Table D1. HMX C–H bond distances (Å) obtained from various refinements.

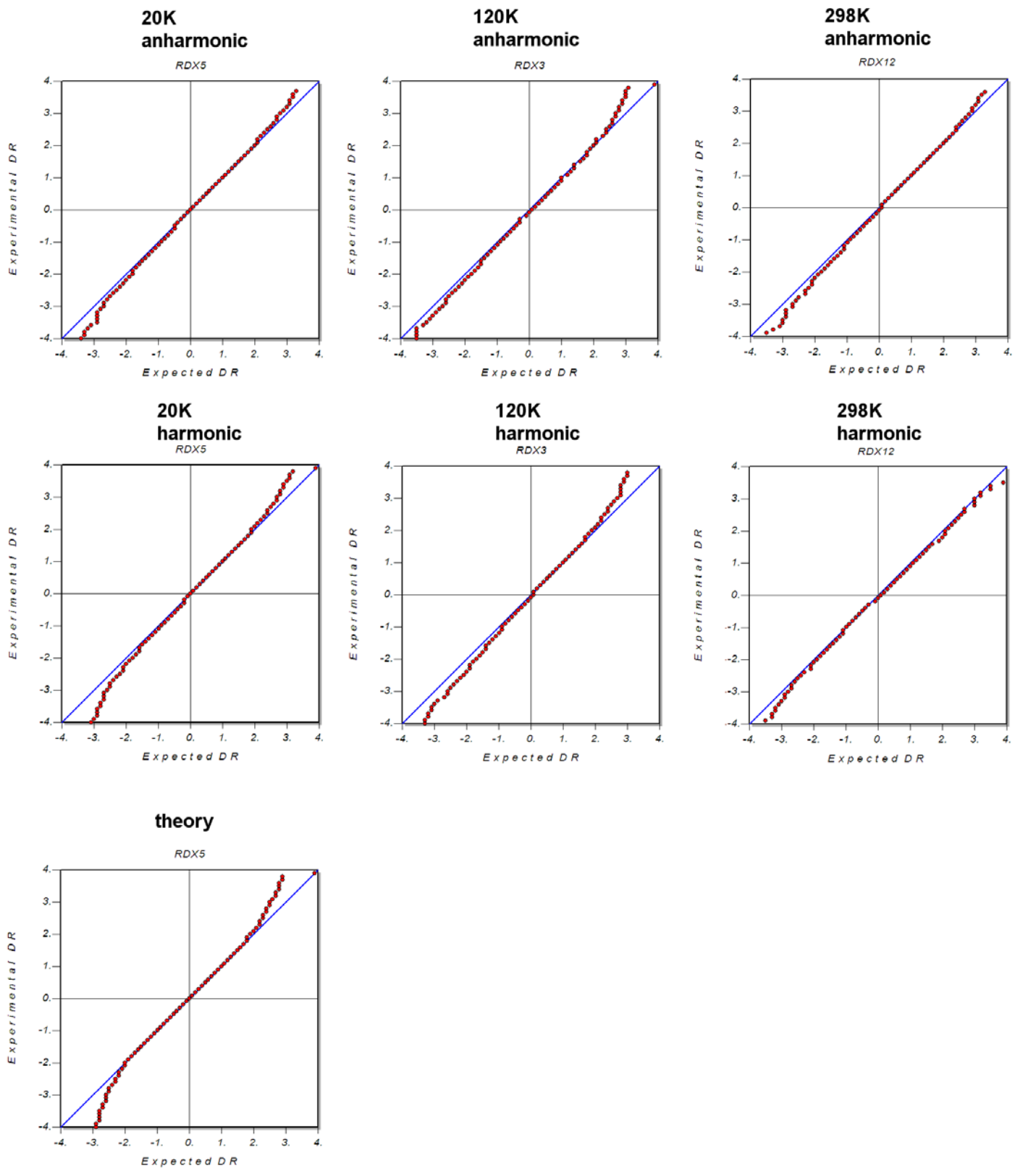
Bond	1	2	3	4
C(1) – H(1A)	1.104(16)	1.110(15)	1.084(9)	1.088(11)
C(1) – H(1B)	1.079(12)	1.078(12)	1.073(8)	1.076(10)
C(2) – H(2A)	1.091(15)	1.095(14)	1.094(9)	1.093(10)
C(2) – H(2B)	1.115(13)	1.113(13)	1.090(8)	1.087(10)

1– 20K, anharmonic refinement, 2 – 20 K harmonic refinement, 3– 120K, anharmonic refinement, 4 – 120 K harmonic refinement. Average neutron distance is 1.091 Å (Allen & Bruno, 2010).

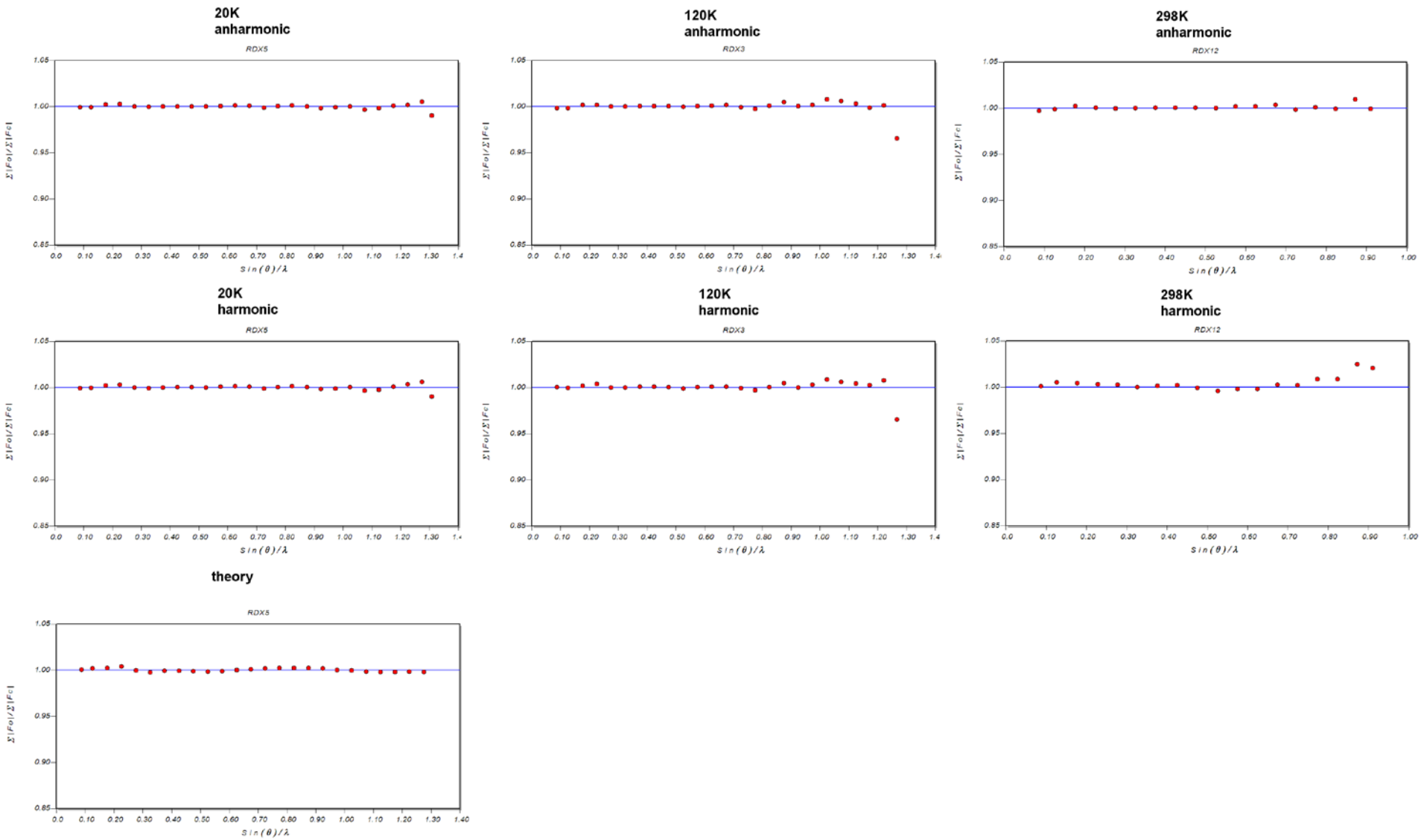
Table D2. Critical point properties for the N – N, O – N and O – O bonding interactions in the RDX crystal as been found at 20K from the anharmonic model refinement.

Bond	ρ, eÅ^{-3}	$\nabla^2\rho$, eÅ^{-5}	R_{ij}, Å	g, a.u.	*v*, a.u.	h_e, a.u.
N(2) – N(6)	0.078	0.93	2.926	0.0081	-0.0066	0.0015
O(6) – N(5)	0.070	0.89	2.865	0.0076	-0.0059	0.0017
O(6) – O(6)	0.069	0.95	2.952	0.0079	-0.0060	0.0019
O(1) – O(5)	0.067	0.97	2.884	0.0080	-0.0060	0.0020
O(1) – O(3)	0.047	0.69	3.019	0.0055	-0.0039	0.0017
O(4) – N(1)	0.058	0.80	3.052	0.0066	-0.0048	0.0018
O(3) – O(3)	0.040	0.59	3.002	0.0047	-0.0032	0.0015
O(6) – N(1)	0.034	0.44	3.320	0.0035	-0.0024	0.0011
O(2) – O(4)	0.025	0.36	3.277	0.0027	-0.0018	0.0010

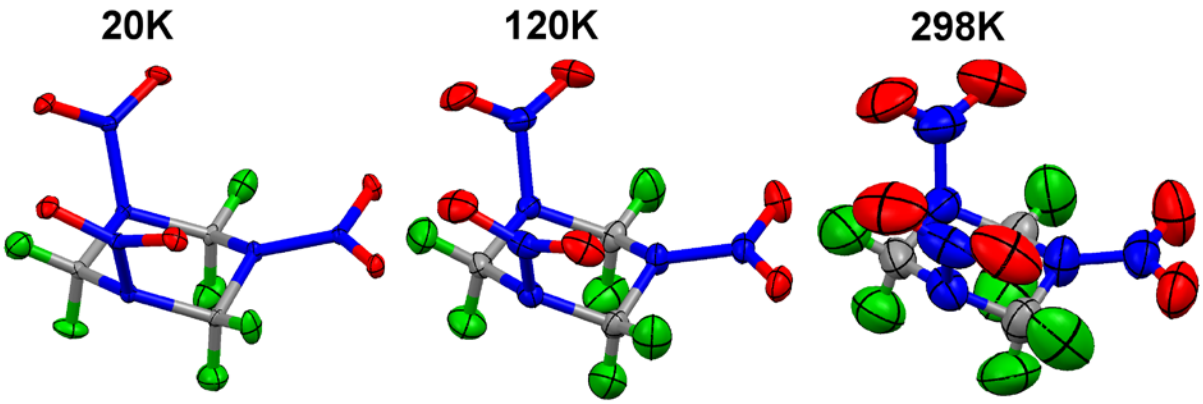
All interactions are intermolecular; ρ is the electron density; $\nabla^2\rho$ is the Laplacian; R_{ij} is interatomic distance, *g*, *v* and h_e are the kinetic, potential and total electronic energies at the critical point, respectively. All virial paths have been verified.



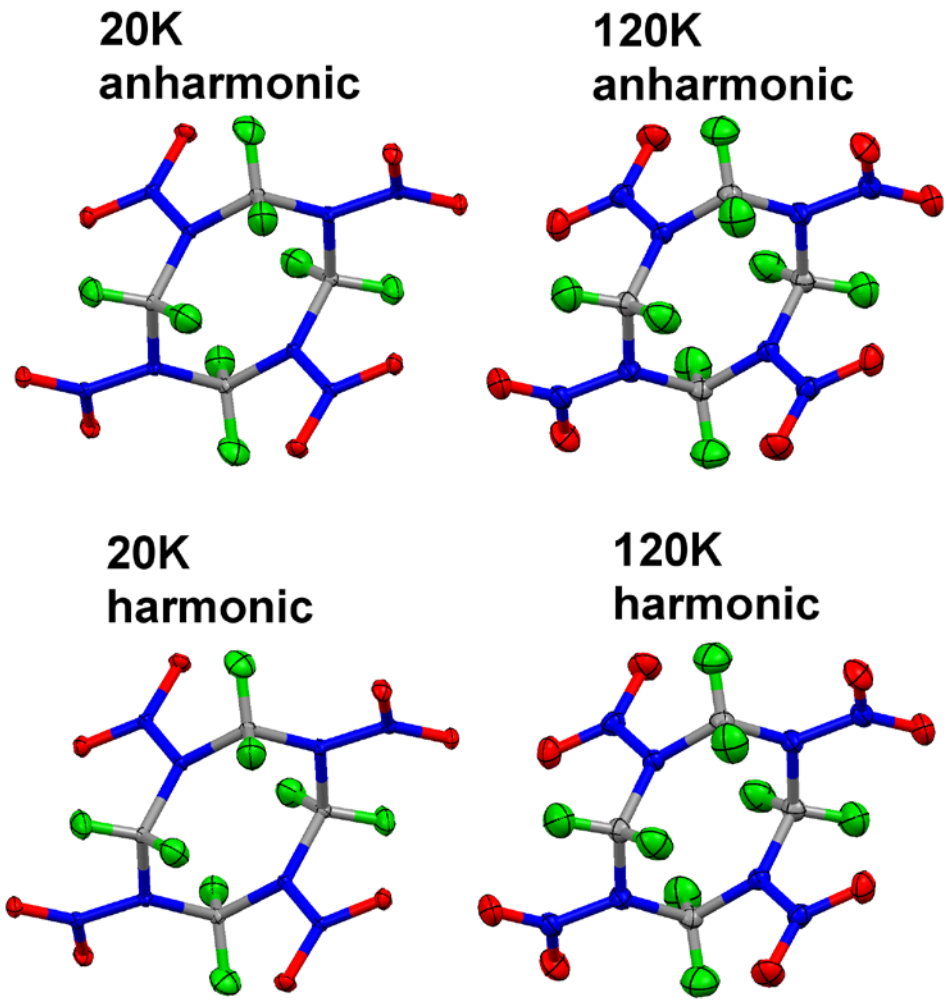
FigD1. Normal probability plots for various RDX refinements at different temperatures.



FigD2. Variation of scale factor, $\Sigma|F_{obs}|/\Sigma|F_{calc}|$, with respect to resolution for various RDX refinements at different temperatures.



FigD3. RDX atomic thermal ellipsoids at the 75% probability level from harmonic model refinements.



FigD4. HMX atomic thermal ellipsoids at the 75% probability level.

Table D3. Bond critical points in the RDX crystal: intramolecular bonds.

Bond		ρ, eÅ^{-3}	$\nabla^2\rho$, eÅ^{-5}	R, Å	d_1, Å	d_2, Å	λ_1, eÅ^{-5}	λ_2, eÅ^{-5}	λ_3, eÅ^{-5}	ε	n_{topo}
O(1) – N(4)	1	3.347	-12.70	1.229	0.631	0.597	-31.238	-28.588	47.124	0.093	1.86
	2	3.372	-14.59	1.226	0.623	0.604	-31.527	-28.741	45.678	0.097	1.85
	3	3.314	-12.11	1.229	0.633	0.596	-29.967	-27.885	45.739	0.075	1.85
	4	3.351	-17.34	1.225	0.647	0.579	-31.346	-28.875	42.883	0.086	1.77
	5	3.146	-3.22	1.219	0.636	0.582	-26.221	-25.319	48.325	0.036	1.89
	6	3.430	-19.73	1.231	0.689	0.549	-34.920	-30.530	45.724	0.144	1.80
	7	3.233	-11.52	1.229	0.627	0.602	-28.607	-26.854	43.942	0.065	1.79
O(2) – N(4)	1	3.301	-12.53	1.235	0.642	0.593	-30.845	-28.309	46.621	0.090	1.83
	2	3.314	-13.93	1.231	0.633	0.598	-31.070	-28.338	45.474	0.096	1.81
	3	3.243	-10.02	1.233	0.636	0.597	-28.838	-26.921	45.740	0.071	1.83
	4	3.283	-15.74	1.227	0.624	0.603	-29.391	-26.258	39.911	0.119	1.74
	5	3.165	-4.48	1.224	0.641	0.584	-26.971	-25.379	47.875	0.063	1.88
	6	3.585	-28.56	1.213	0.683	0.535	-36.740	-30.982	39.163	0.186	1.74
	7	3.188	-10.93	1.235	0.629	0.606	-28.154	-26.441	43.661	0.065	1.76
O(3) – N(5)	1	3.443	-14.98	1.222	0.631	0.591	-31.790	-30.622	47.432	0.038	1.90
	2	3.450	-16.12	1.219	0.622	0.597	-31.742	-30.521	46.147	0.040	1.88
	3	3.405	-14.83	1.219	0.636	0.584	-30.488	-30.066	45.720	0.014	1.87
	4	3.370	-15.51	1.221	0.648	0.573	-30.560	-29.585	44.633	0.033	1.82
	5	3.333	-7.87	1.208	0.639	0.570	-28.110	-27.560	47.798	0.020	1.94
	6	3.159	-7.63	1.241	0.692	0.568	-35.227	-23.625	51.218	0.491	1.82
	7	3.263	-12.33	1.222	0.625	0.597	-28.964	-27.408	44.041	0.057	1.80
O(4) – N(5)	1	3.339	-10.94	1.223	0.628	0.596	-30.124	-28.552	47.733	0.055	1.89
	2	3.350	-11.86	1.220	0.617	0.603	-29.878	-28.303	46.323	0.056	1.88
	3	3.396	-13.73	1.222	0.633	0.589	-30.482	-29.297	46.044	0.040	1.88
	4	3.496	-21.63	1.216	0.638	0.578	-32.951	-30.941	42.265	0.065	1.80
	5	3.281	-7.06	1.212	0.637	0.576	-28.210	-26.790	47.941	0.053	1.92
	6	3.667	-28.48	1.200	0.689	0.515	-35.818	-32.301	39.638	0.109	1.80
	7	3.259	-11.93	1.223	0.627	0.597	-28.827	-27.303	44.196	0.056	1.80
O(5) – N(6)	1	3.333	-10.61	1.222	0.624	0.598	-30.186	-28.116	47.695	0.074	1.89
	2	3.349	-12.23	1.218	0.611	0.607	-30.067	-28.121	45.954	0.069	1.87
	3	3.431	-14.10	1.221	0.633	0.588	-30.939	-29.472	46.315	0.050	1.90
	4	3.551	-23.24	1.212	0.619	0.594	-33.309	-30.471	40.536	0.093	1.81
	5	3.198	-2.62	1.214	0.634	0.580	-25.847	-25.586	48.816	0.010	1.94
	6	4.037	-49.38	1.188	0.733	0.464	-47.398	-36.487	34.508	0.299	1.69
	7	3.270	-11.78	1.222	0.626	0.597	-28.890	-27.256	44.366	0.060	1.81
O(6) – N(6)	1	3.391	-13.99	1.227	0.631	0.596	-31.449	-29.747	47.202	0.057	1.87
	2	3.397	-15.64	1.223	0.628	0.595	-31.471	-29.910	45.738	0.052	1.85
	3	3.341	-12.36	1.225	0.632	0.593	-29.540	-28.895	46.073	0.022	1.86
	4	3.331	-15.25	1.225	0.656	0.570	-30.698	-29.385	44.832	0.045	1.80
	5	3.275	-6.55	1.210	0.636	0.575	-27.777	-27.088	48.311	0.025	1.92
	6	3.358	-16.11	1.242	0.704	0.573	-37.421	-30.604	51.918	0.223	1.82
	7	3.224	-11.87	1.227	0.628	0.599	-28.493	-27.231	43.849	0.046	1.78
N(1) – N(4)	1	2.447	-10.63	1.359	0.664	0.695	-22.328	-17.817	29.514	0.253	1.36
	2	2.434	-10.23	1.359	0.661	0.698	-22.031	-17.537	29.342	0.256	1.38
	3	2.455	-10.36	1.356	0.658	0.698	-22.071	-17.384	29.091	0.270	1.42
	4	2.452	-9.94	1.358	0.666	0.693	-22.060	-17.483	29.607	0.262	1.42
	5	2.451	-10.22	1.350	0.670	0.680	-21.780	-18.036	29.593	0.208	1.40
	6	2.457	-10.71	1.352	0.659	0.694	-21.399	-16.408	27.095	0.304	1.52
	7	2.365	-8.14	1.359	0.663	0.696	-21.331	-16.565	29.756	0.288	1.39
N(2) – N(5)	1	2.214	-8.35	1.406	0.682	0.724	-19.961	-15.708	27.321	0.271	1.23
	2	2.210	-8.33	1.406	0.677	0.729	-19.817	-15.594	27.083	0.271	1.24
	3	2.243	-9.03	1.405	0.682	0.723	-20.137	-16.03	27.135	0.256	1.24
	4	2.238	-8.83	1.406	0.685	0.722	-20.139	-15.993	27.306	0.259	1.23

	5	2.205	-6.46	1.403	0.698	0.705	-18.753	-15.896	28.190	0.180	1.31
	6	2.204	-7.81	1.405	0.691	0.714	-18.946	-14.641	25.776	0.294	1.35
	7	2.140	-5.52	1.406	0.685	0.721	-18.715	-14.757	27.950	0.268	1.28
N(3) – N(6)	1	2.231	-8.47	1.403	0.685	0.718	-19.980	-16.231	27.739	0.231	1.22
	2	2.233	-8.59	1.404	0.68	0.724	-19.910	-16.095	27.415	0.237	1.24
	3	2.259	-9.80	1.403	0.682	0.722	-20.463	-16.303	26.964	0.255	1.22
	4	2.237	-8.89	1.404	0.684	0.721	-20.139	-15.946	27.193	0.263	1.23
	5	2.213	-6.91	1.394	0.689	0.706	-19.390	-15.542	28.022	0.248	1.30
	6	2.253	-8.71	1.401	0.703	0.699	-20.024	-15.916	27.232	0.258	1.28
	7	2.158	-5.77	1.403	0.681	0.722	-18.584	-15.067	27.878	0.233	1.30
N(1) – C(1)	1	1.810	-15.05	1.463	0.841	0.623	-14.026	-13.209	12.181	0.062	0.75
	2	1.799	-15.30	1.462	0.844	0.619	-13.938	-13.100	11.735	0.064	0.74
	3	1.788	-14.31	1.465	0.846	0.619	-13.640	-12.814	12.141	0.064	0.74
	4	1.774	-14.21	1.463	0.845	0.619	-13.505	-12.550	11.846	0.076	0.74
	5	1.808	-14.67	1.455	0.857	0.599	-13.273	-12.185	10.789	0.089	0.79
	6	1.814	-14.54	1.458	0.835	0.624	-14.027	-12.026	11.513	0.166	0.78
	7	1.695	-9.40	1.463	0.821	0.642	-12.970	-11.887	15.455	0.091	0.70
N(1) – C(2)	1	1.789	-14.11	1.466	0.841	0.625	-13.809	-12.677	12.374	0.089	0.75
	2	1.791	-14.27	1.465	0.839	0.627	-13.828	-12.674	12.236	0.091	0.75
	3	1.771	-13.63	1.466	0.849	0.617	-13.480	-12.301	12.152	0.096	0.74
	4	1.765	-13.18	1.465	0.847	0.618	-13.343	-11.946	12.108	0.117	0.75
	5	1.751	-12.86	1.453	0.859	0.595	-12.221	-11.507	10.869	0.062	0.77
	6	1.700	-12.18	1.462	0.896	0.568	-11.830	-10.277	9.930	0.151	0.74
	7	1.683	-8.85	1.466	0.823	0.643	-12.891	-11.530	15.570	0.118	0.70
N(2) – C(2)	1	1.813	-14.82	1.455	0.836	0.620	-13.527	-13.453	12.160	0.005	0.76
	2	1.814	-14.78	1.455	0.831	0.624	-13.486	-13.451	12.154	0.003	0.76
	3	1.841	-14.44	1.455	0.834	0.622	-13.743	-13.490	12.789	0.019	0.79
	4	1.833	-14.44	1.455	0.832	0.623	-13.562	-13.402	12.520	0.012	0.79
	5	1.814	-13.57	1.451	0.837	0.614	-12.869	-12.326	11.622	0.044	0.81
	6	1.935	-17.32	1.447	0.829	0.619	-14.810	-14.045	11.530	0.054	0.85
	7	1.733	-9.95	1.455	0.815	0.64	-12.923	-12.651	15.624	0.022	0.73
N(2) – C(3)	1	1.801	-14.13	1.465	0.841	0.625	-13.452	-13.146	12.467	0.023	0.76
	2	1.791	-14.20	1.466	0.845	0.621	-13.337	-12.986	12.120	0.027	0.75
	3	1.764	-13.63	1.467	0.849	0.619	-13.160	-12.674	12.208	0.038	0.73
	4	1.751	-13.75	1.465	0.849	0.618	-12.988	-12.596	11.838	0.031	0.72
	5	1.695	-11.22	1.458	0.842	0.616	-11.686	-11.069	11.534	0.056	0.73
	6	1.766	-14.57	1.464	0.875	0.590	-12.995	-11.831	10.258	0.098	0.75
	7	1.696	-9.45	1.465	0.821	0.645	-12.589	-12.360	15.497	0.018	0.70
N(3) – C(1)	1	1.802	-14.50	1.457	0.836	0.621	-13.483	-13.179	12.158	0.023	0.76
	2	1.799	-14.55	1.456	0.833	0.624	-13.445	-13.163	12.061	0.021	0.75
	3	1.820	-13.64	1.456	0.836	0.621	-13.401	-13.061	12.827	0.026	0.79
	4	1.824	-13.56	1.457	0.832	0.626	-13.396	-12.975	12.816	0.032	0.80
	5	1.739	-11.78	1.450	0.846	0.605	-11.722	-11.473	11.419	0.022	0.77
	6	1.932	-16.08	1.450	0.815	0.636	-14.677	-13.670	12.262	0.074	0.87
	7	1.737	-9.67	1.457	0.814	0.643	-12.896	-12.588	15.814	0.024	0.74
N(3) – C(3)	1	1.771	-13.84	1.468	0.848	0.621	-13.354	-12.708	12.226	0.051	0.74
	2	1.759	-13.81	1.467	0.850	0.618	-13.185	-12.522	11.896	0.053	0.73
	3	1.762	-13.72	1.469	0.851	0.619	-13.290	-12.622	12.194	0.053	0.73
	4	1.751	-13.66	1.467	0.845	0.623	-13.192	-12.494	12.022	0.056	0.72
	5	1.819	-13.43	1.461	0.825	0.637	-13.109	-12.610	12.293	0.040	0.81
	6	1.823	-13.73	1.466	0.833	0.633	-13.339	-12.702	12.315	0.050	0.80
	7	1.687	-9.05	1.468	0.822	0.647	-12.551	-12.116	15.618	0.036	0.70
C(1) – H(1A)	1	1.921	-23.50	1.070	0.747	0.323	-19.901	-19.269	15.675	0.033	0.86
	2	1.900	-23.06	1.069	0.761	0.308	-20.017	-19.460	16.413	0.029	0.84
	3	1.971	-23.01	1.065	0.684	0.381	-18.906	-17.986	13.878	0.051	0.98

	4	1.887	-22.10	1.083	0.746	0.337	-18.982	-18.124	15.011	0.047	0.89
	5	1.832	-19.84	1.063	0.724	0.341	-17.293	-16.260	13.716	0.064	0.95
	6	1.795	-19.11	1.090	0.757	0.337	-18.233	-15.805	14.931	0.154	0.91
	7	2.023	-24.50	1.071	0.715	0.356	-20.600	-19.816	15.916	0.040	0.94
C(1) - H(1B)	1	1.878	-21.27	1.085	0.732	0.353	-18.574	-17.747	15.051	0.047	0.92
	2	1.872	-21.20	1.089	0.739	0.350	-18.531	-17.780	15.108	0.042	0.91
	3	1.861	-19.60	1.072	0.737	0.335	-18.519	-18.054	16.975	0.026	0.92
	4	1.879	-20.09	1.064	0.702	0.362	-17.846	-17.379	15.131	0.027	0.96
	5	1.755	-17.78	1.090	0.744	0.346	-16.237	-15.759	14.219	0.030	0.93
	6	1.736	-16.73	1.090	0.624	0.467	-14.091	-12.845	10.206	0.097	1.03
	7	1.950	-22.26	1.085	0.713	0.372	-19.238	-18.632	15.614	0.033	0.95
C(2) – H(2A)	1	1.968	-23.67	1.059	0.718	0.341	-19.746	-19.038	15.114	0.037	0.92
	2	1.955	-23.31	1.056	0.724	0.332	-19.789	-19.075	15.550	0.037	0.92
	3	1.991	-23.72	1.043	0.674	0.369	-19.168	-18.780	14.227	0.021	0.97
	4	1.936	-23.12	1.052	0.715	0.337	-19.329	-18.932	15.138	0.021	0.91
	5	1.819	-19.91	1.063	0.716	0.349	-16.917	-16.175	13.186	0.046	0.94
	6	1.817	-19.83	1.090	0.733	0.360	-17.113	-16.395	13.681	0.044	0.93
	7	2.079	-26.22	1.060	0.706	0.354	-21.340	-20.610	15.734	0.035	0.94
C(2) – H(2B)	1	1.898	-22.04	1.089	0.736	0.353	-18.829	-18.091	14.875	0.041	0.91
	2	1.898	-21.98	1.088	0.735	0.354	-18.790	-18.024	14.832	0.042	0.92
	3	1.882	-21.76	1.088	0.754	0.334	-19.429	-18.617	16.290	0.044	0.88
	4	1.898	-22.45	1.089	0.737	0.352	-19.04	-18.216	14.806	0.045	0.90
	5	1.795	-19.68	1.105	0.750	0.355	-16.878	-16.070	13.267	0.050	0.92
	6	1.873	-21.05	1.090	0.711	0.379	-17.685	-17.019	13.656	0.039	0.95
	7	1.935	-22.05	1.089	0.719	0.371	-19.142	-18.520	15.607	0.034	0.94
C(3) – H(3A)	1	1.911	-22.54	1.058	0.726	0.332	-19.520	-18.634	15.614	0.048	0.89
	2	1.890	-21.80	1.056	0.736	0.320	-19.454	-18.626	16.276	0.044	0.88
	3	1.886	-22.82	1.080	0.749	0.331	-19.687	-18.679	15.547	0.054	0.85
	4	1.857	-22.18	1.079	0.759	0.320	-19.426	-18.342	15.590	0.059	0.84
	5	1.812	-20.69	1.087	0.734	0.354	-16.823	-16.508	12.637	0.019	0.91
	6	1.821	-19.38	1.090	0.708	0.382	-16.526	-15.845	12.987	0.043	0.97
	7	2.059	-25.52	1.058	0.707	0.351	-21.242	-20.321	16.040	0.045	0.94
C(3) – H(3B)	1	1.907	-23.03	1.079	0.734	0.345	-19.191	-18.559	14.716	0.034	0.89
	2	1.900	-22.85	1.077	0.741	0.336	-19.271	-18.753	15.177	0.028	0.88
	3	1.901	-23.21	1.090	0.740	0.350	-19.368	-18.451	14.607	0.050	0.87
	4	1.884	-23.27	1.096	0.752	0.345	-19.149	-18.261	14.137	0.049	0.86
	5	1.825	-21.00	1.085	0.726	0.360	-17.101	-16.550	12.654	0.033	0.91
	6	1.837	-20.04	1.090	0.725	0.366	-17.253	-16.333	13.544	0.056	0.95
	7	2.008	-24.88	1.079	0.720	0.360	-20.678	-19.756	15.550	0.047	0.91

1– 20K, anharmonic refinement, 2 – 20 K harmonic refinement, 3– 120K, anharmonic refinement, 4 – 120 K harmonic refinement, 5– 298K, anharmonic refinement, 6 – 298 K harmonic refinement, 7 – theory; ρ is the electron density; $\nabla^2\rho$ is the Laplacian; R_{ij} is interatomic distance, d_1 and d_2 are the distances from the critical point to atoms 1 and 2, λ_1, λ_2, λ_3 are principle curvatures, ε is bond ellipticity, n_{topo} is topological bond order.

Table D4. Hydrogen bond angles calculated after anharmonic refinement of 20K data.

Hydrogen bond	∠O–H–C, °
O(1) ··· H(3B) – C(3)$^{(1)}$	135.9
O(2) ··· H(1A) – C(1)$^{(4)}$	149.9
O(4) ··· H(2B) – C(2)$^{(2)}$	118.4
O(1) ··· H(1B) – C(1)$^{(1)}$	132.9
O(3) ··· H(3B) – C(3)$^{(3)}$	115.8
O(1) ··· H(2A) – C(2)$^{(6)}$	127.0
O(6) ··· H(3B) – C(3)$^{(5)}$	110.4
O(2) ··· H(2B) – C(2)$^{(1)}$	149.2
O(5) ··· H(1B) – C(1)$^{(7)}$	150.6

Symmetry operators: (1) (1/2+x, y, 1/2-z); (2) (x, 1/2-y, -1/2+z); (3) (1/2+x, 1/2-y, -z); (4) (1-x, -1/2+y, 1/2-z); (5) (1/2-x, 1/2+y, z); (6) (1-x, 1/2+y, 1/2-z); (7) (1/2-x, 1-y, -1/2+z).

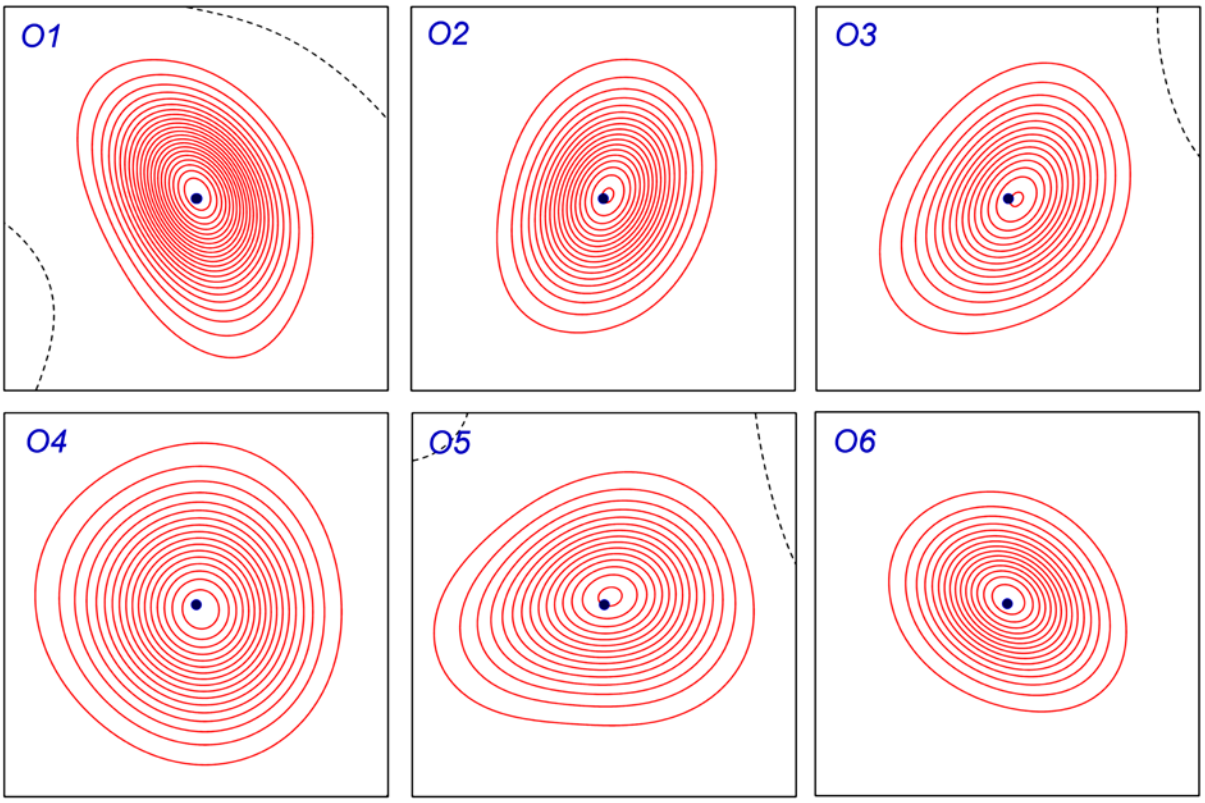


Fig.D5. The total (all orders of cumulants) single particle vibrational probability density function (pdf) maps for oxygen atoms in RDX at 298K plotted in planes perpendicular to c* through atomic centers. Blue dots denote nuclear positions. Picture size is ±0.8 A. Contour intervals are 500 A^{-3}.

Table D5. Anisotropic atomic displacements in RDX at 298K. For each atom, the harmonic refinement data are in the first row, anharmonic ones are in the second, neutron data (Choi & Prince, 1972) are in the third.

Atom	U_{11}, A^2	U_{22}, A^2	U_{33}, A^2	U_{12}, A^2	U_{13}, A^2	U_{23}, A^2
H(1A)	0.056(8)	0.030(6)	0.109(12)	-0.010(6)	0.009(8)	-0.014(7)
H(1A)	0.051(4)	0.051(5)	0.084(5)	0.001(4)	-0.023(3)	-0.010(4)
H(1A)	0.0709(47)	0.0342(37)	0.0965(54)	-0.0075(35)	-0.0255(43)	-0.0161(37)
H(1B)	0.069(8)	0.075(7)	0.040(5)	0.009(6)	0.013(5)	-0.009(5)
H(1B)	0.048(4)	0.067(4)	0.036(3)	0.008(3)	-0.000(3)	-0.008(3)
H(1B)	0.0674(46)	0.0714(47)	0.0471(42)	0.0179(41)	-0.0018(38)	-0.0162(39)
H(2A)	0.051(7)	0.048(8)	0.076(8)	0.004(6)	-0.014(6)	-0.009(7)
H(2A)	0.061(5)	0.042(4)	0.064(4)	0.001(3)	-0.018(4)	-0.001(3)
H(2A)	0.0762(49)	0.0460(44)	0.0807(56)	0.0137(39)	-0.0215(44)	0.0022(35)
H(2B)	0.070(8)	0.066(7)	0.053(7)	-0.037(6)	0.007(6)	0.016(6)
H(2B)	0.065(5)	0.051(3)	0.046(4)	-0.019(3)	-0.004(3)	0.006(3)
H(2B)	0.0762(47)	0.0664(47)	0.0398(35)	-0.0032(38)	0.0058(38)	0.0101(32)
H(3A)	0.053(7)	0.077(8)	0.041(6)	0.011(6)	0.002(6)	0.004(6)
H(3A)	0.048(3)	0.065(3)	0.040(4)	0.003(3)	-0.004(3)	0.003(3)
H(3A)	0.0548(42)	0.0756(44)	0.0470(43)	0.0020(34)	-0.0185(37)	-0.0023(39)
H(3B)	0.039(6)	0.056(6)	0.054(7)	0.000(5)	0.009(5)	-0.006(5)
H(3B)	0.038(4)	0.048(3)	0.051(4)	-0.009(3)	0.007(3)	-0.000(2)
H(3B)	0.0333(33)	0.0752(47)	0.0588(38)	-0.0144(34)	0.0113(34)	-0.0020(34)
O(1)	0.0408(5)	0.0593(6)	0.0408(5)	-0.0119(5)	-0.0113(4)	-0.0009(5)
O(1)	0.0421(3)	0.0628(4)	0.0419(4)	-0.0161(4)	-0.0126(3)	-0.0013(3)
O(1)	0.0418(22)	0.0528(24)	0.0433(20)	-0.0166(18)	-0.0109(19)	-0.0016(20)
O(2)	0.0423(6)	0.0564(9)	0.0689(8)	0.0073(6)	-0.0204(6)	0.0066(8)
O(2)	0.0413(3)	0.0627(4)	0.0682(4)	0.0069(4)	-0.0159(4)	0.0124(5)
O(2)	0.0418(22)	0.0515(24)	0.0717(29)	0.0086(20)	-0.0155(23)	0.0104(22)
O(3)	0.0568(8)	0.0612(10)	0.0714(10)	0.0101(8)	0.0229(8)	-0.0085(9)
O(3)	0.0583(6)	0.0619(7)	0.0771(7)	0.0126(5)	0.0252(3)	-0.0122(2)
O(3)	0.0559(29)	0.0526(25)	0.0816(34)	0.0079(23)	0.0234(27)	-0.0115(25)
O(4)	0.0726(10)	0.0821(10)	0.0264(4)	-0.0031(10)	0.0094(5)	-0.0055(5)
O(4)	0.0790(5)	0.0821(5)	0.0275(3)	-0.0062(5)	0.0117(4)	-0.0070(4)
O(4)	0.0724(32)	0.0740(32)	0.0312(20)	0.0028(27)	0.0056(22)	-0.0079(20)
O(5)	0.0911(12)	0.0640(10)	0.0471(7)	0.0182(10)	0.0220(8)	0.0221(7)
O(5)	0.0887(5)	0.0653(4)	0.0481(4)	0.0178(5)	0.0189(4)	0.0249(4)
O(5)	0.0909(33)	0.0540(25)	0.0422(27)	0.0198(24)	0.0175(27)	0.0194(22)
O(6)	0.0523(8)	0.0417(7)	0.1001(11)	-0.0062(6)	0.0263(8)	0.0076(9)
O(6)	0.0541(6)	0.0409(5)	0.1079(7)	-0.0078(4)	0.0294(3)	0.0082(5)
O(6)	0.0483(27)	0.0327(20)	0.1132(41)	-0.0067(19)	0.0318(28)	0.0072(25)

N(1)	0.0339(2)	0.0319(3)	0.0383(2)	-0.0010(2)	-0.0127(2)	-0.0010(2)
N(1)	0.03502(16)	0.03163(18)	0.0406(2)	-0.00053(19)	-0.0129(3)	-0.00134(17)
N(1)	0.0337(10)	0.0318(11)	0.0338(10)	0.0000(10)	-0.0138(10)	0.0001(10)
N(2)	0.0289(2)	0.0371(3)	0.02528(18)	-0.00503(19)	0.00113(17)	-0.00411(19)
N(2)	0.0282(4)	0.0397(3)	0.0261(3)	-0.0054(4)	0.0011(4)	-0.0042(3)
N(2)	0.0289(10)	0.0347(11)	0.0267(11)	-0.0047(9)	0.0019(10)	-0.0044(9)
N(3)	0.0273(2)	0.0353(3)	0.0359(2)	0.0015(2)	0.00031(19)	0.0057(2)
N(3)	0.0295(2)	0.03497(17)	0.0365(2)	0.0007(3)	0.0005(3)	0.0048(3)
N(3)	0.0266(10)	0.0317(11)	0.0374(11)	0.0011(9)	0.0018(10)	0.0042(10)
N(4)	0.02999(15)	0.0465(2)	0.02858(14)	-0.00488(15)	-0.00636(12)	0.00632(15)
N(4)	0.0308(4)	0.0462(5)	0.0293(3)	-0.0038(2)	-0.0061(3)	0.0072(2)
N(4)	0.0305(11)	0.0441(13)	0.0275(10)	-0.0033(11)	-0.0070(10)	0.0100(11)
N(5)	0.04057(19)	0.0432(2)	0.03390(18)	-0.00748(18)	0.01102(15)	-0.00976(15)
N(5)	0.0411(3)	0.0442(4)	0.0356(3)	-0.0079(4)	0.0109(4)	-0.0095(3)
N(5)	0.0388(13)	0.0400(13)	0.0360(14)	-0.0067(10)	0.0091(11)	-0.0091(11)
N(6)	0.0399(2)	0.0346(2)	0.0559(3)	0.00943(19)	0.01869(19)	0.01223(19)
N(6)	0.0399(3)	0.0357(4)	0.0556(3)	0.0090(3)	0.0177(4)	0.0118(4)
N(6)	0.0408(13)	0.0324(13)	0.0576(18)	0.0098(11)	0.0199(13)	0.0132(11)
C(1)	0.0377(2)	0.0347(2)	0.0376(2)	0.00117(18)	-0.00672(17)	-0.00722(18)
C(1)	0.0397(4)	0.0333(4)	0.0389(4)	0.0015(4)	-0.0053(4)	-0.0062(3)
C(1)	0.0376(16)	0.0261(18)	0.0408(19)	0.0009(15)	-0.0089(16)	-0.0087(14)
C(2)	0.0421(2)	0.0295(2)	0.03100(18)	-0.00463(17)	-0.00540(16)	0.00395(15)
C(2)	0.0422(4)	0.0297(4)	0.0327(4)	-0.0052(4)	-0.0049(3)	0.0042(3)
C(2)	0.0420(20)	0.0222(18)	0.0319(18)	-0.0039(15)	-0.0043(16)	0.0043(14)
C(3)	0.02192(15)	0.0459(2)	0.02935(16)	-0.00240(15)	-0.00089(12)	-0.00013(17)
C(3)	0.0219(3)	0.0477(5)	0.0292(3)	-0.0029(3)	-0.0006(2)	-0.0008(3)
C(3)	0.0184(14)	0.0436(16)	0.0295(19)	-0.0022(14)	0.0010(16)	-0.0001(16)

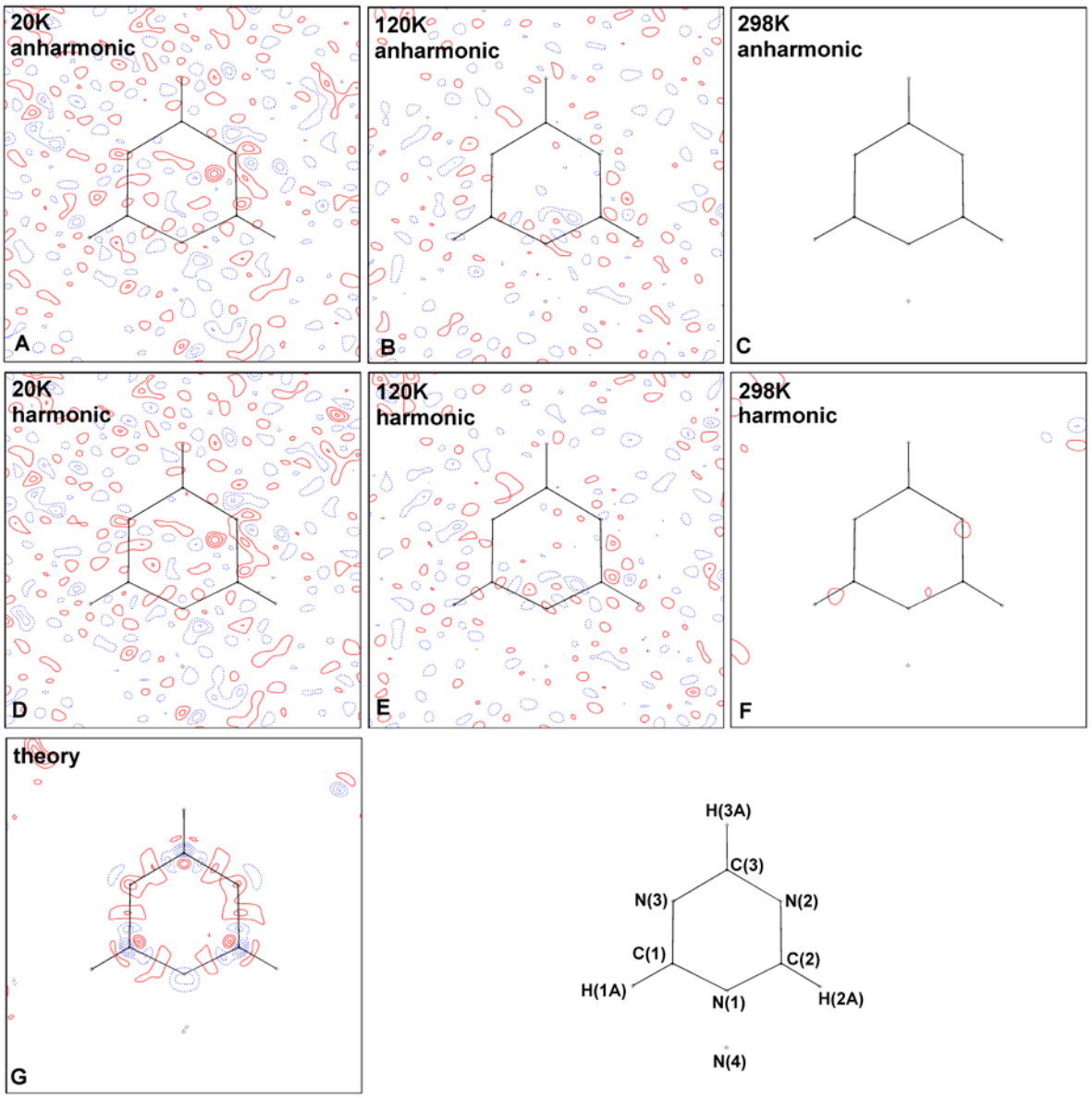


Fig.D6 . Residual electron density maps of RDX in the plane of the C(1),C(2) & C(3) atoms: A – anharmonic model refinement at 20 K, B – anharmonic refinement at 120 K, C – anharmonic refinement at 298 K, D – harmonic model refinement at 20 K, E – harmonic refinement at 120 K, F – harmonic refinement at 298 K, G – multipole model refinement on theoretical data. Contour intervals are 0.05 eÅ^{-3}. Positive contours are red and negative contours are blue dashed lines.