Inter- and Intra-molecular Bonding in 1,3,5-Triamino-2,4,6-trinitrobenzene (TATB) – an Experimental and Theoretical QTAIM Analysis

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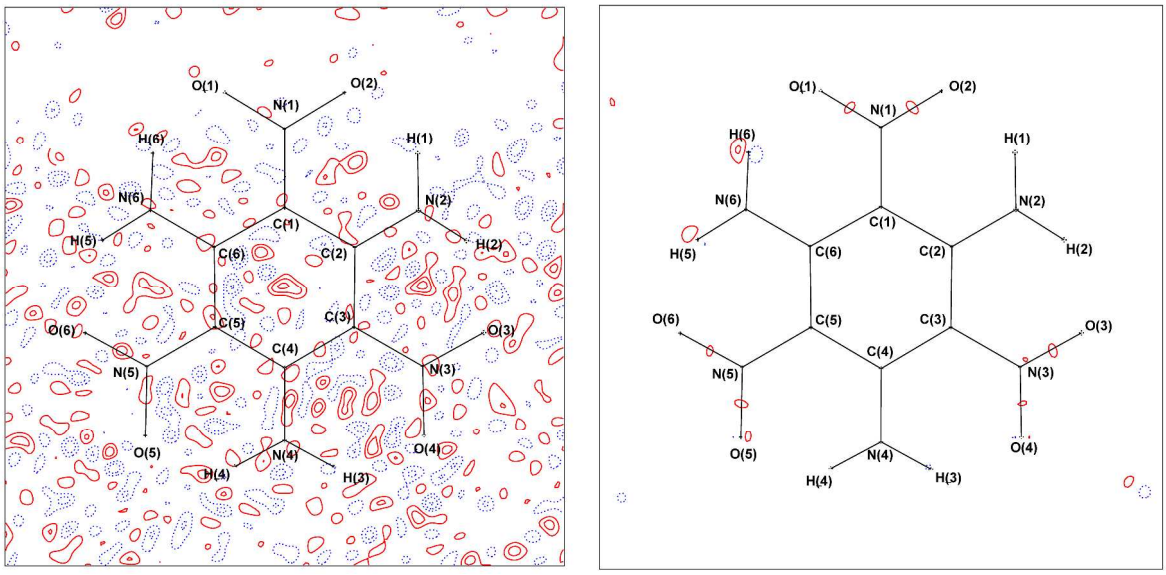
SUPPLEMENTARY MATERIAL

Abstract

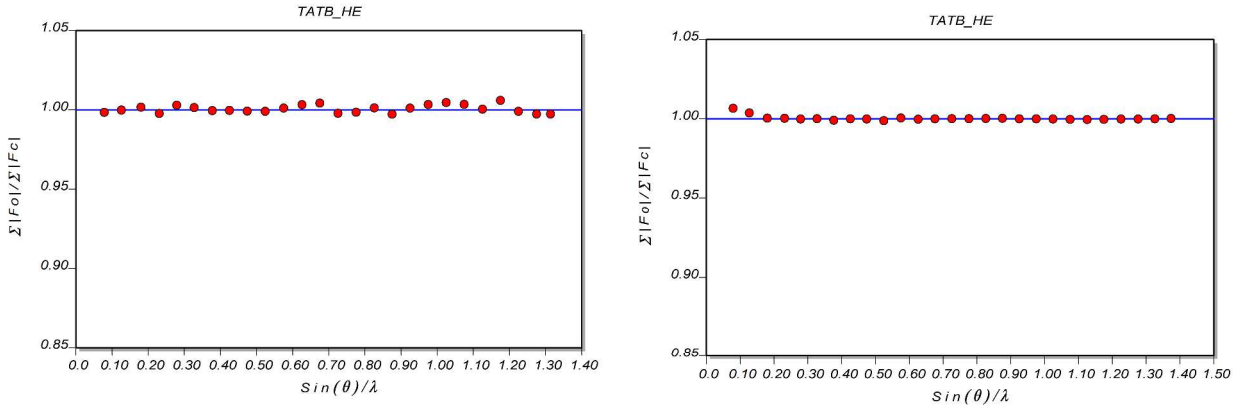
Chemical bonding in the triclinic phase of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) has been analyzed based on the experimental electron density derived from X-ray diffraction data obtained at 20K. The results have been compared with those from solid state theoretical calculations. The total electron density has been analyzed in terms of the Quantum Theory of Atoms in Molecules (QTAIM). Features of the covalent bonds demonstrate the presence of multiple bonds of various order. Strong intramolecular hydrogen bonds and weaker intermolecular bonds within the layer structure are characterized by the properties of their (3,-1) critical points. Weaker interactions, predominantly O ⋯ O, between the layers have also been characterized. Atomic charges are also reported. The importance of correcting the primary X-ray data for λ/2 contamination is discussed.

Contents



a) b)

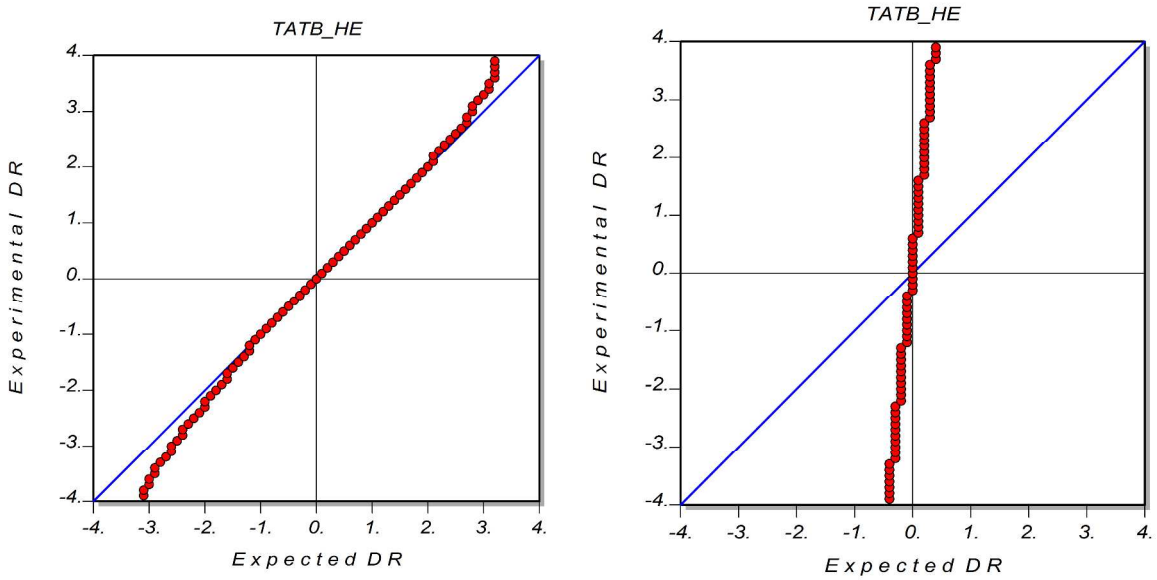
Fig. S1. a) Residual map, all experimental data, b) residual map, theoretical structure factors.



Contour level 0.05 eÅ^{-3}.

a) b)

Fig S2. Plot of average scale factor with respect to resolution; a) experimental data, b) theoretical structure factors.



a) b)

Fig. S3. Normal probability plots for a) experimental data, b) theoretical data with unit weights.

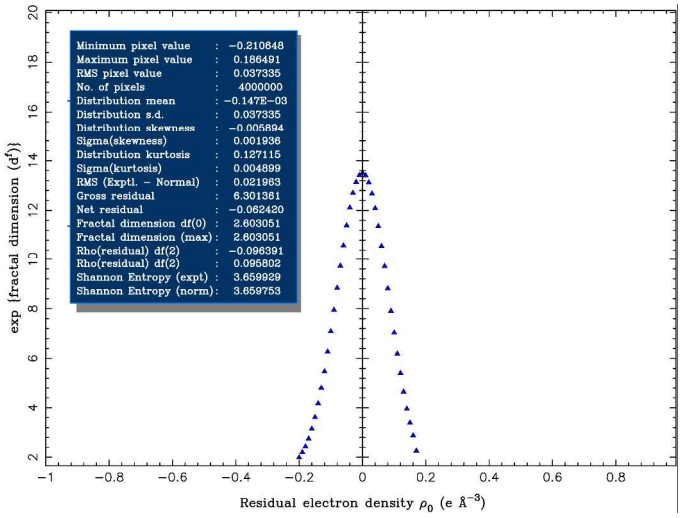


Fig S4. Fractal dimension plot.

Table S1: Properties of the Intramolecular and Intermolecular Bond Critical Points in DCBQ. 1st row: experimental multipole. 2nd row: theoretical structure factors (TSF) multipole. 3rd row: Wave functions from TOPOND. 4th row: DFT calculations from Stephens *et al.[1]*

Bond	ρ(r) (e/Å^3)	$\nabla^2\rho$(r) (e/Å^5)	Rij (Å)	d_1 (Å)	d_2 (Å)	Hessian Eigenvalues (e/Å^5)			Ellipt	g (au)	v (au)	h (au)	Bond order
Intramolecular - covalent													
O(1) - N(1)	3.160	-10.05	1.252	0.647	0.605	-28.503	-26.862	45.314	0.061	0.7414	-1.5871	-0.8457	1.8
	3.055	-11.75	1.252	0.648	0.604	-26.824	-24.311	39.385	0.103	0.6850	-1.4919	-0.8069	1.6
	3.111	-19.28	1.252	0.654	0.598	-29.135	-26.171	36.028	0.113	0.6566	-1.5131	-0.8566	1.5
	3.290	-24.10	1.236	0.647	0.589	-30.800	-27.800	34.500	0.110	0.3586	-0.9662	-0.6076	1.4
O(2) - N(1)	3.175	-12.84	1.261	0.653	0.608	-29.212	-27.962	44.336	0.045	0.7286	-1.5904	-0.8618	1.7
	2.992	-10.79	1.261	0.651	0.610	-26.150	-23.689	39.043	0.104	0.6657	-1.4433	-0.7777	1.6
	3.043	-17.98	1.261	0.657	0.604	-28.316	-25.521	35.859	0.110	0.6372	-1.4609	-0.8237	1.5
	3.290	-24.10	1.236	0.646	0.589	-30.900	-27.800	34.500	0.110	0.3586	-0.9676	-0.6090	1.4
O(3) - N(3)	3.208	-12.83	1.251	0.653	0.599	-29.336	-28.088	44.592	0.044	0.7425	-1.6182	-0.8757	1.7
	3.062	-12.02	1.251	0.648	0.604	-26.903	-24.433	39.320	0.101	0.6862	-1.4971	-0.8109	1.6
	3.111	-19.38	1.251	0.654	0.597	-29.208	-26.219	36.052	0.114	0.6559	-1.5128	-0.8569	1.5
	3.290	-24.10	1.236	0.647	0.589	-30.900	-27.800	34.500	0.110	0.3586	-0.9676	-0.6090	1.4
O(4) - N(3)	3.182	-10.63	1.256	0.649	0.607	-29.034	-27.018	45.420	0.075	0.7465	-1.6034	-0.8568	1.8
	3.023	-11.41	1.256	0.650	0.606	-26.522	-24.047	39.159	0.103	0.6739	-1.4662	-0.7923	1.6
	3.077	-18.70	1.256	0.655	0.600	-28.774	-25.882	35.931	0.112	0.6463	-1.4867	-0.8403	1.5
	3.290	-24.10	1.236	0.646	0.589	-30.900	-27.800	34.500	0.110	0.3586	-0.9676	-0.6090	1.4

O(5) - N(5)	3.166	-10.42	1.254	0.650	0.604	-28.666	-26.922	45.166	0.065	0.7414	-1.5909	-0.8495	1.8
	3.044	-11.57	1.254	0.648	0.605	-26.680	-24.209	39.319	0.102	0.6817	-1.4834	-0.8017	1.6
	3.097	-19.01	1.253	0.654	0.599	-28.991	-26.051	36.004	0.112	0.6527	-1.5026	-0.8499	1.5
	3.290	-24.10	1.236	0.646	0.589	-30.900	-27.800	34.500	0.110	0.3586	-0.9676	-0.6090	1.4
O(6) - N(5)	3.114	-8.54	1.260	0.645	0.615	-27.710	-26.485	45.656	0.046	0.7322	-1.5530	-0.8208	1.8
	2.993	-10.82	1.260	0.651	0.608	-26.194	-23.722	39.100	0.104	0.6659	-1.4440	-0.7781	1.6
	3.050	-18.15	1.260	0.657	0.603	-28.437	-25.593	35.859	0.111	0.6389	-1.4660	-0.8271	1.5
	3.290	-24.10	1.236	0.646	0.589	-30.900	-27.800	34.500	0.110	0.3586	-0.9676	-0.6090	1.4
N(2) - H(1)	2.120	-35.25	1.013	0.785	0.228	-31.546	-29.986	26.285	0.052	0.1731	-0.7120	-0.5388	0.5
	2.222	-34.31	1.013	0.758	0.255	-30.409	-29.524	25.624	0.030	0.2134	-0.7828	-0.5694	0.6
	2.254	-45.38	0.991	0.771	0.220	-32.798	-31.810	19.207	0.031	0.1478	-0.7664	-0.6186	0.6
	2.230	-44.30	0.994	0.774	0.220	-32.100	-31.000	18.800	0.030	0.0504	-0.5616	-0.5112	0.7
N(2) - H(2)	2.124	-35.49	1.014	0.785	0.229	-31.246	-30.307	26.059	0.031	0.1728	-0.7137	-0.5410	0.5
	2.217	-34.47	1.014	0.760	0.254	-30.442	-29.478	25.449	0.033	0.2108	-0.7792	-0.5684	0.6
	2.247	-45.50	0.992	0.773	0.218	-32.798	-31.834	19.134	0.031	0.1447	-0.7614	-0.6167	0.6
	2.230	-44.30	0.994	0.774	0.220	-32.100	-31.000	18.800	0.030	0.0504	-0.5616	-0.5112	0.7
N(4) - H(3)	2.140	-35.23	1.013	0.781	0.232	-31.353	-30.110	26.229	0.041	0.1799	-0.7253	-0.5454	0.5
	2.221	-34.83	1.013	0.761	0.253	-30.609	-29.674	25.451	0.032	0.2095	-0.7804	-0.5709	0.6
	2.254	-45.59	0.991	0.772	0.218	-32.871	-31.907	19.183	0.030	0.1463	-0.7656	-0.6193	0.6
	2.230	-44.30	0.994	0.774	0.220	-32.100	-31.000	18.800	0.030	0.0504	-0.5616	-0.5112	0.7

N(4) - H(4)	2.123	-35.57	1.013	0.788	0.225	-31.677	-30.407	26.511	0.042	0.1719	-0.7128	-0.5409	0.5
	2.228	-34.79	1.013	0.759	0.255	-30.584	-29.633	25.427	0.032	0.2123	-0.7856	-0.5732	0.6
	2.254	-45.57	0.991	0.772	0.219	-32.871	-31.907	19.207	0.031	0.1465	-0.7657	-0.6192	0.6
	2.230	-44.30	0.994	0.774	0.220	-32.100	-31.000	18.800	0.030	0.0504	-0.5616	-0.5112	0.7
N(6) - H(5)	2.084	-33.64	1.013	0.790	0.224	-30.921	-29.487	26.764	0.049	0.1726	-0.6942	-0.5216	0.5
	2.223	-35.04	1.013	0.761	0.253	-30.672	-29.754	25.386	0.031	0.2089	-0.7814	-0.5724	0.6
	2.254	-45.62	0.991	0.772	0.218	-32.871	-31.931	19.183	0.030	0.1461	-0.7655	-0.6194	0.6
	2.230	-44.30	0.994	0.774	0.220	-32.100	-31.000	18.800	0.030	0.0504	-0.5616	-0.5112	0.7
N(6) - H(6)	2.103	-34.06	1.014	0.784	0.230	-31.035	-29.351	26.325	0.057	0.1757	-0.7048	-0.5291	0.5
	2.219	-35.33	1.014	0.763	0.252	-30.767	-29.749	25.187	0.034	0.2054	-0.7773	-0.5719	0.6
	2.247	-45.69	0.992	0.774	0.217	-32.871	-31.931	19.086	0.030	0.1433	-0.7607	-0.6173	0.6
	2.230	-44.30	0.994	0.774	0.220	-32.100	-31.000	18.800	0.030	0.0504	-0.5616	-0.5112	0.7
N(1) - C(1)	1.938	-18.83	1.416	0.878	0.538	-15.948	-11.779	8.893	0.354	0.2287	-0.6528	-0.4241	0.9
	1.901	-15.64	1.416	0.865	0.551	-14.764	-10.942	10.069	0.349	0.2393	-0.6409	-0.4016	0.9
	1.910	-17.52	1.415	0.889	0.526	-15.086	-10.700	8.266	0.410	0.2291	-0.6399	-0.4108	0.9
	1.850	-14.90	1.430	0.914	0.516	-13.300	-9.400	7.800	0.420	0.2030	-0.5601	-0.3571	1.1
N(2) - C(2)	2.417	-30.93	1.321	0.831	0.490	-20.086	-17.956	7.110	0.119	0.3047	-0.9304	-0.6256	1.2
	2.392	-26.50	1.321	0.778	0.543	-19.306	-16.405	9.208	0.177	0.3263	-0.9276	-0.6013	1.2
	2.402	-28.22	1.321	0.800	0.521	-20.363	-17.134	9.278	0.189	0.3183	-0.9293	-0.6110	1.2
	2.350	-23.90	1.321	0.833	0.488	-18.400	-16.100	10.600	0.140	0.2593	-0.7676	-0.5083	1.4

N(3) - C(3)	1.919	-18.73	1.420	0.884	0.537	-15.579	-11.829	8.680	0.317	0.2235	-0.6413	-0.4178	0.8
	1.882	-15.23	1.420	0.867	0.553	-14.516	-10.827	10.109	0.341	0.2365	-0.6310	-0.3945	0.9
	1.896	-17.54	1.420	0.889	0.531	-14.965	-10.748	8.169	0.393	0.2248	-0.6316	-0.4068	0.9
	1.850	-14.90	1.430	0.914	0.516	-13.300	-9.400	7.800	0.420	0.2030	-0.5601	-0.3571	1.1
N(4) - C(4)	2.436	-30.75	1.318	0.814	0.504	-20.353	-17.514	7.120	0.162	0.3128	-0.9447	-0.6320	1.2
	2.404	-27.17	1.318	0.781	0.537	-19.430	-16.556	8.811	0.174	0.3260	-0.9339	-0.6079	1.2
	2.423	-28.58	1.317	0.800	0.517	-20.629	-17.303	9.350	0.191	0.3230	-0.9425	-0.6195	1.2
	2.350	-23.90	1.321	0.833	0.488	-18.400	-16.100	10.600	0.140	0.2593	-0.7661	-0.5068	1.4
N(5) - C(5)	1.973	-21.07	1.414	0.877	0.536	-16.660	-13.070	8.658	0.275	0.2241	-0.6667	-0.4427	0.8
	1.906	-15.74	1.414	0.865	0.548	-14.832	-10.945	10.039	0.355	0.2404	-0.6440	-0.4036	0.9
	1.917	-17.54	1.413	0.890	0.523	-15.134	-10.724	8.314	0.413	0.2310	-0.6440	-0.4130	0.9
	1.850	-14.90	1.430	0.914	0.516	-13.300	-9.400	7.800	0.420	0.2030	-0.5601	-0.3571	1.1
N(6) - C(6)	2.424	-30.60	1.318	0.816	0.502	-19.905	-17.749	7.053	0.121	0.3096	-0.9366	-0.6271	1.2
	2.401	-26.81	1.318	0.778	0.539	-19.344	-16.470	9.009	0.175	0.3277	-0.9334	-0.6058	1.2
	2.423	-28.58	1.317	0.799	0.518	-20.629	-17.279	9.326	0.195	0.3230	-0.9425	-0.6195	1.2
	2.350	-23.90	1.321	0.833	0.488	-18.400	-16.100	10.600	0.140	0.2593	-0.7676	-0.5083	1.4
C(1) - C(2)	1.917	-15.52	1.448	0.717	0.730	-14.603	-12.234	11.312	0.194	0.2451	-0.6512	-0.4061	1.1
	1.878	-14.12	1.448	0.702	0.746	-13.797	-11.214	10.888	0.230	0.2430	-0.6326	-0.3895	1.2
	1.896	-16.34	1.447	0.715	0.732	-14.339	-11.808	9.808	0.213	0.2331	-0.6358	-0.4026	1.1
	1.920	-17.60	1.440	0.707	0.733	-14.200	-11.500	8.100	0.240	0.0830	-0.3497	-0.2667	1.2

C(2) - C(3)	1.942	-15.49	1.445	0.728	0.717	-14.835	-12.230	11.574	0.213	0.2531	-0.6670	-0.4139	1.2
	1.888	-14.30	1.445	0.744	0.702	-13.896	-11.298	10.893	0.230	0.2447	-0.6378	-0.3931	1.2
	1.903	-16.51	1.445	0.733	0.712	-14.459	-11.857	9.808	0.219	0.2340	-0.6393	-0.4053	1.1
	1.920	-17.60	1.440	0.733	0.707	-14.200	-11.500	8.100	0.240	0.0830	-0.3497	-0.2667	1.2
C(3) - C(4)	1.955	-16.62	1.447	0.716	0.730	-15.087	-12.862	11.327	0.173	0.2491	-0.6706	-0.4215	1.1
	1.885	-14.31	1.447	0.702	0.744	-13.873	-11.314	10.880	0.226	0.2437	-0.6358	-0.3921	1.2
	1.903	-16.44	1.446	0.714	0.733	-14.387	-11.857	9.808	0.214	0.2345	-0.6395	-0.4050	1.1
	1.920	-17.60	1.440	0.707	0.733	-14.200	-11.500	8.100	0.240	0.0830	-0.3497	-0.2667	1.2
C(4) - C(5)	1.920	-15.60	1.449	0.721	0.729	-14.655	-12.341	11.396	0.188	0.2453	-0.6525	-0.4072	1.1
	1.875	-14.12	1.449	0.745	0.704	-13.765	-11.253	10.903	0.223	0.2420	-0.6305	-0.3885	1.2
	1.890	-16.31	1.449	0.733	0.716	-14.291	-11.833	9.832	0.208	0.2313	-0.6318	-0.4005	1.1
	1.920	-17.60	1.440	0.733	0.707	-14.200	-11.500	8.100	0.240	0.0830	-0.3497	-0.2667	1.2
C(5) - C(6)	1.937	-15.46	1.448	0.717	0.731	-14.755	-12.248	11.543	0.205	0.2518	-0.6640	-0.4122	1.2
	1.878	-14.11	1.448	0.702	0.746	-13.784	-11.218	10.893	0.229	0.2429	-0.6322	-0.3893	1.2
	1.896	-16.31	1.448	0.715	0.733	-14.339	-11.808	9.808	0.214	0.2333	-0.6359	-0.4026	1.1
	1.920	-17.60	1.440	0.707	0.733	-14.200	-11.500	8.100	0.240	0.0830	-0.3497	-0.2667	1.2
C(6) - C(1)	1.936	-16.26	1.449	0.724	0.725	-14.837	-12.714	11.286	0.167	0.2457	-0.6602	-0.4145	1.1
	1.873	-13.99	1.449	0.746	0.704	-13.750	-11.172	10.931	0.231	0.2424	-0.6300	-0.3876	1.2
	1.890	-16.24	1.449	0.716	0.733	-14.291	-11.784	9.808	0.212	0.2318	-0.6320	-0.4003	1.1
	1.920	-17.60	1.440	0.733	0.707	-14.200	-11.500	8.100	0.240	0.0830	-0.3497	-0.2667	1.2

Bond	ρ(r) (e/Å^3)	$\nabla^2\rho$(r) (e/Å^5)	Rij (Å)	d_1 (Å)	d_2 (Å)	Hessian Eigenvalues (e/Å^5)			Ellipt	g (au)	v (au)	h (au)	BDE (kJ/mol[1])	Bond order
Intramolecular - non-covalent														
O(1) - H(6)	0.304	4.82	1.695	1.129	0.577	-1.687	-1.463	7.971	0.153	0.0497	-0.0495	0.0003	-64.9	0.1
	0.315	4.31	1.695	1.124	0.575	-1.852	-1.572	7.731	0.178	0.0472	-0.0497	-0.0025	-65.2	0.1
	0.337	4.07	1.726	1.115	0.612	-2.000	-1.976	8.073	0.013	0.0477	-0.0531	-0.0054	-69.6	0.1
O(2) - H(1)	0.300	4.64	1.720	1.129	0.606	-1.582	-1.400	7.620	0.130	0.0481	-0.0481	0.0000	-63.1	0.1
	0.322	4.15	1.720	1.123	0.606	-1.836	-1.543	7.531	0.190	0.0467	-0.0503	-0.0036	-66.1	0.1
	0.324	4.00	1.754	1.125	0.629	-1.856	-1.832	7.663	0.015	0.0459	-0.0502	-0.0044	-66.0	0.1
O(3) - H(2)	0.315	4.55	1.702	1.128	0.589	-1.776	-1.552	7.876	0.145	0.0488	-0.0505	-0.0016	-66.2	0.1
	0.325	4.30	1.702	1.121	0.588	-1.896	-1.585	7.781	0.197	0.0480	-0.0514	-0.0034	-67.5	0.1
	0.337	4.07	1.734	1.117	0.617	-1.976	-1.928	7.977	0.024	0.0477	-0.0531	-0.0054	-69.6	0.1
O(4) - H(3)	0.313	4.43	1.715	1.133	0.596	-1.838	-1.490	7.759	0.234	0.0479	-0.0497	-0.0019	-65.3	0.1
	0.320	4.17	1.715	1.125	0.598	-1.838	-1.537	7.544	0.195	0.0467	-0.0501	-0.0034	-65.8	0.1
	0.331	4.00	1.747	1.123	0.624	-1.880	-1.856	7.736	0.014	0.0465	-0.0515	-0.0050	-67.6	0.1
O(5) - H(4)	0.301	4.65	1.713	1.135	0.592	-1.679	-1.354	7.685	0.240	0.0483	-0.0483	0.0000	-63.4	0.1
	0.312	4.21	1.713	1.127	0.591	-1.829	-1.484	7.520	0.232	0.0462	-0.0488	-0.0026	-64.1	0.1
	0.331	4.00	1.745	1.121	0.624	-1.928	-1.856	7.784	0.036	0.0465	-0.0515	-0.0050	-67.6	0.1
O(6) - H(5)	0.313	4.68	1.707	1.128	0.599	-1.718	-1.500	7.899	0.146	0.0495	-0.0505	-0.0010	-66.3	0.1
	0.319	4.24	1.707	1.123	0.589	-1.868	-1.540	7.644	0.213	0.0470	-0.0501	-0.0031	-65.8	0.1
	0.331	4.02	1.738	1.120	0.618	-1.952	-1.904	7.880	0.018	0.0467	-0.0516	-0.0049	-67.7	0.1

Intermolecular (in-plane)													
Bond	ρ(r) (e/Å^3)	$\nabla^2\rho$(r) (e/Å^5)	Rij (Å)	d_1 (Å)	d_2 (Å)	Hessian eigenvalues (e/Å^5)			Ellipt	g (au)	v (au)	h (au)	BDE (kJ/mol[1])
O(1) - H(4)	0.090	1.52	2.265	1.385	0.927	-0.332	-0.279	2.134	0.191	0.0127	-0.0096	0.0031	12.5
	0.090	1.52	2.265	1.381	0.938	-0.350	-0.294	2.168	0.190	0.0127	-0.0096	0.0031	12.6
$x+1, y, z$	0.088	1.33	2.370	1.390	0.980	-0.337	-0.313	1.952	0.119	0.0112	-0.0087	0.0025	11.4
O(2) - H(3)	0.084	1.48	2.253	1.392	0.881	-0.322	-0.233	2.032	0.383	0.0122	-0.0090	0.0032	11.8
	0.084	1.54	2.253	1.391	0.891	-0.335	-0.219	2.099	0.533	0.0126	-0.0092	0.0034	12.1
$x+1, y, z$	0.088	1.30	2.324	1.393	0.931	-0.337	-0.313	1.976	0.090	0.0111	-0.0086	0.0024	11.3
O(3) - H(6)	0.086	1.51	2.275	1.385	0.933	-0.307	-0.269	2.081	0.140	0.0124	-0.0092	0.0032	12.1
	0.092	1.50	2.275	1.377	0.952	-0.354	-0.312	2.168	0.133	0.0126	-0.0096	0.0030	12.6
$x-1, y-1, z$	0.088	1.30	2.022	1.393	0.629	-0.337	-0.289	1.928	0.139	0.0111	-0.0086	0.0024	11.3
O(4) - H(5)	0.088	1.38	2.274	1.394	0.905	-0.331	-0.269	1.978	0.231	0.0116	-0.0089	0.0027	11.7
	0.086	1.48	2.274	1.395	0.909	-0.338	-0.229	2.050	0.480	0.0122	-0.0091	0.0031	12.0
$x-1, y-1, z$	0.088	1.25	2.348	1.403	0.944	-0.337	-0.289	1.880	0.107	0.0107	-0.0085	0.0023	11.1
O(5) - H(2)	0.092	1.42	2.274	1.391	0.930	-0.383	-0.289	2.090	0.323	0.0120	-0.0094	0.0027	12.3
	0.086	1.49	2.274	1.389	0.933	-0.331	-0.271	2.088	0.224	0.0123	-0.0091	0.0031	12.0
$x, y+1, z$	0.088	1.30	2.380	1.396	0.984	-0.337	-0.289	1.904	0.116	0.0111	-0.0086	0.0024	11.3
O(6) - H(1)	0.079	1.50	2.260	1.413	0.869	-0.304	-0.185	1.992	0.642	0.0121	-0.0087	0.0035	11.4
	0.082	1.50	2.260	1.399	0.891	-0.324	-0.213	2.041	0.520	0.0122	-0.0089	0.0033	11.7
$x, y+1, z$	0.088	1.28	2.331	1.398	0.933	-0.337	-0.313	1.928	0.081	0.0109	-0.0085	0.0024	11.2

Intermolecular (between layers)													
O(1) - O(1)	0.021	0.29	3.349	1.675	1.675	-0.044	-0.035	0.366	0.253	0.0022	-0.0014	0.0008	1.8
	0.021	0.30	3.349	1.675	1.675	-0.047	-0.040	0.385	0.167	0.0023	-0.0014	0.0008	1.9
-x + 2, *-y* + 1, *-z* + 1	0.020	0.29	3.352	1.676	1.676	-0.048	-0.048	0.386	0.283	0.0022	-0.0014	0.0008	1.8
O(2) - O(3)	0.043	0.52	3.207	1.601	1.610	-0.095	-0.066	0.685	0.442	0.0043	-0.0031	0.0012	4.0
	0.032	0.51	3.207	1.599	1.609	-0.069	-0.056	0.638	0.217	0.0039	-0.0026	0.0014	3.4
-x + 1, *-y*, *-z* + 1	0.034	0.53	3.212	1.603	1.609	-0.072	-0.072	0.675	0.206	0.0041	-0.0027	0.0014	3.5
O(3) - O(3)	0.010	0.14	3.668	1.834	1.834	-0.015	-0.007	0.161	0.972	0.0010	-0.0006	0.0004	0.8
	0.012	0.16	3.668	1.834	1.834	-0.022	-0.014	0.191	0.560	0.0011	-0.0007	0.0005	0.9
-x, *-y* - 1, *-z*	0.007	0.14	3.671	1.836	1.836	-0.024	-0.024	0.193	0.380	0.0010	-0.0006	0.0005	0.7
O(4) - O(4)	0.042	0.53	3.189	1.595	1.595	-0.087	-0.081	0.701	0.070	0.0043	-0.0031	0.0012	4.0
	0.035	0.52	3.189	1.595	1.595	-0.093	-0.077	0.688	0.216	0.0040	-0.0027	0.0013	3.6
-x, *-y*, *-z* + 1	0.040	0.53	3.192	1.596	1.596	-0.096	-0.072	0.699	0.198	0.0042	-0.0030	0.0013	3.9
O(4) - O(5)	0.044	0.57	3.154	1.577	1.578	-0.093	-0.057	0.720	0.622	0.0046	-0.0033	0.0013	4.3
	0.036	0.57	3.154	1.572	1.581	-0.081	-0.071	0.721	0.130	0.0044	-0.0029	0.0015	3.8
-x, *-y*, *-z*	0.040	0.58	3.158	1.578	1.580	-0.096	-0.072	0.747	0.166	0.0046	-0.0031	0.0014	4.1
O(4) - N(4)	0.042	0.48	3.337	1.632	1.708	-0.074	-0.035	0.586	1.094	0.0039	-0.0029	0.0010	3.7
	0.033	0.44	3.337	1.630	1.731	-0.068	-0.038	0.543	0.786	0.0034	-0.0023	0.0011	3.0
-x, *-y*, *-z*	0.034	0.43	3.349	1.637	1.712	-0.072	-0.048	0.554	0.794	0.0034	-0.0023	0.0011	3.1
O(6) - O(6)	0.052	0.66	3.086	1.543	1.543	-0.116	-0.086	0.862	0.351	0.0054	-0.0040	0.0014	5.3

	0.043	0.65	3.086	1.543	1.543	-0.111	-0.096	0.860	0.159	0.0052	-0.0035	0.0016	4.6
-*x* + 1, -*y* + 1, -*z*	0.047	0.67	3.088	1.544	1.544	-0.120	-0.120	0.892	0.098	0.0054	-0.0038	0.0016	5.0
O(6) - N(6)	0.042	0.52	3.255	1.586	1.673	-0.087	-0.056	0.667	0.539	0.0042	-0.0030	0.0012	4.0
	0.034	0.48	3.255	1.604	1.666	-0.073	-0.062	0.618	0.171	0.0038	-0.0025	0.0013	3.3
-*x* + 1, -*y* + 1, -*z*	0.034	0.48	3.258	1.604	1.654	-0.072	-0.048	0.627	0.398	0.0038	-0.0025	0.0012	3.3
N(2) – N(2)	0.043	0.45	3.440	1.720	1.720	-0.066	-0.023	0.537	1.866	0.0037	-0.0028	0.0009	3.7
	0.032	0.41	3.440	1.720	1.720	-0.054	-0.023	0.489	1.334	0.0032	-0.0022	0.0010	2.9
-*x* + 1, -*y*, -*z* + 1	0.034	0.39	3.445	1.722	1.722	-0.048	-0.024	0.458	1.590	0.0031	-0.0022	0.0009	2.9
N(4) – N(4)	0.041	0.43	3.438	1.719	1.719	-0.078	-0.015	0.522	4.208	0.0036	-0.0027	0.0009	3.5
	0.032	0.40	3.438	1.719	1.719	-0.065	-0.026	0.492	1.484	0.0032	-0.0021	0.0010	2.8
-*x*, -*y*, -*z*	0.034	0.39	3.446	1.723	1.723	-0.072	-0.024	0.482	2.136	0.0031	-0.0022	0.0009	2.9

1. Stephen AD, Srinivasan P, Kumaradhas P (2011) Bond charge depletion, bond strength and the impact sensitivity of high energetic 1,3,5-triamino 2,4,6-trinitrobenzene (TATB) molecule: A theoretical charge density analysis. Computational and Theoretical Chemistry 967 (2-3):250-256. doi:10.1016/j.comptc.2011.04.026

Table S2. Crystal09 Calculation for TATB

```
title : tatb (6311G** for H, Valenzano 2006 for C, O, Heyd_2005 for N)
CRYSTAL
0 0 0
2
8.9970 9.0201 6.5975 108.8702 92.3837 119.9599
24
8     0.837386    0.311045    0.287465  O1
8     0.695661    0.030333    0.270609  O2
8     0.049966   -0.294391    0.240465  O3
8    -0.084506   -0.151824    0.251646  O4
8     0.233983    0.476837    0.221647  O5
8     0.512407    0.618374    0.236783  O6
7     0.693989    0.169920    0.273491  N1
7     0.368947   -0.148769    0.236152  N2
7     0.054884   -0.151875    0.246530  N3
7     0.069491    0.171244    0.260264  N4
7     0.372990    0.476017    0.232391  N5
7     0.684233    0.471699    0.252332  N6
6     0.534815    0.166551    0.260237  C1
6     0.372174    0.001919    0.248127  C2
6     0.213326    0.005440    0.247738  C3
6     0.212852    0.166046    0.249730  C4
6     0.373835    0.322008    0.241522  C5
6     0.536937    0.325982    0.251198  C6
1     0.482873   -0.146284    0.240343  H1
1     0.251713   -0.262021    0.224485  H2
1    -0.040966    0.059629    0.26507   H3
1     0.075393    0.286975    0.262787  H4
1     0.678518    0.577931    0.240112  H5
1     0.795237    0.468368    0.26176   H6
KEEPSYMM
ENDG
1 4
0 0 3 1. 1.
    33.8650000            0.0254938
     5.0947900            0.1903730
     1.1587900            0.8521610
0 0 1 0. 1.
     0.3258400            1.0000000
0 0 1 0. 1.
     0.1027410            1.0000000
0 2 1 0. 1.
     0.7500000            1.0000000
6 6
0 0 6 2.0 1.00
 0.4563240000D+04 0.1966650000D-02
 0.6820240000D+03 0.1523060000D-01
 0.1549730000D+03 0.7612690000D-01
 0.4445530000D+02 0.2608010000D+00
 0.1302900000D+02 0.6164620000D+00
 0.1827730000D+01 0.2210060000D+00
0 1 3 4.0 1.00
 0.2096420000D+02 0.1146600000D+00 0.4024870000D-01
 0.4803310000D+01 0.9199990000D+00 0.2375940000D+00
```

```
 0.1459330000D+01 -0.3030680000D-02 0.8158540000D+00
0 1 1 0.0 1.00
 0.4834560000D+00 0.1000000000D+01 0.1000000000D+01
0 1 1 0.0 1.00
 0.1455850000D+00 0.1000000000D+01 0.1000000000D+01
0 3 1 0.0 1.0
 2.0 .1000000000D+01
0 3 1 0.0 1.0
 0.6 .1000000000D+01
7 5
0 0 6 2. 1.
      6293.48000        0.196979000E-02
      949.044000        0.149613000E-01
      218.776000        0.735006000E-01
      63.6916000        0.248937000
      18.8282000        0.602460000
      2.72023000        0.256202000
0 1 3 5. 1.
      30.6331000        0.111906000       0.383119000E-01
      7.02614000        0.921666000       0.237403000
      2.11205000       -0.256919000E-02   0.817592000
0 1 1 0. 1.
     0.684009000         1.00000000        1.00000000
0 1 1 0. 1.
     0.200878000         1.00000000        1.00000000
0 3 1 0. 1.
     0.913000000         1.00000000
8 6
0 0 8 2.0 1.0
 8020. 0.001080
 1338. 0.008040
 255.4 0.053240
 69.22 0.168100
 23.90 0.358100
 9.264 0.385500
 3.851 0.146800
 1.212 0.072800
0 1 4 6. 1.0
 49.43 -0.008830 0.009580
 10.47 -0.091500 0.069600
 3.235 -0.040200 0.206500
 1.217 0.379000 0.347000
0 1 1 0. 1.0
 0.486 1. 1.
0 1 1 0. 1.0
 0.1925 1. 1.
0 3 1 0. 1.
 2.0 1.
0 3 1 0. 1.
 0.500 1.
99 0
END
DFT
B3LYP
XLGRID
END
```

```
SHRINK
4 8
LEVSHIFT
10 1
TOLINTEG
9 9 9 9 30
EXCHSIZE
15000000
BIPOSIZE
15000000
FMIXING
50
MAXCYCLE
150
SCFDIR
END
+++ ENERGIES IN A.U. +++
 ::: EXT EL-POLE                      -5.4493581684076E+03
 ::: EXT EL-SPHEROPOLE                    3.8565730607934E+01
 ::: BIELET ZONE E-E                   5.9878406220557E+03
 ::: TOTAL E-E                        5.7704818425606E+02
 ::: TOTAL E-N + N-E                   -3.9884760921097E+03
 ::: TOTAL N-N                        -4.2104999207712E+02
 ::: KINETIC ENERGY                    2.0151060515477E+03
 ::: PSEUDO TOTAL   ENERGY                -1.8173718483831E+03
 ::: VIRIAL COEFFICIENT                1.0515943492246E+00
 TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3      TELAPSE   132363.05 TCPU   132342.28
 NUMERICALLY INTEGRATED DENSITY    264.0001025062
 TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT      TELAPSE   132490.38 TCPU   132469.56
 CYC  27 ETOT(AU) -2.023323307676E+03 DETOT -7.04E-07 tst  3.74E-07 PX  6.78E-05
 == SCF ENDED - CONVERGENCE ON ENERGY      E(AU) -2.0233233076763E+03 CYCLES  27
 ENERGY EXPRESSION=HARTREE+FOCK EXCH*0.20000+(BECKE  EXCH)*0.80000+LYP    CORR
 TOTAL ENERGY(DFT)(AU)( 27) -2.0233233076763E+03 DE-7.0E-07 tester 3.7E-07
```

Table S3. Multipole populations from theoretical structure factors.

```
loop_
_atom_rho_multipole_atom_label
_atom_rho_multipole_coeff_Pv
_atom_rho_multipole_coeff_P00
_atom_rho_multipole_coeff_P11
_atom_rho_multipole_coeff_P1-1
_atom_rho_multipole_coeff_P10
_atom_rho_multipole_coeff_P20
_atom_rho_multipole_coeff_P21
_atom_rho_multipole_coeff_P2-1
_atom_rho_multipole_coeff_P22
_atom_rho_multipole_coeff_P2-2
_atom_rho_multipole_coeff_P30
_atom_rho_multipole_coeff_P31
_atom_rho_multipole_coeff_P3-1
_atom_rho_multipole_coeff_P32
_atom_rho_multipole_coeff_P3-2
_atom_rho_multipole_coeff_P33
_atom_rho_multipole_coeff_P3-3
_atom_rho_multipole_coeff_P40
_atom_rho_multipole_coeff_P41
_atom_rho_multipole_coeff_P4-1
_atom_rho_multipole_coeff_P42
_atom_rho_multipole_coeff_P4-2
_atom_rho_multipole_coeff_P43
_atom_rho_multipole_coeff_P4-3
_atom_rho_multipole_coeff_P44
_atom_rho_multipole_coeff_P4-4
_atom_rho_multipole_kappa
_atom_rho_multipole_kappa_prime0
_atom_rho_multipole_kappa_prime1
_atom_rho_multipole_kappa_prime2
_atom_rho_multipole_kappa_prime3
_atom_rho_multipole_kappa_prime4
_atom_rho_multipole_radial_slater_n0
_atom_rho_multipole_radial_slater_zeta0
_atom_rho_multipole_radial_slater_n1
_atom_rho_multipole_radial_slater_zeta1
_atom_rho_multipole_radial_slater_n2
_atom_rho_multipole_radial_slater_zeta2
_atom_rho_multipole_radial_slater_n3
_atom_rho_multipole_radial_slater_zeta3
_atom_rho_multipole_radial_slater_n4
_atom_rho_multipole_radial_slater_zeta4
O(1C) 2.0059(3) 0 -0.00450(15) -0.00440(15) 0.01150(18)
-0.0111(3) 0 0 -0.0026(2) 0
0.0012(4) 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
0.99133(15) 1 0.8 0.8 1.2 1
2 4.4974 2 4.4974 2 4.4974 3 4.4974 4 4.4974
O(2C) 2.0058(3) 0 0 0 0.01420(18)
-0.0107(3) 0 0 -0.0023(2) 0
0.0012(4) 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
```

0.99133(15) 1 0.8 0.8 1.2 1
2 4.4974 2 4.4974 2 4.4974 3 4.4974 4 4.4974
O(3C) 2.0060(3) 0 0 0 0.01350(18)
-0.0111(3) 0 0 -0.0024(2) 0
0.0012(4) 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
0.99133(15) 1 0.8 0.8 1.2 1
2 4.4974 2 4.4974 2 4.4974 3 4.4974 4 4.4974
O(4C) 2.0058(3) 0 -0.00300(15) 0 0.00960(18)
-0.0110(3) 0 0 -0.0024(2) 0
0.0010(4) 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
0.99133(15) 1 0.8 0.8 1.2 1
2 4.4974 2 4.4974 2 4.4974 3 4.4974 4 4.4974
O(5C) 2.0059(3) 0 0 0 0.00980(18)
-0.0111(3) 0 0 -0.0024(2) 0
0.0013(4) 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
0.99133(15) 1 0.8 0.8 1.2 1
2 4.4974 2 4.4974 2 4.4974 3 4.4974 4 4.4974
O(6C) 2.0057(3) 0 0.00360(15) 0 0.00820(18)
-0.0110(3) 0 0 -0.0024(2) 0
0.0011(4) 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
0.99133(15) 1 0.8 0.8 1.2 1
2 4.4974 2 4.4974 2 4.4974 3 4.4974 4 4.4974
O(1) 6.300(2) 0 0.0013(4) -0.0024(4) -0.0909(5)
-0.1178(6) 0.0001(4) -0.0112(4) -0.0867(5) 0.0121(4)
0.1039(15) 0.0039(11) -0.0130(11) 0.0319(12) -0.0053(11) 0.0004(10) -0.0036(10)
0.0496(13) 0.0009(10) -0.0053(10) 0.0134(11) -0.0020(11) 0.0001(11) -0.0027(11)
-0.0005(9) -0.0002(9)
0.98142(13) 1 1.342(4) 1.105(2) 0.691(2) 0.810(5)
2 4.4974 2 4.4974 2 4.4974 3 4.4974 4 4.4974
O(2) 6.311(2) 0 0.0032(3) -0.0027(3) -0.0911(5)
-0.1236(6) 0.0013(4) -0.0117(4) -0.0818(5) -0.0009(4)
0.1047(15) -0.0020(11) -0.0101(11) 0.0284(12) 0.0001(11) -0.0019(10) -0.0014(10)
0.0499(13) -0.0006(10) -0.0044(10) 0.0114(11) -0.0002(11) -0.0005(10)
-0.0015(11) -0.0020(9) -0.0002(9)
0.98142(13) 1 1.342(4) 1.105(2) 0.691(2) 0.810(5)
2 4.4974 2 4.4974 2 4.4974 3 4.4974 4 4.4974
O(3) 6.300(2) 0 0.0005(3) -0.0064(3) -0.0916(5)
-0.1169(6) -0.0001(4) -0.0110(4) -0.0877(5) -0.0015(4)
0.1053(15) -0.0008(11) -0.0131(11) 0.0321(12) 0.0010(11) 0.0000(10) -0.0042(10)
0.0495(13) 0.0000(10) -0.0052(10) 0.0117(11) 0.0016(11) -0.0007(11) -0.0021(11)
-0.0010(9) 0.0004(9)
0.98142(13) 1 1.342(4) 1.105(2) 0.691(2) 0.810(5)
2 4.4974 2 4.4974 2 4.4974 3 4.4974 4 4.4974
O(4) 6.312(2) 0 0.0009(4) -0.0075(3) -0.0896(5)
-0.1203(6) 0.0003(4) -0.0116(4) -0.0831(5) -0.0013(4)
0.1089(15) 0.0002(11) -0.0113(11) 0.0299(12) 0.0013(11) 0.0000(10) -0.0020(10)
0.0521(13) 0.0005(10) -0.0062(10) 0.0115(11) 0.0005(11) 0.0003(10) -0.0021(11)
-0.0017(9) -0.0005(9)
0.98142(13) 1 1.342(4) 1.105(2) 0.691(2) 0.810(5)
2 4.4974 2 4.4974 2 4.4974 3 4.4974 4 4.4974
O(5) 6.305(2) 0 0.0014(3) -0.0005(3) -0.0905(5)
-0.1189(6) 0.0002(4) -0.0119(4) -0.0849(5) -0.0153(4)

0.1046(15) -0.0026(11) -0.0120(11) 0.0296(12) 0.0063(11) -0.0001(10) -0.0045(10)
0.0500(13) -0.0001(10) -0.0067(10) 0.0115(11) 0.0008(11) 0.0001(11) -0.0029(11)
-0.0007(9) -0.0002(9)
0.98142(13) 1 1.342(4) 1.105(2) 0.691(2) 0.810(5)
2 4.4974 2 4.4974 2 4.4974 3 4.4974 4 4.4974
O(6) 6.317(2) 0 -0.0011(4) -0.0036(3) -0.0891(5)
-0.1225(6) -0.0019(4) -0.0122(4) -0.0816(5) -0.0028(4)
0.1076(15) 0.0003(11) -0.0104(11) 0.0289(12) 0.0010(11) 0.0003(10) -0.0041(10)
0.0518(13) 0.0009(10) -0.0059(10) 0.0122(11) -0.0007(11) -0.0002(10) -0.0025(11)
-0.0010(9) -0.0007(9)
0.98142(13) 1 1.342(4) 1.105(2) 0.691(2) 0.810(5)
2 4.4974 2 4.4974 2 4.4974 3 4.4974 4 4.4974
N(1C) 2.0099(3) 0 -0.00230(11) -0.00250(11) 0
0.0035(2) 0 0 0.0050(2) 0
0 0 0 0 0 -0.0024(3) 0
0 0 0 0 0 0 0 0 0 0
0.98911(19) 1 1 0.6 1.2 1
2 3.81056 2 3.81056 2 3.81056 3 3.81056 4 3.81056
N(2C) 2.0037(3) 0 0.00280(15) 0 -0.00110(12)
0.0104(2) 0.0003(2) 0.0000(2) -0.0069(2) 0
0 0 0 0 0 -0.0014(3) 0
0 0 0 0 0 0 0 0 0 0
0.99190(18) 1 1 0.6 1.2 1
2 3.81056 2 3.81056 2 3.81056 3 3.81056 4 3.81056
N(3C) 2.0100(3) 0 -0.00190(11) 0 0.00120(11)
0.0034(2) 0 0 0.0051(2) 0
0 0 0 0 0 -0.0025(3) 0
0 0 0 0 0 0 0 0 0 0
0.98911(19) 1 1 0.6 1.2 1
2 3.81056 2 3.81056 2 3.81056 3 3.81056 4 3.81056
N(4C) 2.0037(3) 0 -0.00220(15) -0.00380(13) -0.00140(12)
0.0104(3) -0.0007(2) -0.0006(2) -0.0063(2) 0
0 0 0 0 0 -0.0014(3) 0
0 0 0 0 0 0 0 0 0 0
0.99190(18) 1 1 0.6 1.2 1
2 3.81056 2 3.81056 2 3.81056 3 3.81056 4 3.81056
N(5C) 2.0100(3) 0 -0.00170(11) 0 0
0.0036(2) 0 0 0.0052(2) 0
0 0 0 0 0 -0.0025(3) 0
0 0 0 0 0 0 0 0 0 0
0.98911(19) 1 1 0.6 1.2 1
2 3.81056 2 3.81056 2 3.81056 3 3.81056 4 3.81056
N(6C) 2.0037(3) 0 0.00150(15) 0 0
0.0100(3) 0.0008(2) -0.0006(2) -0.0062(2) 0
0 0 0 0 0 -0.0016(3) 0
0 0 0 0 0 0 0 0 0 0
0.99190(18) 1 1 0.6 1.2 1
2 3.81056 2 3.81056 2 3.81056 3 3.81056 4 3.81056
N(1) 4.951(5) 0 0.083(2) 0.0041(10) 0.0073(9)
-0.285(2) -0.0030(15) 0.0048(14) 0.028(2) -0.0031(17)
-0.0024(11) 0.0044(12) -0.0003(11) -0.0011(12) -0.0021(11) 0.295(2) 0.0012(11)
0.072(3) 0.003(2) -0.004(2) 0.000(2) 0.004(2) 0.009(2) 0.001(2) 0.047(3)
-0.007(3)
0.9871(4) 1 0.828(7) 0.5906(16) 0.834(2) 0.625(6)
2 3.81056 2 3.81056 2 3.81056 3 3.81056 4 3.81056
N(2) 4.914(5) 0 -0.0266(8) -0.0011(4) 0.0012(5)

-0.0664(18) 0.0076(16) 0.0044(18) -0.080(2) -0.0029(16)
0.0032(11) 0.0438(12) 0.0014(11) 0.0014(12) -0.0120(14) 0.246(2) 0.0009(15)
0.0296(17) -0.0022(14) -0.0045(14) 0.0286(15) 0.0007(15) -0.0029(14) -0.0005(18)
-0.0168(17) -0.0002(14)
1.0049(3) 1 1.361(19) 0.684(5) 0.825(2) 0.833(9)
2 3.81056 2 3.81056 2 3.81056 3 3.81056 4 3.81056
N(3) 4.942(5) 0 0.085(2) 0.0047(10) -0.0004(10)
-0.290(2) 0.0032(15) -0.0001(14) 0.022(2) -0.0055(17)
0.0002(11) 0.0012(11) -0.0017(11) 0.0008(12) -0.0002(11) 0.296(2) 0.0018(11)
0.072(3) -0.001(2) -0.002(2) -0.003(2) 0.005(2) -0.005(2) -0.002(2) 0.059(3)
0.004(3)
0.9871(4) 1 0.828(7) 0.5906(16) 0.834(2) 0.625(6)
2 3.81056 2 3.81056 2 3.81056 3 3.81056 4 3.81056
N(4) 4.910(5) 0 -0.0251(8) 0.0012(5) 0.0006(5)
-0.0716(19) -0.0091(16) 0.0023(18) -0.082(2) -0.0038(16)
0.0049(11) 0.0442(12) -0.0006(11) 0.0023(12) 0.0127(14) 0.247(2) 0.0015(15)
0.0305(17) 0.0000(14) 0.0064(14) 0.0292(15) -0.0004(15) -0.0045(14) 0.0008(18)
-0.0155(17) 0.0025(14)
1.0049(3) 1 1.361(19) 0.684(5) 0.825(2) 0.833(9)
2 3.81056 2 3.81056 2 3.81056 3 3.81056 4 3.81056
N(5) 4.949(5) 0 0.088(2) 0.0052(10) -0.0064(9)
-0.283(2) -0.0004(15) -0.0035(14) 0.029(2) -0.0073(17)
0.0018(11) 0.0032(12) -0.0008(11) 0.0000(12) -0.0001(11) 0.293(2) -0.0003(11)
0.069(3) -0.004(2) 0.000(2) -0.008(2) 0.003(2) -0.005(2) 0.001(2) 0.049(3)
0.003(3)
0.9871(4) 1 0.828(7) 0.5906(16) 0.834(2) 0.625(6)
2 3.81056 2 3.81056 2 3.81056 3 3.81056 4 3.81056
N(6) 4.913(5) 0 -0.0258(8) -0.0028(4) -0.0014(4)
-0.0759(19) -0.0028(15) 0.0124(18) -0.087(2) 0.0002(16)
-0.0033(11) 0.0470(12) 0.0011(11) -0.0040(12) -0.0124(14) 0.249(2) 0.0021(15)
0.0327(17) 0.0013(14) -0.0036(14) 0.0287(15) -0.0017(15) 0.0009(14) -0.0024(18)
-0.0214(17) -0.0003(14)
1.0049(3) 1 1.361(19) 0.684(5) 0.825(2) 0.833(9)
2 3.81056 2 3.81056 2 3.81056 3 3.81056 4 3.81056
C(1C) 2.0068(3) 0 0 0.00110(12) 0
0.0043(2) 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
0.99031(16) 1 1 1 1 1
2 3.1303 2 3.1303 2 3.1303 3 3.1303 4 3.1303
C(2C) 2.0126(3) 0 -0.00220(11) -0.00350(11) 0
-0.00160(18) 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
0.98432(15) 1 1 1 1 1
2 3.1303 2 3.1303 2 3.1303 3 3.1303 4 3.1303
C(3C) 2.0069(3) 0 -0.00340(12) -0.00260(12) 0
0.0044(2) 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
0.99031(16) 1 1 1 1 1
2 3.1303 2 3.1303 2 3.1303 3 3.1303 4 3.1303
C(4C) 2.0127(3) 0 -0.00120(11) 0.00180(11) 0
-0.00160(18) 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0

0.98432(15) 1 1 1 1 1
2 3.1303 2 3.1303 2 3.1303 3 3.1303 4 3.1303
C(5C) 2.0069(3) 0 -0.00160(12) 0 -0.00170(12)
0.0043(2) 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
0.99031(16) 1 1 1 1 1
2 3.1303 2 3.1303 2 3.1303 3 3.1303 4 3.1303
C(6C) 2.0125(3) 0 -0.00040(11) 0 -0.00150(11)
-0.00150(18) 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
0.98432(15) 1 1 1 1 1
2 3.1303 2 3.1303 2 3.1303 3 3.1303 4 3.1303
C(1) 3.644(8) 0 0.0281(14) 0.0546(19) -0.0018(10)
0.0181(8) 0.0015(6) 0.0021(6) 0.0238(8) -0.0382(10)
-0.0024(13) 0.0018(13) 0.0024(13) -0.0020(14) 0.0107(14) 0.220(3) 0.0085(15)
0.0077(10) 0.0001(8) 0.0008(8) 0.0021(8) -0.0035(9) 0.0006(8) 0.0002(9)
-0.0032(8) -0.0057(9)
1.0195(5) 1 1.051(11) 1.194(11) 0.948(4) 1.36(4)
2 3.1303 2 3.1303 2 3.1303 3 3.1303 4 3.1303
C(2) 4.269(8) 0 0 0 0
-0.343(2) 0.0025(14) 0.0020(14) 0.0006(16) 0.0022(16)
0.0015(14) 0.0015(14) 0.0012(15) 0.0029(16) -0.0005(15) 0.377(4) -0.0163(17)
0.041(2) 0.0004(15) 0.0003(16) 0.0019(17) -0.0052(17) 0.0006(16) 0.0021(19)
-0.0129(18) -0.0154(19)
0.9793(5) 1 1 0.7936(17) 0.877(2) 0.942(11)
2 3.1303 2 3.1303 2 3.1303 3 3.1303 4 3.1303
C(3) 3.631(8) 0 0.0317(14) 0.057(2) 0.0016(10)
0.0170(8) 0.0004(6) -0.0010(6) 0.0242(8) -0.0400(11)
0.0026(13) 0.0014(13) 0.0029(13) -0.0017(14) -0.0042(14) 0.221(3) 0.0090(15)
0.0071(10) 0.0003(8) -0.0005(8) 0.0021(8) -0.0039(9) -0.0003(8) -0.0006(9)
-0.0023(8) -0.0043(9)
1.0195(5) 1 1.051(11) 1.194(11) 0.948(4) 1.36(4)
2 3.1303 2 3.1303 2 3.1303 3 3.1303 4 3.1303
C(4) 4.262(8) 0 0 0 0
-0.345(2) -0.0023(14) -0.0029(14) -0.0051(16) 0.0029(16)
0.0004(14) 0.0002(14) 0.0016(15) 0.0005(16) 0.0037(15) 0.376(4) -0.0088(17)
0.043(2) 0.0011(15) -0.0001(16) 0.0025(17) -0.0027(17) 0.0002(16) -0.0018(19)
-0.0099(18) -0.0161(19)
0.9793(5) 1 1 0.7936(17) 0.877(2) 0.942(11)
2 3.1303 2 3.1303 2 3.1303 3 3.1303 4 3.1303
C(5) 3.635(8) 0 0.0301(14) 0.054(2) 0.0023(10)
0.0166(8) -0.0021(6) -0.0015(6) 0.0231(8) -0.0389(11)
-0.0008(13) 0.0023(13) 0.0006(13) 0.0035(14) -0.0085(14) 0.221(3) 0.0066(15)
0.0069(10) -0.0002(8) -0.0007(8) 0.0020(8) -0.0035(9) -0.0004(8) 0.0001(9)
-0.0035(9) -0.0055(9)
1.0195(5) 1 1.051(11) 1.194(11) 0.948(4) 1.36(4)
2 3.1303 2 3.1303 2 3.1303 3 3.1303 4 3.1303
C(6) 4.273(8) 0 0 0 0
-0.342(2) -0.0013(14) -0.0004(14) -0.0046(16) 0.0067(16)
-0.0017(14) 0.0009(14) 0.0001(15) -0.0016(16) 0.0011(15) 0.377(4) -0.0117(17)
0.040(2) 0.0022(15) 0.0003(16) 0.0042(17) -0.0032(17) -0.0003(16) -0.0028(19)
-0.0098(18) -0.0142(19)
0.9793(5) 1 1 0.7936(17) 0.877(2) 0.942(11)
2 3.1303 2 3.1303 2 3.1303 3 3.1303 4 3.1303

H(1) 0.7938(18) 0 -0.0019(13) -0.0065(14) 0.1982(12)
0.1097(17) -0.0023(16) -0.0241(17) -0.0054(16) -0.0009(16)
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.2 1.2 1.2 1.2 1.2 1.2
0 1.9154 1 1.9154 2 1.9154 3 1.9154 4 1.9154
H(2) 0.7901(18) 0 -0.0148(13) -0.0222(14) 0.1994(12)
0.1109(17) -0.0062(16) -0.0290(17) -0.0026(16) -0.0012(16)
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.2 1.2 1.2 1.2 1.2 1.2
0 1.9154 1 1.9154 2 1.9154 3 1.9154 4 1.9154
H(3) 0.7867(18) 0 0.0352(13) -0.0181(14) 0.1958(12)
0.1108(17) 0.0170(16) -0.0283(17) -0.0027(16) -0.0005(16)
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.2 1.2 1.2 1.2 1.2 1.2
0 1.9154 1 1.9154 2 1.9154 3 1.9154 4 1.9154
H(4) 0.7938(18) 0 0.0200(13) -0.0316(14) 0.2004(12)
0.1135(17) 0.0156(16) -0.0348(17) -0.0015(16) -0.0023(16)
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.2 1.2 1.2 1.2 1.2 1.2
0 1.9154 1 1.9154 2 1.9154 3 1.9154 4 1.9154
H(5) 0.7868(18) 0 0.0250(13) -0.0248(14) 0.1956(12)
0.1137(17) 0.0130(16) -0.0278(17) -0.0033(16) -0.0004(16)
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.2 1.2 1.2 1.2 1.2 1.2
0 1.9154 1 1.9154 2 1.9154 3 1.9154 4 1.9154
H(6) 0.7793(18) 0 0.0070(13) -0.0462(14) 0.1977(12)
0.1104(17) 0.0025(16) -0.0395(17) 0.0002(16) 0.0016(16)
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.2 1.2 1.2 1.2 1.2 1.2
0 1.9154 1 1.9154 2 1.9154 3 1.9154 4 1.9154

##
Local CIF definition in XD - local coordinate systems
##

loop_
_atom_local_axes_atom_label
_atom_local_axes_atom0
_atom_local_axes_ax1
_atom_local_axes_atom1
_atom_local_axes_atom2
_atom_local_axes_ax2
O(1C) N(1) Z O(1) N(6) Y
O(2C) N(1) Z O(2) N(2) Y
O(3C) N(3) Z O(3) N(2) Y
O(4C) N(3) Z O(4) N(4) Y
O(5C) N(5) Z O(5) N(4) Y
O(6C) N(5) Z O(6) N(6) Y
O(1) N(1) Z O(1) N(6) Y
O(2) N(1) Z O(2) N(2) Y

O(3)	N(3)	Z	O(3)	N(2)	Y
O(4)	N(3)	Z	O(4)	N(4)	Y
O(5)	N(5)	Z	O(5)	N(4)	Y
O(6)	N(5)	Z	O(6)	N(6)	Y
N(1C)	C(1)	X	N(1)	O(1)	Y
N(2C)	C(2)	X	N(2)	O(2)	Y
N(3C)	C(3)	X	N(3)	O(3)	Y
N(4C)	C(4)	X	N(4)	O(4)	Y
N(5C)	C(5)	X	N(5)	O(5)	Y
N(6C)	C(6)	X	N(6)	O(6)	Y
N(1)	C(1)	X	N(1)	O(1)	Y
N(2)	C(2)	X	N(2)	O(2)	Y
N(3)	C(3)	X	N(3)	O(3)	Y
N(4)	C(4)	X	N(4)	O(4)	Y
N(5)	C(5)	X	N(5)	O(5)	Y
N(6)	C(6)	X	N(6)	O(6)	Y
C(1C)	C(2)	X	C(1)	C(6)	Y
C(2C)	C(3)	X	C(2)	C(1)	Y
C(3C)	C(4)	X	C(3)	C(2)	Y
C(4C)	C(5)	X	C(4)	C(3)	Y
C(5C)	C(6)	X	C(5)	C(4)	Y
C(6C)	C(1)	X	C(6)	C(5)	Y
C(1)	C(2)	X	C(1)	C(6)	Y
C(2)	C(3)	X	C(2)	C(1)	Y
C(3)	C(4)	X	C(3)	C(2)	Y
C(4)	C(5)	X	C(4)	C(3)	Y
C(5)	C(6)	X	C(5)	C(4)	Y
C(6)	C(1)	X	C(6)	C(5)	Y
H(1)	N(2)	Z	H(1)	O(2)	Y
H(2)	N(2)	Z	H(2)	O(3)	Y
H(3)	N(4)	Z	H(3)	O(4)	Y
H(4)	N(4)	Z	H(4)	O(5)	Y
H(5)	N(6)	Z	H(5)	O(6)	Y
H(6)	N(6)	Z	H(6)	O(1)	Y

Table S4. Reflection statistics in equal volume resolutions shells

Sinθ/λ(max)	N(data)	<I/σ>	Completeness %	R
0.4900	841	145.05	100.0	0.0170
0.6174	826	93.10	100.0	0.0252
0.7067	843	58.97	99.4	0.0317
0.7779	803	42.56	97.9	0.0279
0.8379	791	35.15	94.5	0.0342
0.8904	800	30.42	94.6	0.0359
0.9374	773	27.88	91.3	0.0384
0.9800	750	24.23	90.7	0.0483
1.0193	760	20.99	89.5	0.0553
1.0557	678	18.98	85.3	0.0615
1.0898	749	19.26	80.3	0.0569
1.1219	693	16.97	87.3	0.0626
1.1522	699	15.08	85.7	0.0713
1.1810	694	14.75	81.9	0.0739
1.2085	678	13.69	80.9	0.0778
1.2348	633	13.76	76.1	0.0753
1.2600	687	12.44	74.7	0.0842
1.2842	604	12.42	67.0	0.0839
1.3076	621	8.76	100.0	0.0974
1.3301	379	9.68	40.7	0.0769