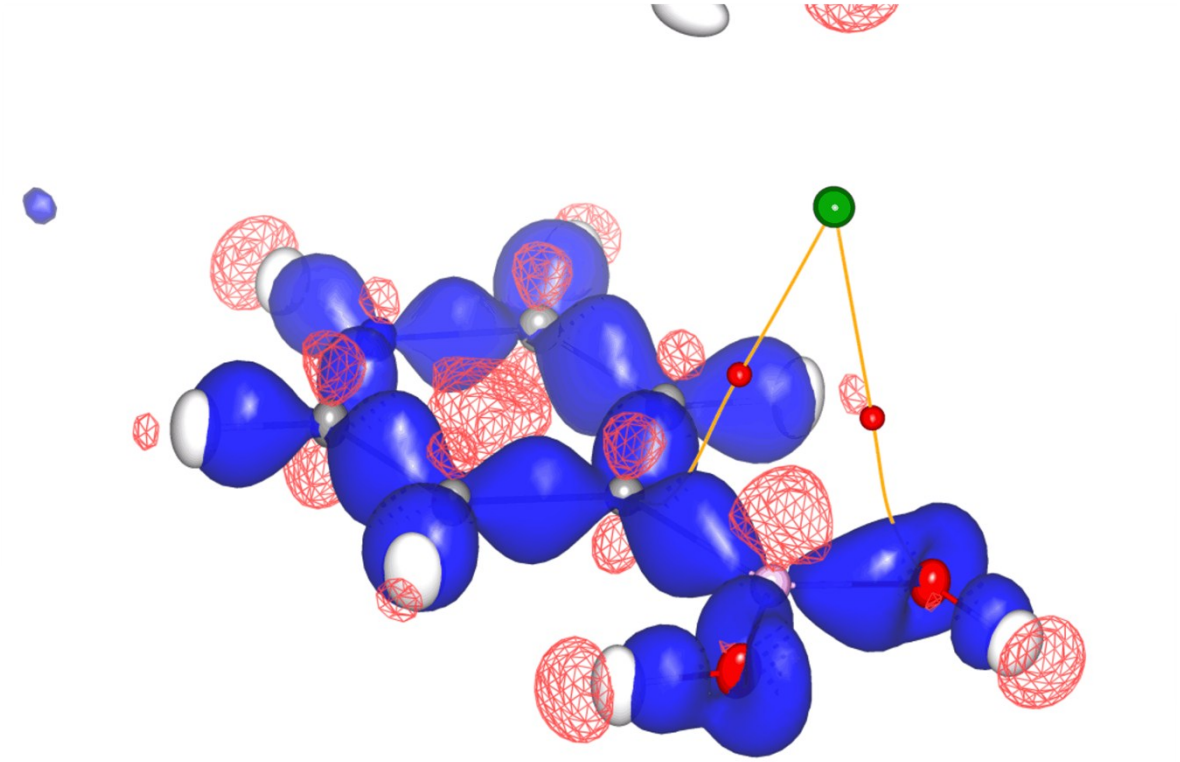

Figure S1. Static electron density deformation of **1**. Isosurface levels at ±0.15 e/Å^3. Blue electron excess, red electron deficient region.

Figure S2 shows the distribution of bond CPs and bond paths in compounds **2** and **3**. In compound **2** only one CP is found that connects the O atoms of the N-oxide group to the oxygen atom of the carboxylate, in good agreement to the experimental findings. In compound three, three bond critical points are found. One corresponding to the p-hole interaction interconnecting the O atom of one nitro group to the N-atom of the adjacent nitro group. In addition, two O-atoms are inter-connected through a bond CP and bond path, thus characterizing the chalcogen-chalcogen interaction. Finally, this O atom is also connected to one aromatic C atom. This distribution of CPs is identical to that found experimentally.

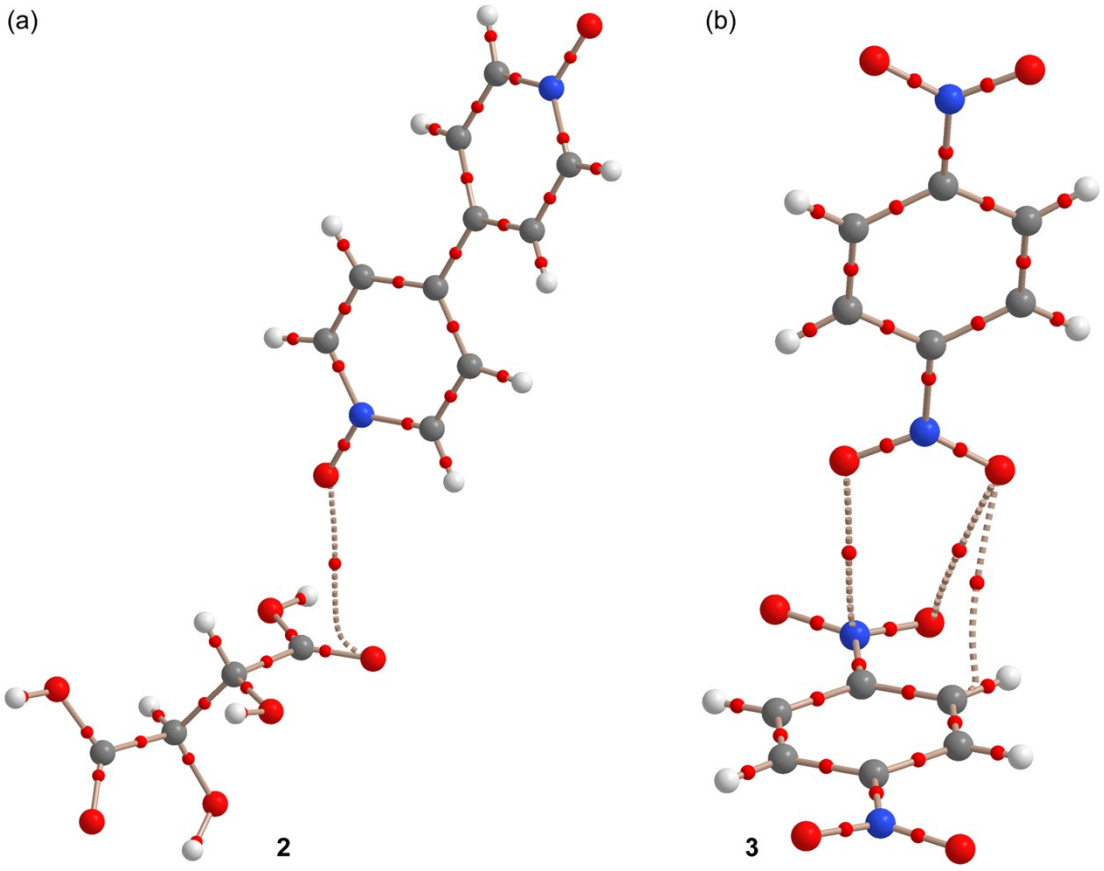

Figure S2. Distribution of bond critical points (red spheres) and bond paths in **2** (a) and compound **3** (b) computed using the M06-2X/def2-TZVP wavefunction.

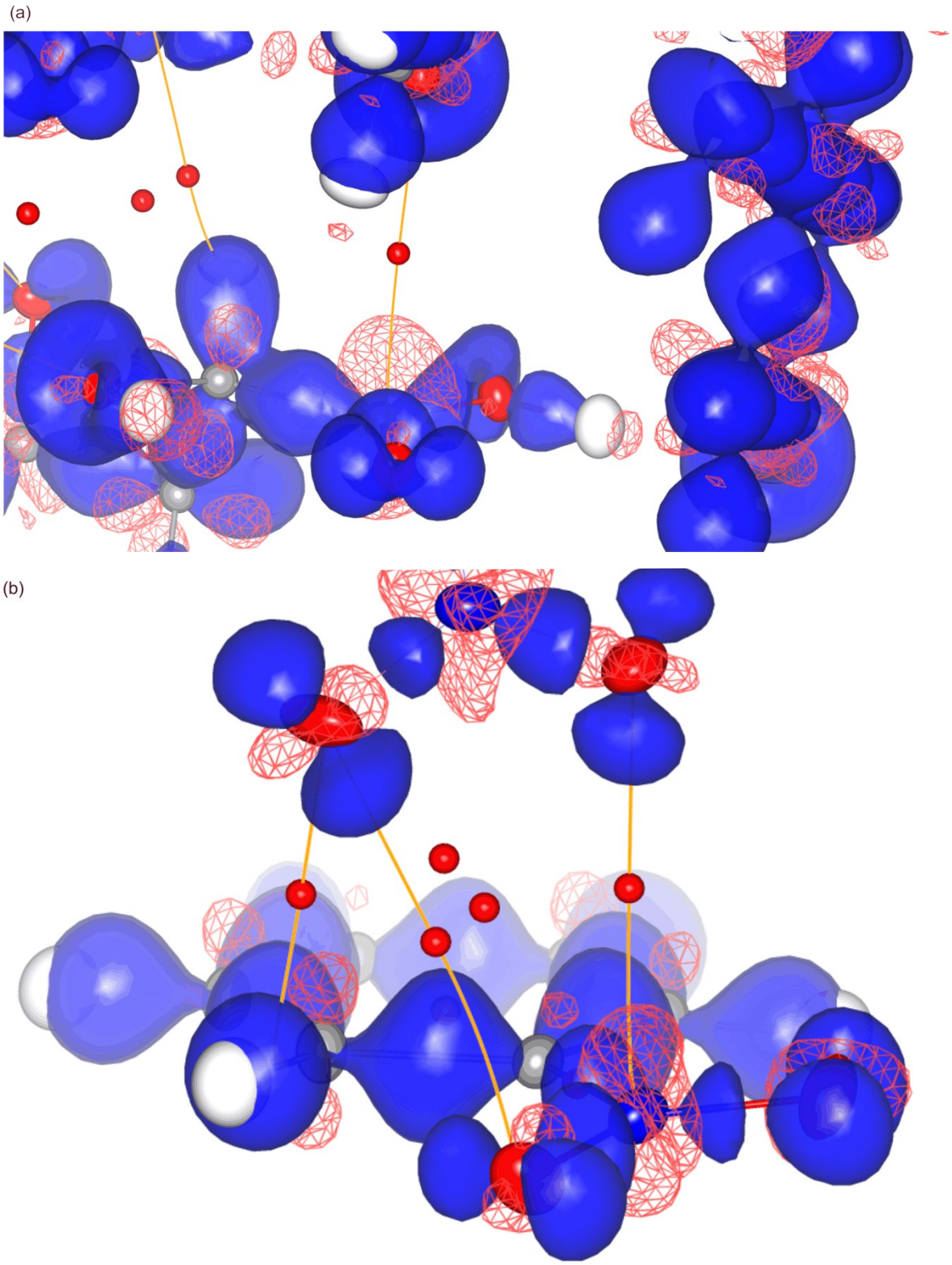

Figure S4. Static electron density deformation of **2** and **3**. Isosurface levels at ±0.15 e/Å^3. Blue electron excess, red electron deficient region.

2. Dynamic deformation density maps

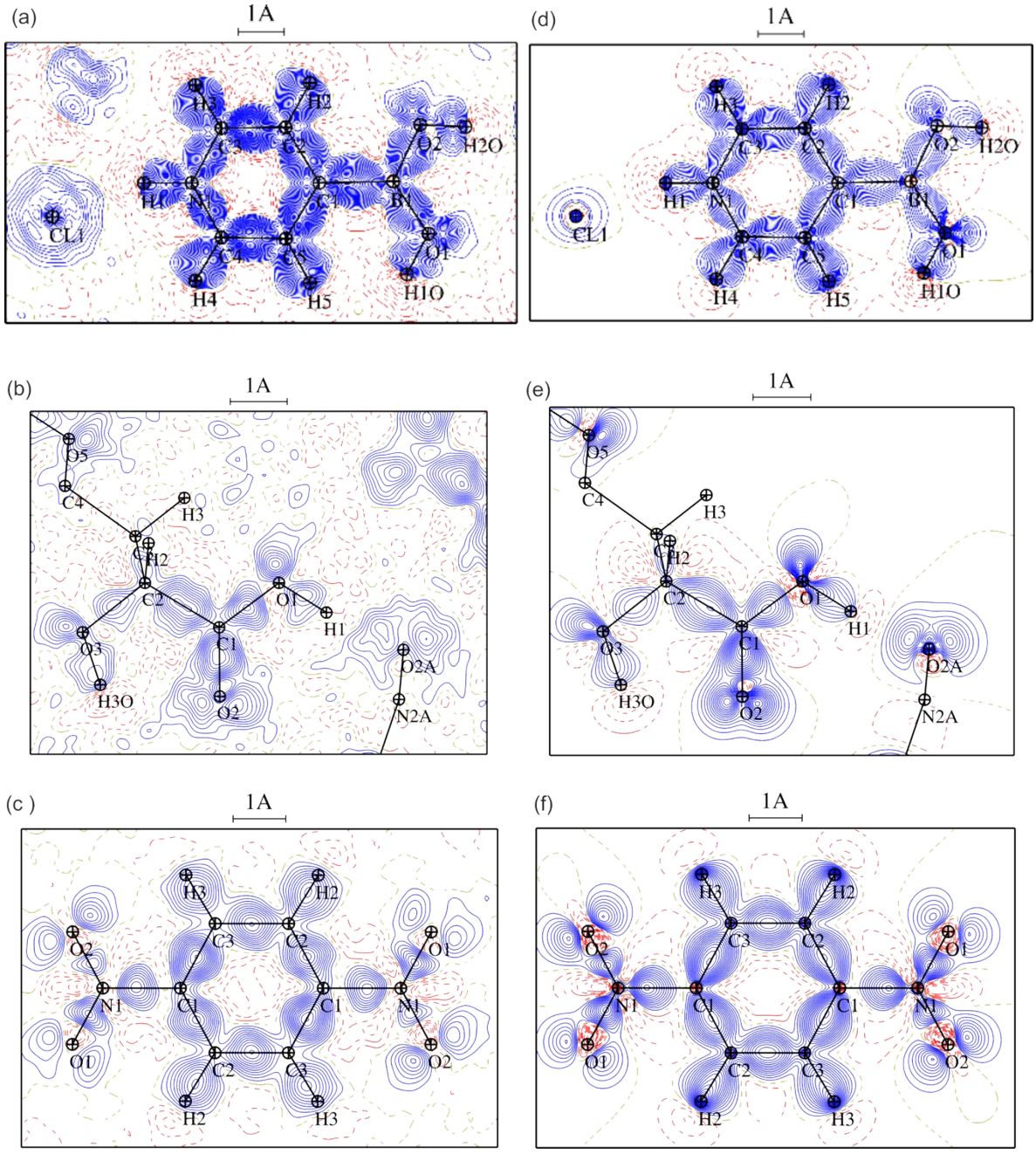

Figure S5. Dynamic deformation density maps of compounds 1, a) (at the pyridomium ring plane), 2, b) (C1-O1-O2 plane) and 3, c) (phenyl ring plane). Static deformation electron density deformation of compounds 1, d), 2, e) and 3, f). Contours levels at 0.05 e/Å^3

3. Fourier residual maps

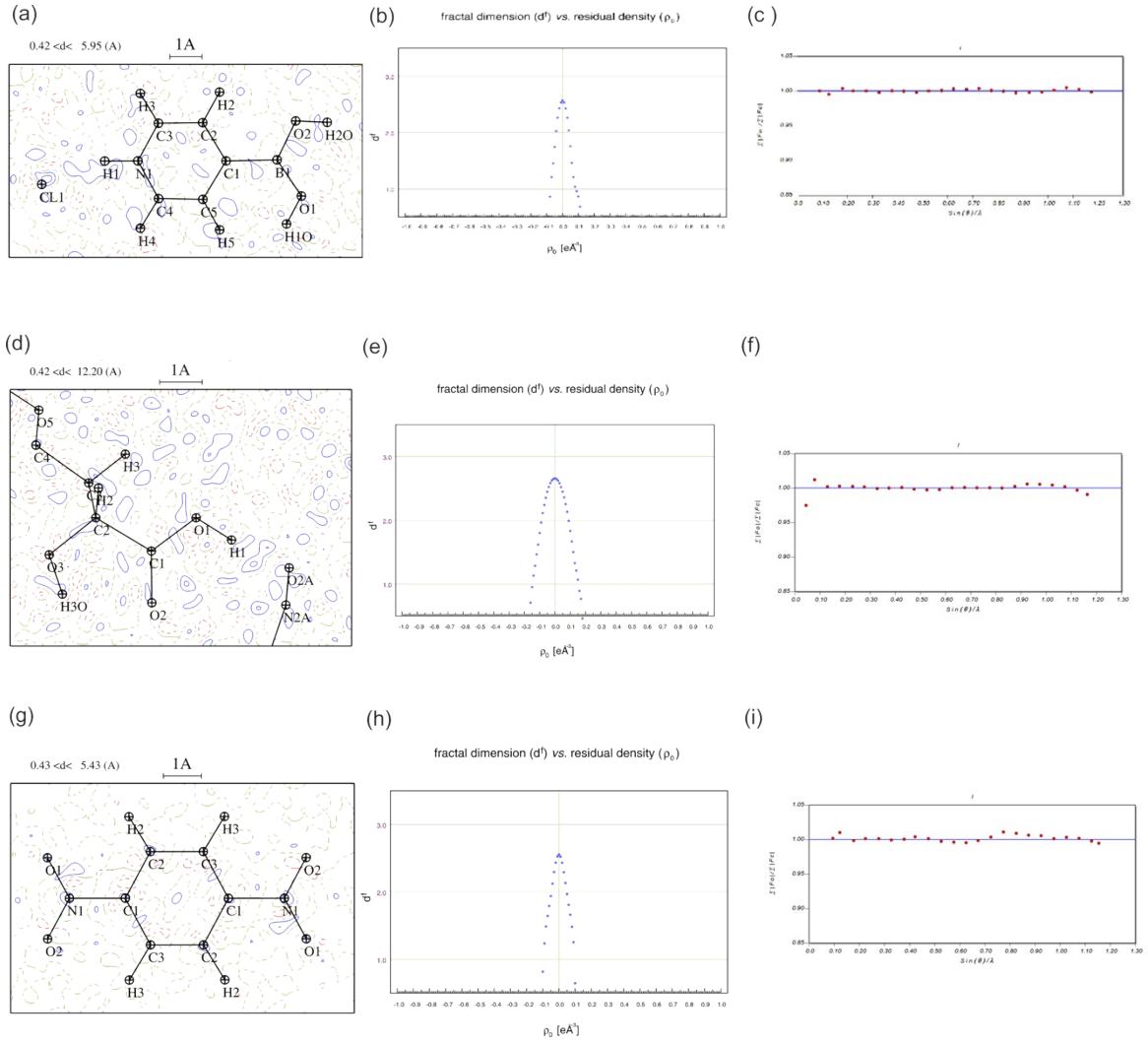

Figure S6. Fourier residual maps (Contours levels at 0.05 e/Å^3), fractal dimension test and scaling factor plots of compounds **1** a), b) and c); **2** d), e) and f); **1** g), h) and i); Plane definition as in Fig. S5.

4. Tables with AIM data Tables with AIM data

Table S1. Compound **1.** Bond energies calculated using the Abramov expression[16], bond distances and distances from the atom to the critical point, in Å. Electron density at the critical point in e/Å^3. Eigen values of the Hessian matrix and ellipticy at the critical point.

		Hartree/Bohr^3		kJ/mol/Bohr^3											
Atom1	**Atom2**	**Gcp**	**Vcp**	**Gcp**	**Vcp**	**DISTIJ**	**DCPI**	**DCPJ**	**DEN**	**LAPL**	**3-EIGEN-VALUES**			**ELLIPTIC**	**TYPE**
O1	B1	0.3099	-0.4847	813.7	-1272.7	1.361	0.907	0.456	1.44	13.0	-14.33	-13.47	40.83	0.064	(3,-1)
O1	H1O	0.2211	-0.8179	580.5	-2147.3	0.991	0.753	0.239	2.28	-36.2	-34.38	-34.27	32.43	0.003	(3,-1)
O2	B1	0.3141	-0.5158	824.6	-1354.4	1.356	0.901	0.455	1.52	10.8	-15.06	-14.70	40.59	0.025	(3,-1)
O2	H2O	0.2139	-0.7824	561.5	-2054.1	0.982	0.748	0.234	2.22	-34.2	-33.33	-33.27	32.41	0.002	(3,-1)
N1	C3	0.3041	-0.8756	798.4	-2298.9	1.343	0.813	0.530	2.31	-25.8	-18.04	-16.38	8.64	0.101	(3,-1)
N1	C4	0.2695	-0.8141	707.6	-2137.4	1.342	0.836	0.506	2.23	-26.5	-17.89	-15.53	6.90	0.152	(3,-1)
N1	H1	0.2066	-0.6669	542.5	-1751.0	1.033	0.774	0.259	1.99	-24.5	-26.65	-25.80	28.00	0.033	(3,-1)
C1	C2	0.2827	-0.7504	742.2	-1970.2	1.402	0.706	0.697	2.09	-17.8	-15.56	-13.51	11.23	0.152	(3,-1)
C1	C5	0.2878	-0.7577	755.7	-1989.4	1.403	0.687	0.715	2.10	-17.6	-16.12	-13.42	11.99	0.201	(3,-1)
C1	B1	0.1051	-0.3050	275.9	-800.7	1.593	1.080	0.514	1.23	-9.1	-9.49	-9.33	9.68	0.017	(3,-1)
C2	C3	0.3085	-0.8382	810.0	-2200.7	1.384	0.648	0.736	2.24	-21.3	-17.52	-14.08	10.28	0.244	(3,-1)
C2	H2	0.2118	-0.6117	556.0	-1605.9	1.089	0.718	0.371	1.87	-18.1	-17.71	-16.68	16.26	0.062	(3,-1)
C3	H3	0.1879	-0.5774	493.3	-1516.0	1.089	0.758	0.331	1.82	-19.4	-18.55	-17.37	16.48	0.068	(3,-1)
C4	C5	0.2997	-0.8245	786.9	-2164.7	1.384	0.733	0.651	2.22	-21.7	-17.50	-14.13	9.93	0.239	(3,-1)
C4	H4	0.1852	-0.5705	486.1	-1497.8	1.089	0.761	0.329	1.80	-19.3	-18.38	-17.03	16.12	0.080	(3,-1)
C5	H5	0.2165	-0.6252	568.3	-1641.3	1.089	0.727	0.362	1.89	-18.5	-18.44	-17.53	17.43	0.052	(3,-1)
Non covalent interactions															
CL1	H1	0.0236	-0.0219	62.0	-57.4	2.100	1.465	0.646	0.178	2.5	-0.67	-0.60	3.71	0.123	(3,-1)
CL1	H2O	0.0202	-0.0188	53.0	-49.3	2.137	1.509	0.633	0.163	2.1	-0.41	-0.40	2.90	0.019	(3,-1)
CL1	H1O	0.0178	-0.0170	46.7	-44.6	2.149	1.504	0.692	0.156	1.8	-0.62	-0.41	2.83	0.492	(3,-1)
O1	H5	0.0082	-0.0059	21.5	-15.4	2.765	1.598	1.178	0.063	1.0	-0.19	-0.05	1.26	3.211	(3,-1)
H3	O1	0.0079	-0.0057	20.7	-14.9	2.432	1.058	1.420	0.062	1.0	-0.23	-0.21	1.41	0.094	(3,-1)
CL1	H3	0.0064	-0.0045	16.7	-11.9	2.680	1.726	0.979	0.053	0.8	-0.18	-0.13	1.11	0.355	(3,-1)
CL1	H5	0.0059	-0.0040	15.6	-10.6	2.701	1.799	0.964	0.046	0.8	-0.12	-0.06	0.93	1.129	(3,-1)
CL1	C1	0.0041	-0.0033	10.7	-8.5	3.537	1.833	1.725	0.050	0.5	-0.12	-0.08	0.67	0.477	(3,-1)
CL1	O2	0.0037	-0.0028	9.8	-7.4	3.557	1.891	1.683	0.043	0.5	-0.10	-0.07	0.62	0.496	(3,-1)
CL1	C3	0.0035	-0.0026	9.1	-6.7	3.575	1.892	1.721	0.040	0.4	-0.06	-0.02	0.50	2.723	(3,-1)
CL1	H2	0.0026	-0.0017	6.9	-4.6	3.216	1.928	1.316	0.027	0.3	-0.05	-0.05	0.44	0.026	(3,-1)
C4	O1	0.0025	-0.0017	6.5	-4.4	3.527	1.786	1.754	0.027	0.3	-0.05	-0.04	0.40	0.325	(3,-1)

Table S2. Compound **2.** Bond energies calculated using the Abramov expression[16], bond distances and distances from the atom to the critical point, in Å. Electron density at the critical point in e/Å^3. Eigen values of the Hessian matrix and ellipticy at the critical point.

		Hartree/Bohr^3		kJ/mol/Bohr^3											
Atom1	**Atom2**	**Gcp**	**Vcp**	**Gcp**	**Vcp**	**DISTIJ**	**DCPI**	**DCPJ**	**DEN**	**LAPL**	**3-EIGEN-VALUES**			**ELLIPTIC**	**TYPE**
O1	C1	0.2990	-0.8997	785.0	-2362.1	1.310	0.816	0.494	2.365	-29.08	-20.56	-19.23	10.71	0.070	(3,-1)
H1A	C1A	0.1909	-0.5867	501.1	-1540.2	1.084	0.340	0.744	1.834	-19.76	-18.63	-17.55	16.42	0.062	(3,-1)
C1	O2	0.5109	-1.3512	1341.4	-3547.5	1.216	0.425	0.791	2.968	-31.75	-30.09	-26.87	25.22	0.120	(3,-1)
C1	C2	0.2126	-0.5572	558.3	-1463.0	1.522	0.775	0.747	1.742	-12.72	-12.84	-11.28	11.40	0.139	(3,-1)
H2A	C2A	0.1853	-0.5503	486.6	-1444.7	1.082	0.341	0.741	1.758	-17.31	-17.02	-16.35	16.05	0.041	(3,-1)
H2	C2	0.2080	-0.5776	546.2	-1516.4	1.095	0.368	0.727	1.794	-15.57	-17.00	-16.56	17.99	0.026	(3,-1)
C2	O3	0.2544	-0.6306	668.0	-1655.6	1.408	0.588	0.820	1.861	-11.73	-13.79	-13.78	15.84	0.001	(3,-1)
C2	C3	0.1948	-0.4922	511.3	-1292.2	1.543	0.770	0.773	1.609	-9.90	-11.10	-10.53	11.73	0.054	(3,-1)
O3	H3O	0.1725	-0.7575	452.8	-1988.8	0.976	0.761	0.215	2.212	-39.77	-35.80	-34.95	30.98	0.024	(3,-1)
H3	C3	0.2084	-0.5748	547.1	-1509.2	1.096	0.372	0.724	1.788	-15.24	-17.01	-16.34	18.11	0.041	(3,-1)
C3	C4	0.2133	-0.5631	560.1	-1478.3	1.527	0.749	0.779	1.755	-13.15	-13.15	-11.39	11.39	0.155	(3,-1)
C3	O4	0.2457	-0.6198	645.1	-1627.2	1.402	0.580	0.822	1.847	-12.38	-13.64	-13.60	14.86	0.003	(3,-1)
C4	O6	0.5118	-1.3681	1343.6	-3591.9	1.211	0.423	0.788	2.995	-33.21	-31.57	-27.55	25.91	0.146	(3,-1)
C4	O5	0.2841	-0.8587	745.9	-2254.4	1.325	0.510	0.815	2.301	-28.00	-20.11	-18.36	10.47	0.095	(3,-1)
H4A	C4A	0.1900	-0.5639	498.9	-1480.5	1.082	0.340	0.742	1.784	-17.72	-17.36	-16.75	16.39	0.037	(3,-1)
H4	O4	0.2092	-0.8305	549.2	-2180.4	0.978	0.227	0.751	2.319	-39.73	-36.59	-35.61	32.47	0.027	(3,-1)
O5	H5O	0.1933	-0.6434	507.5	-1689.1	0.980	0.772	0.208	1.956	-24.75	-30.64	-30.48	36.38	0.005	(3,-1)
H5A	C5A	0.1932	-0.5879	507.2	-1543.6	1.082	0.345	0.738	1.835	-19.43	-18.38	-17.41	16.35	0.056	(3,-1)
O2A	N2A	0.5747	-1.0920	1508.9	-2867.1	1.332	0.657	0.675	2.466	5.54	-19.69	-18.55	43.78	0.062	(3,-1)
C3A	C4A	0.2796	-0.7458	734.1	-1958.1	1.402	0.714	0.688	2.081	-17.99	-16.43	-13.02	11.46	0.262	(3,-1)
C3A	C6A	0.2381	-0.6109	625.0	-1603.8	1.476	0.742	0.734	1.836	-12.99	-14.17	-11.85	13.03	0.196	(3,-1)
C3A	C2A	0.2827	-0.7547	742.3	-1981.4	1.399	0.713	0.686	2.096	-18.24	-16.43	-13.20	11.38	0.245	(3,-1)
C4A	C5A	0.2948	-0.7989	773.9	-2097.6	1.385	0.674	0.711	2.173	-20.18	-17.24	-13.39	10.44	0.287	(3,-1)
C5A	N1A	0.2839	-0.8135	745.3	-2135.9	1.352	0.476	0.876	2.213	-23.69	-18.29	-14.72	9.32	0.243	(3,-1)
C6A	C7A	0.2820	-0.7586	740.5	-1991.6	1.404	0.702	0.702	2.104	-18.75	-16.71	-13.46	11.42	0.242	(3,-1)
C6A	C10A	0.2815	-0.7489	739.0	-1966.3	1.399	0.708	0.691	2.085	-17.93	-16.30	-13.33	11.70	0.223	(3,-1)
C7A	C8A	0.3031	-0.8197	795.9	-2152.2	1.382	0.694	0.688	2.206	-20.58	-17.79	-13.68	10.89	0.301	(3,-1)
C7A	H7A	0.1950	-0.5908	511.9	-1551.0	1.083	0.750	0.333	1.839	-19.36	-18.46	-17.70	16.80	0.043	(3,-1)

Table S2 Continuation.

		Hartree/Bohr^3		kJ/mol/Bohr^3											
Atom1	**Atom2**	**Gcp**	**Vcp**	**Gcp**	**Vcp**	**DISTIJ**	**DCPI**	**DCPJ**	**DEN**	**LAPL**	**3-EIGEN-VALUES**			**ELLIPTIC**	**TYPE**
C8A	N2A	0.2885	-0.8232	757.3	-2161.4	1.354	0.495	0.859	2.228	-23.74	-17.66	-15.17	9.09	0.164	(3,-1)
C8A	H8A	0.2000	-0.5891	525.0	-1546.6	1.082	0.734	0.348	1.830	-18.23	-18.08	-17.18	17.03	0.053	(3,-1)
C9A	C10A	0.3043	-0.8181	799.0	-2147.9	1.383	0.707	0.676	2.202	-20.19	-17.51	-13.86	11.17	0.263	(3,-1)
C9A	N2A	0.2939	-0.8296	771.7	-2178.2	1.348	0.482	0.866	2.235	-23.31	-17.65	-15.22	9.56	0.159	(3,-1)
C9A	H9A	0.1955	-0.5864	513.4	-1539.6	1.082	0.734	0.348	1.829	-18.83	-18.23	-17.27	16.68	0.055	(3,-1)
C10A	H10A	0.2058	-0.5984	540.4	-1571.0	1.081	0.722	0.359	1.844	-18.00	-17.68	-16.96	16.64	0.043	(3,-1)
C2A	C1A	0.2992	-0.8139	785.7	-2136.8	1.379	0.667	0.712	2.198	-20.76	-17.64	-13.60	10.48	0.297	(3,-1)
O1A	N1A	0.5791	-1.1131	1520.4	-2922.3	1.326	0.658	0.668	2.501	4.35	-20.12	-18.81	43.28	0.069	(3,-1)
C1A	N1A	0.2872	-0.8253	754.0	-2166.9	1.350	0.480	0.870	2.233	-24.19	-18.87	-14.51	9.19	0.301	(3,-1)
Non covalent interactions															
H5O	O1A	0.0653	-0.0786	171.4	-206.3	1.546	0.496	1.050	0.443	5.01	-2.75	-2.69	10.45	0.021	(3,-1)
O3	H4	0.0409	-0.0335	107.3	-87.8	1.707	1.181	0.529	0.208	4.66	-0.72	-0.71	6.09	0.013	(3,-1)
H3O	O2	0.0164	-0.0140	43.0	-36.8	2.022	0.778	1.263	0.128	1.80	-0.55	-0.50	2.86	0.095	(3,-1)
O6	H10A	0.0115	-0.0079	30.2	-20.8	2.224	1.372	0.856	0.071	1.45	-0.25	-0.25	1.95	0.020	(3,-1)
H4A	O4	0.0089	-0.0063	23.5	-16.6	2.340	0.942	1.416	0.065	1.11	-0.23	-0.23	1.58	0.013	(3,-1)
O4	H9A	0.0085	-0.0062	22.3	-16.3	2.418	1.416	1.039	0.067	1.04	-0.24	-0.23	1.50	0.050	(3,-1)
O5	H3	0.0067	-0.0047	17.5	-12.2	2.515	1.476	1.073	0.053	0.83	-0.16	-0.14	1.13	0.177	(3,-1)
H5A	O6	0.0065	-0.0046	17.0	-12.1	2.556	1.167	1.446	0.054	0.80	-0.17	-0.16	1.13	0.084	(3,-1)
H2	O1	0.0058	-0.0040	15.2	-10.6	2.602	1.151	1.503	0.048	0.73	-0.13	-0.11	0.96	0.131	(3,-1)
O3	H9A	0.0050	-0.0035	13.2	-9.2	2.744	1.548	1.240	0.044	0.63	-0.11	-0.09	0.84	0.217	(3,-1)
C4A	C10A	0.0045	-0.0034	11.7	-8.9	3.230	1.608	1.625	0.049	0.53	-0.07	-0.04	0.64	0.744	(3,-1)
O6	H4A	0.0035	-0.0022	9.1	-5.8	2.784	1.579	1.237	0.029	0.45	-0.08	-0.06	0.59	0.355	(3,-1)
O2	O2A	0.0033	-0.0022	8.7	-5.7	3.373	1.878	1.594	0.030	0.43	-0.07	-0.04	0.54	0.739	(3,-1)
O6	C5A	0.0033	-0.0021	8.7	-5.6	3.335	1.607	1.735	0.029	0.43	-0.06	-0.03	0.53	1.059	(3,-1)
H10A	O4	0.0032	-0.0021	8.3	-5.5	2.944	1.348	1.651	0.030	0.41	-0.08	-0.05	0.54	0.579	(3,-1)
O6	O1A	0.0030	-0.0020	8.0	-5.2	3.390	1.912	1.581	0.028	0.39	-0.06	-0.03	0.49	0.819	(3,-1)
N1A	C3A	0.0023	-0.0016	6.2	-4.1	3.587	1.784	1.813	0.026	0.30	-0.03	-0.01	0.34	2.200	(3,-1)
O2	H4	0.0005	-0.0003	1.4	-0.7	3.542	1.956	1.594	0.005	0.07	-0.01	0.00	0.09	1.768	(3,-1)

Table S 1. Compound **3.** Bond energies calculated using the Abramov expression[16], bond distances and distances from the atom to the critical point, in Å. Electron density at the critical point in e/Å^3. Eigen values of the Hessian matrix and ellipticy at the critical point.

		Hartree/Bohr^3		kJ/mol/Bohr^3										
Atom1	**Atom2**	**Gcp**	**Vcp**	**Gcp**	**Vcp**	**DISTIJ**	**DCPI**	**DCPJ**	**DEN**	**LAPL**	**3-EIGEN-VALUES**			**ELLIPTIC**	**TYPE**
N1	O1	0.8322	-1.8173	2184.99	-4771.27	1.227	0.591	0.635	3.44	-14.73	-31.61	-28.84	45.72	0.096	(3,-1)
N1	O2	0.7900	-1.6957	2074.08	-4452.05	1.224	0.592	0.632	3.29	-11.16	-28.93	-27.52	45.29	0.051	(3,-1)
N1	C1	0.2129	-0.5602	559.00	-1470.83	1.470	0.893	0.578	1.75	-12.95	-12.48	-10.66	10.19	0.170	(3,-1)
C1	C2	0.2862	-0.7846	751.52	-2059.86	1.389	0.708	0.681	2.15	-20.44	-16.03	-13.38	8.97	0.199	(3,-1)
C1	C3	0.3028	-0.8277	794.88	-2173.24	1.391	0.732	0.660	2.22	-21.42	-16.47	-13.82	8.87	0.192	(3,-1)
C2	C3	0.2822	-0.7770	740.99	-2040.11	1.391	0.701	0.691	2.14	-20.49	-15.54	-13.28	8.33	0.170	(3,-1)
C2	H2	0.2116	-0.6276	555.58	-1647.72	1.077	0.707	0.370	1.90	-19.70	-17.88	-17.11	15.30	0.045	(3,-1)
C3	H3	0.2035	-0.5957	534.18	-1564.08	1.077	0.708	0.369	1.84	-18.20	-16.83	-16.40	15.03	0.026	(3,-1)
Non covalent interactions															
N1	O1	0.0067	-0.0046	17.45	-12.11	2.965	1.487	1.488	0.05	0.84	-0.14	-0.05	1.02	1.904	(3,-1)
C2	O2	0.0040	-0.0027	10.58	-7.15	3.278	1.752	1.554	0.04	0.51	-0.10	-0.09	0.70	0.203	(3,-1)
O1	O2	0.0032	-0.0020	8.51	-5.27	3.271	1.650	1.636	0.03	0.43	-0.06	-0.04	0.53	0.419	(3,-1)

5. Crystallographic Table

Table S4. Crystallographic table of the refinements of **1**, **2** and **3**. Data collected at 90K using Mo *Kα* radiation.

Compound	**1**		**3**		**2**	
Empirical formula	$C_5 H_7 B Cl N O_2$		$C_6 H_4 N_2 O_4$		$C_{14} H_{14} N_2 O_8$	
Formula weight	159.38		168.11		142.13	
Crystal system /	Monoclinic		Monoclinic		Orthorhombic	
Space group	*Pc*		$P2_1/n$		$P2_12_12_1$	
$Friedif_{stat}$	124		-		7	
Unit cell dimensions	a = 6.20620(5)Å α= 90° b = 5.25334(4)Å β = 105.5034(8)° c = 11.18373(9)Å γ = 90°		a = 5.66357(3)Å α= 90° b = 5.37326(3)Å β = 92.0201(5)° c = 10.91612(7)Å γ = 90°		a = 4.54400(10)Å α= 90° b = 15.2652(2)Å β = 90° c = 20.3342(2)Å γ = 90°	
Volume	351.359(5) $Å^3$		331.991(3) $Å^3$		1409.47(3) $Å^3$	
Z	2		2		4	
Density (calc.)	1.506 Mg/m^3		1.682 Mg/m^3		1.594 Mg/m^3	
Abs. coefficient	0.467 mm^{-1}		0.145 mm^{-1}		0.133 mm^{-1}	
F(000)	164		172		704	
Crystal size	0.3 x 0.3 x 0.25 mm^3		0.35 x 0.3 x 0.2 mm^3		0.3 x 0.2 x 0.2 mm^3	
Refls. collected	31805		33917		90175	
Abs. correction	Multi-scan		Multi-scan		Multi-scan	
Refinement model	Spherical	Multipolar	Spherical	Multipolar	Spherical	Multipolar
Theta range	3.24 to 58.52°	3.24 to 58.52°	3.74 to 55.16°	3.74 to 55.52°	1.67 to 57.35°	1.67 to 57.35°
Index ranges	$-11 \le h \le 15$ $-16 \le k \le 14$ $-37 \le l \le 31$	$-13 \le h \le 13$ $0 \le k \le 15$ $0 \le l \le 36$	$-13 \le h \le 13$ $-12 \le k \le 11$ $-25 \le l \le 25$	$-13 \le h \le 13$ $0 \le k \le 12$ $0 \le l \le 25$	$-8 \le h \le 10$ $-36 \le k \le 35$ $-48 \le l \le 38$	$-8 \le h \le 10$ $-36 \le k \le 35$ $-48 \le l \le 38$
Indep. reflections	7501[R_{int} = 0.0121]		4276[R_{int} = 0.0251]		19571[R_{int} = 0.0338]	
Completeness	94.9%		99.0%		98.3%	
Data / restraints / parameters	7501/ 2/ 119	7501/ 154/ 334	4276/ 0/ 63	4276/ 80/ 207	18682/ 0/ 273	18682/361/747
GOOF on F^2	1.113	0.989	1.139	0.928	1.001	1.036
Final R indices [I>2sigma(I)]	R_1 = 0.0134 wR_2 = 0.0399		R_1 = 0.0288 wR_2 = 0.1041		R_1 = 0.0308 wR_2 = 0.0796	
R indices (all data)*	R_1 = 0.0134 wR_2 = 0.0399	R_1 = 0.0063 wR_2 = 0.0139	R_1 = 0.0296 wR_2 = 0.1110	R_1 = 0.0107 wR_2 = 0.0241	R_1 = 0.0382 wR_2 = 0.0827	R_1 = 0.0215 wR_2 = 0.0307
Hooft/Parsons parameter	y = 0.003(5) z=0.005(4)	y =0.009(5)	-	-	y =0.07(10) z=0.09(12)	y =-0.03(7)
Largest diff. peak and hole	0.41/-0.19 $e.Å^{-3}$	0.12/-0.09 $e.Å^{-3}$	0.61/-0.48 $e.Å^{-3}$	0.10/-0.10 $e.Å^{-3}$	0.57/-0.23 $e.Å^{-3}$	0.18/-0.16 $e.Å^{-3}$
RBT (non H)		2.4 x 10^{-4}		1.4 x 10^{-4}		2.0 x 10^{-4}

* $I/\sigma(I)$=0.1 for the multipolar refinement.