

Supplementary Information for Publication: Non-invasive detection of hazardous materials with thermal-to-epithermal neutron station: a feasibility study towards practical application

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S1. Performance of dispersion-corrected density functional approximations

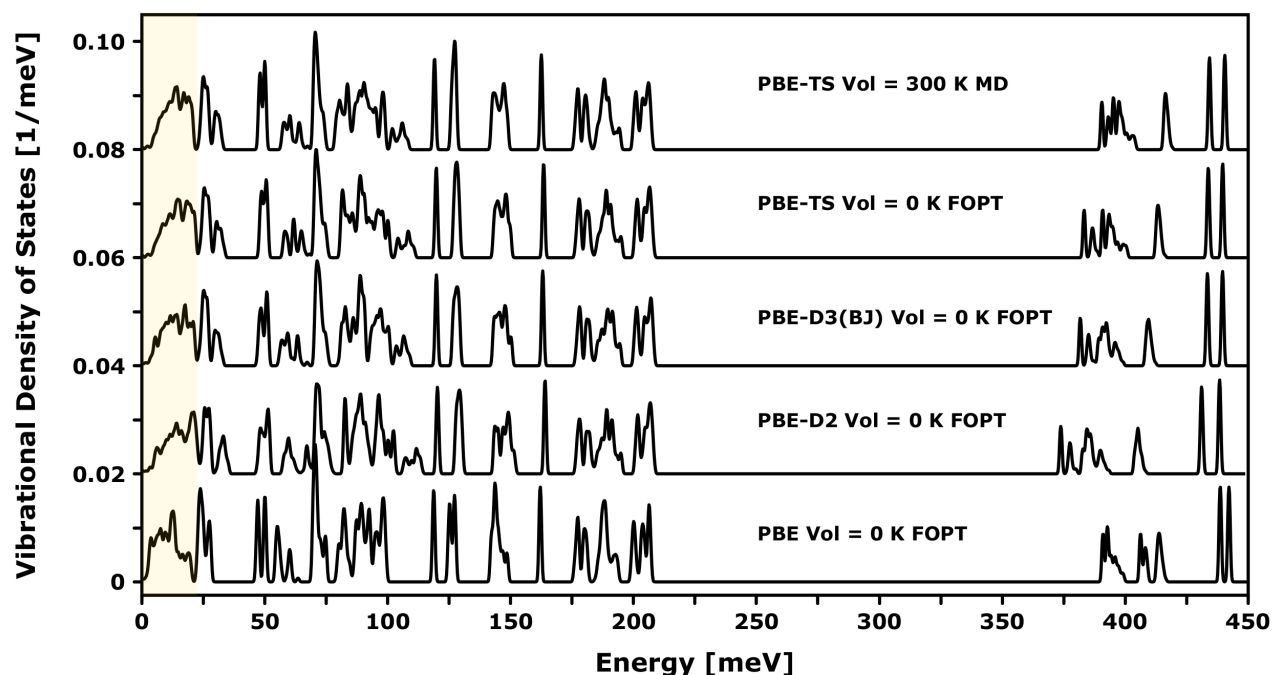


Figure S1. Theoretical vibrational density of states (VDoS) for the $P2_1/a$ phase of melamine according to different density functional approximations. The shaded regime highlights the external phonon modes. The cell volume was either fully optimised at 0 K (FOPT) or derived from AIMD simulations at 300 K (MD).

S2. Analysis of the zone-centre phonon modes

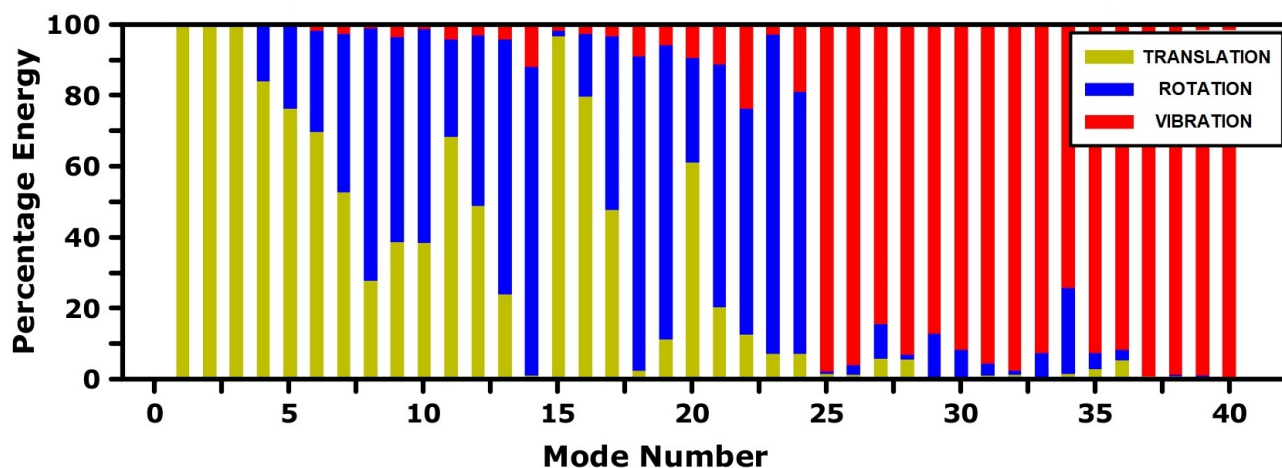


Figure S2. Vibrational energy decomposition of the zone-centre modes for the $P2_1/a$ phase of melamine according to harmonic lattice dynamics (linear response using PBE-TS functional). The contributions from external modes are further decomposed into translation and rotation of the molecular centroids (presented as yellow and blue bars, respectively). The contributions from internal modes are shown as red bars.

No.	meV [$\Gamma_{\text{Symm.}}$]	No.	meV [$\Gamma_{\text{Symm.}}$]	No.	meV [$\Gamma_{\text{Symm.}}$]	No.	meV [$\Gamma_{\text{Symm.}}$]	No.	meV [$\Gamma_{\text{Symm.}}$]
1	0.0 [Au]	37	48.1 [Ag]	73	88.3 [Ag]	109	143.8 [Au]	145	200.4 [Au]
2	0.0 [Bu]	38	48.3 [Bg]	74	88.7 [Bg]	110	144.0 [Bu]	146	200.5 [Bu]
3	0.0 [Bu]	39	49.4 [Au]	75	88.8 [Ag]	111	144.8 [Ag]	147	201.7 [Ag]
4	8.8 [Ag]	40	49.6 [Bu]	76	89.1 [Au]	112	145.0 [Bg]	148	201.8 [Bg]
5	9.5 [Bu]	41	50.2 [Ag]	77	89.3 [Bu]	113	145.2 [Au]	149	204.3 [Bg]
6	9.9 [Au]	42	50.3 [Bg]	78	89.8 [Bg]	114	145.8 [Ag]	150	205.1 [Au]
7	10.7 [Bg]	43	50.7 [Au]	79	90.4 [Bu]	115	146.4 [Bu]	151	205.3 [Bu]
8	11.1 [Au]	44	50.8 [Bu]	80	90.6 [Au]	116	147.5 [Au]	152	205.4 [Ag]
9	12.9 [Au]	45	58.3 [Au]	81	91.6 [Bg]	117	148.0 [Bg]	153	206.2 [Ag]
10	13.3 [Bg]	46	59.2 [Bu]	82	92.5 [Ag]	118	148.2 [Ag]	154	206.9 [Bu]
11	13.6 [Ag]	47	61.2 [Ag]	83	92.9 [Bu]	119	149.7 [Bg]	155	207.1 [Bg]
12	14.1 [Au]	48	62.7 [Au]	84	94.2 [Au]	120	150.0 [Bu]	156	207.6 [Au]
13	14.8 [Ag]	49	64.1 [Bg]	85	94.4 [Bg]	121	163.3 [Ag]	157	383.2 [Ag]
14	15.4 [Bu]	50	68.8 [Bu]	86	95.6 [Au]	122	163.3 [Bg]	158	383.4 [Bg]
15	15.6 [Bg]	51	69.8 [Ag]	87	97.3 [Ag]	123	163.5 [Bu]	159	386.6 [Au]
16	17.0 [Bg]	52	70.3 [Bg]	88	97.3 [Bu]	124	163.6 [Au]	160	388.8 [Bu]
17	17.9 [Ag]	53	70.6 [Au]	89	98.3 [Bg]	125	177.1 [Au]	161	390.8 [Bg]
18	18.3 [Bu]	54	70.6 [Ag]	90	98.4 [Ag]	126	177.3 [Bu]	162	390.9 [Ag]
19	19.0 [Au]	55	70.9 [Bg]	91	99.1 [Bu]	127	177.5 [Bg]	163	392.4 [Bu]
20	19.5 [Ag]	56	71.3 [Bu]	92	100.4 [Au]	128	177.7 [Ag]	164	393.4 [Au]
21	19.9 [Bu]	57	71.4 [Au]	93	105.1 [Au]	129	180.2 [Ag]	165	393.8 [Ag]
22	21.2 [Bg]	58	72.3 [Bg]	94	106.3 [Bu]	130	180.3 [Bg]	166	395.8 [Au]
23	21.3 [Bg]	59	72.5 [Ag]	95	107.6 [Ag]	131	181.3 [Au]	167	398.6 [Bg]
24	21.8 [Ag]	60	72.5 [Bu]	96	108.2 [Bg]	132	182.0 [Bu]	168	400.8 [Bu]
25	24.1 [Au]	61	74.7 [Bu]	97	119.4 [Ag]	133	186.1 [Ag]	169	412.6 [Ag]
26	25.0 [Au]	62	75.4 [Au]	98	119.6 [Au]	134	186.4 [Bu]	170	412.7 [Au]
27	25.1 [Bg]	63	80.9 [Au]	99	119.6 [Bg]	135	187.2 [Bg]	171	413.1 [Bg]
28	25.6 [Ag]	64	81.1 [Bg]	100	120.0 [Bu]	136	187.9 [Au]	172	413.3 [Bu]
29	25.9 [Bu]	65	81.5 [Ag]	101	126.9 [Au]	137	188.5 [Au]	173	433.6 [Ag]
30	26.8 [Bu]	66	83.3 [Bg]	102	127.2 [Ag]	138	189.0 [Ag]	174	433.7 [Bg]
31	27.5 [Bg]	67	83.7 [Ag]	103	127.5 [Bg]	139	190.6 [Bu]	175	433.9 [Au]
32	27.7 [Ag]	68	83.9 [Bu]	104	127.5 [Bu]	140	190.8 [Bg]	176	434.1 [Bu]
33	29.9 [Ag]	69	84.5 [Au]	105	128.0 [Bu]	141	190.9 [Bg]	177	439.5 [Ag]
34	30.1 [Bu]	70	85.3 [Ag]	106	128.1 [Bg]	142	191.8 [Ag]	178	439.6 [Au]
35	31.2 [Au]	71	86.8 [Bu]	107	128.5 [Ag]	143	192.6 [Au]	179	439.6 [Bu]
36	31.8 [Bg]	72	88.2 [Bg]	108	128.8 [Au]	144	194.1 [Bu]	180	439.6 [Bg]

Table S1. The full set of the Γ -point vibrations of melamine crystal ($P2_1/a$). The phonon eigenenergies (in meV) were obtained from harmonic linear-response calculations using PBE-TS functional. The phonon symmetries are given in square brackets.

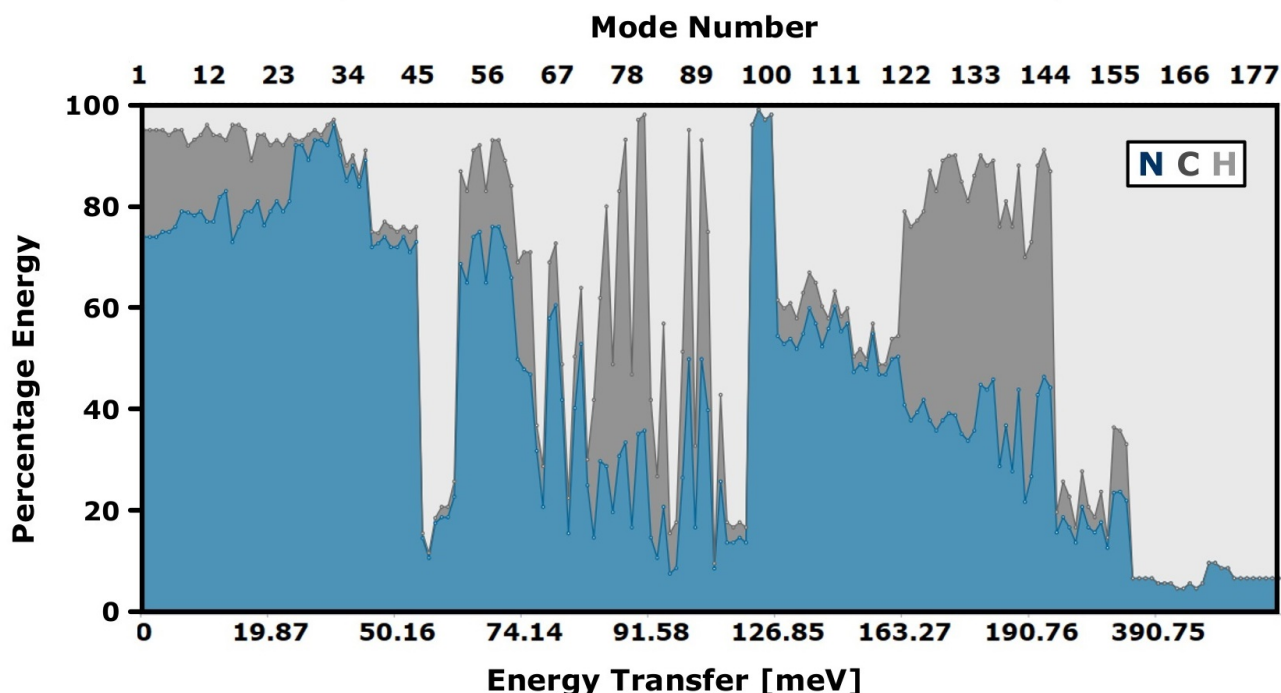


Figure S3. Percentage nuclear contributions to the zone-centre modes in the melamine crystal ($P2_1/a$) according to harmonic linear-response calculations with PBE-TS.

ID	INS	HLD	MD	Assignment	ID	INS	HLD	MD	Assignment
<i>i</i>	404.7	392.4 (No. 163)	398.5	$\nu_s(\text{H-N-H})$	<i>xii</i>	84.1	83.9 (No. 68)	79.8	R6-ring
<i>ii</i>	204.3	206.2 (No. 153)	203.7	$\delta(\text{H-N-H})$	<i>xiii</i>	79.6	81.1 (No. 64)	79.6	$\tau(\text{H-N-H})$
<i>iii</i>	191.5	190.8 (No. 140)	187.1	$\nu_s(\text{C-N-C}) + \delta(\text{H-N-H})$	<i>xiv</i>	73.5	72.3 (No. 58)	71.2	$\nu_{as}(\text{C-N-C})$
<i>iv</i>	179.5	177.5 (No. 127)	178.2	$\nu_{as}(\text{C-N-C}) + \rho(\text{H-N-H})$	<i>xv</i>	59.9	64.1 (No. 49)	62.0	$\gamma(\text{N-H-N})$
<i>v</i>	163.3	163.5 (No. 123)	160.1	$\nu_{as}(\text{C-N-C}) + \rho(\text{H-N-H})$	<i>xvi</i>	54.4	58.3 (No. 45)	56.0	$\gamma(\text{N-H-N})$
<i>vi</i>	145.5	145.2 (No. 113)	143.1	$\rho(\text{H-N-H})$	<i>xvii</i>	49.3	50.3 (No. 42)	49.5	$\delta(\text{N-C-NH}_2)$
<i>vii</i>	128.4	128.5 (No. 107)	125.2	$\rho(\text{H-N-H})$	<i>xviii</i>	47.6	48.3 (No. 38)	46.9	$\delta(\text{N-C-NH}_2)$
<i>viii</i>	120.4	119.6 (No. 99)	113.3	R3-ring	<i>xix</i>	31.2	31.2 (No. 35)	29.9	$\gamma(\text{N-C-NH}_2)$
<i>ix</i>	110.1	107.6 (No. 95)	108.5	$\omega(\text{H-N-H})$	<i>xx</i>	30.1	30.1 (No. 34)	27.3	$\gamma(\text{N-C-NH}_2)$
<i>x</i>	98.7	94.2 (No. 84)	94.3	$\tau(\text{H-N-H})$	<i>xxi</i>	26.8	27.7 (No. 32)	24.9	$\gamma(\text{N-C-NH}_2)$
<i>xi</i>	90.6	89.1 (No. 76)	86.5	γ -ring	<i>xxii</i>	24.9	25.1 (No. 27)	23.6	$\tau(\text{N-C-N})$

Table S2. Main spectral features (ID) in the INS spectrum of melamine, assigned to the fundamental internal vibrational transitions. The experimentally observed (INS) energy transfers (in meV) are compared to the calculated ones in terms of both harmonic lattice dynamics (HLD) at 0 K and *ab initio* molecular dynamics simulations (MD) at 300 K. The labelling of normal mode in the HLD columns stay in line with Table S1 and Figs. S4–S15. Legend: ν_s , ν_{as} – symmetric and antisymmetric stretching; δ – bending; ρ – rocking; ω – wagging; τ – twisting; R3 – symmetric ring stretching; R6 – ring breathing; γ – out-of-plane deformation.

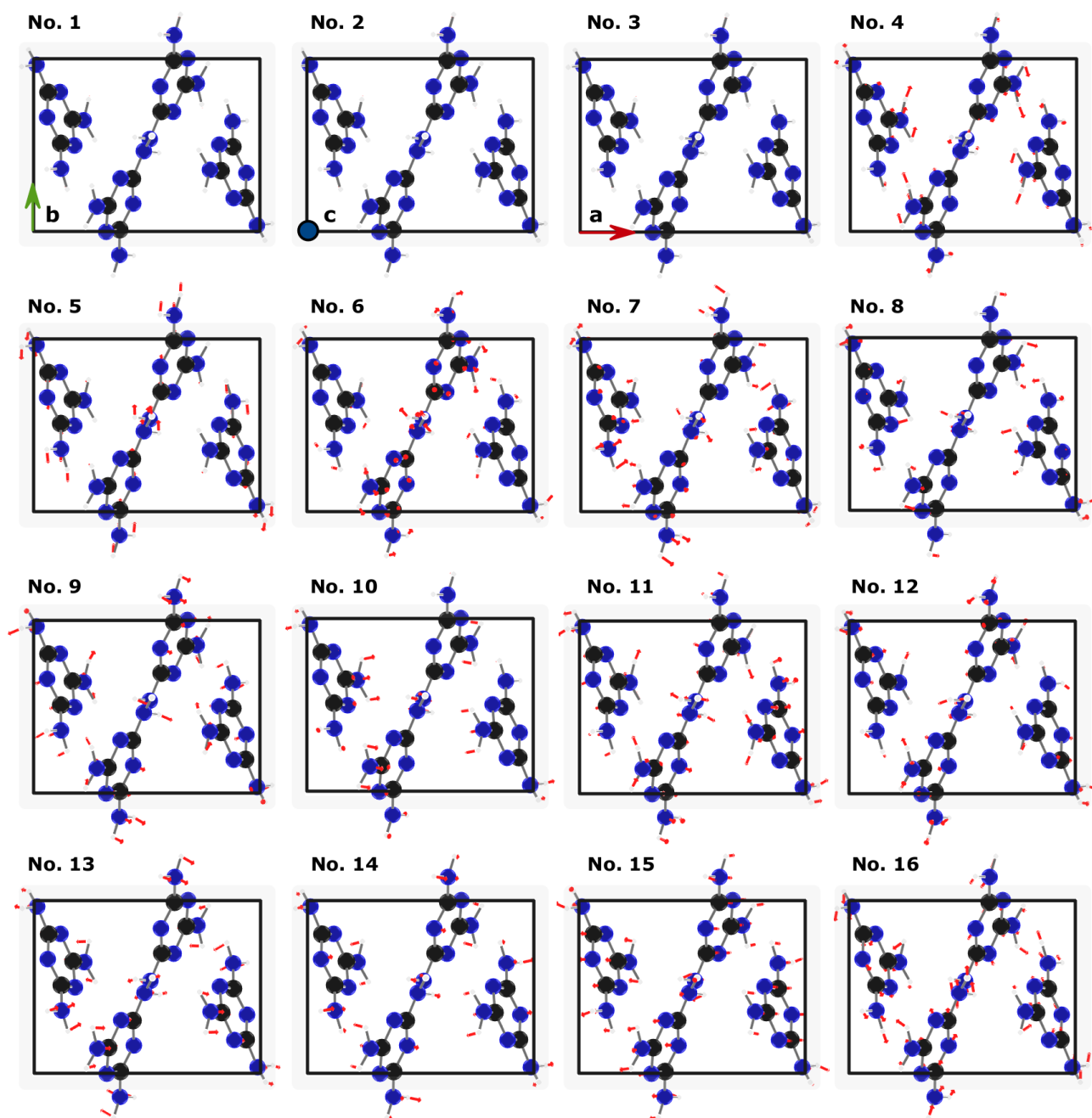


Figure S4. Schematic representation of the zone-centre modes eigenvectors (No. 1 - 16), according to harmonic lattice dynamics calculations (linear-response with PBE-TS). Atoms are shown as solid spheres: hydrogen (grey), carbon (black), and nitrogen (blue). Atomic displacements are shown as solid red vectors.

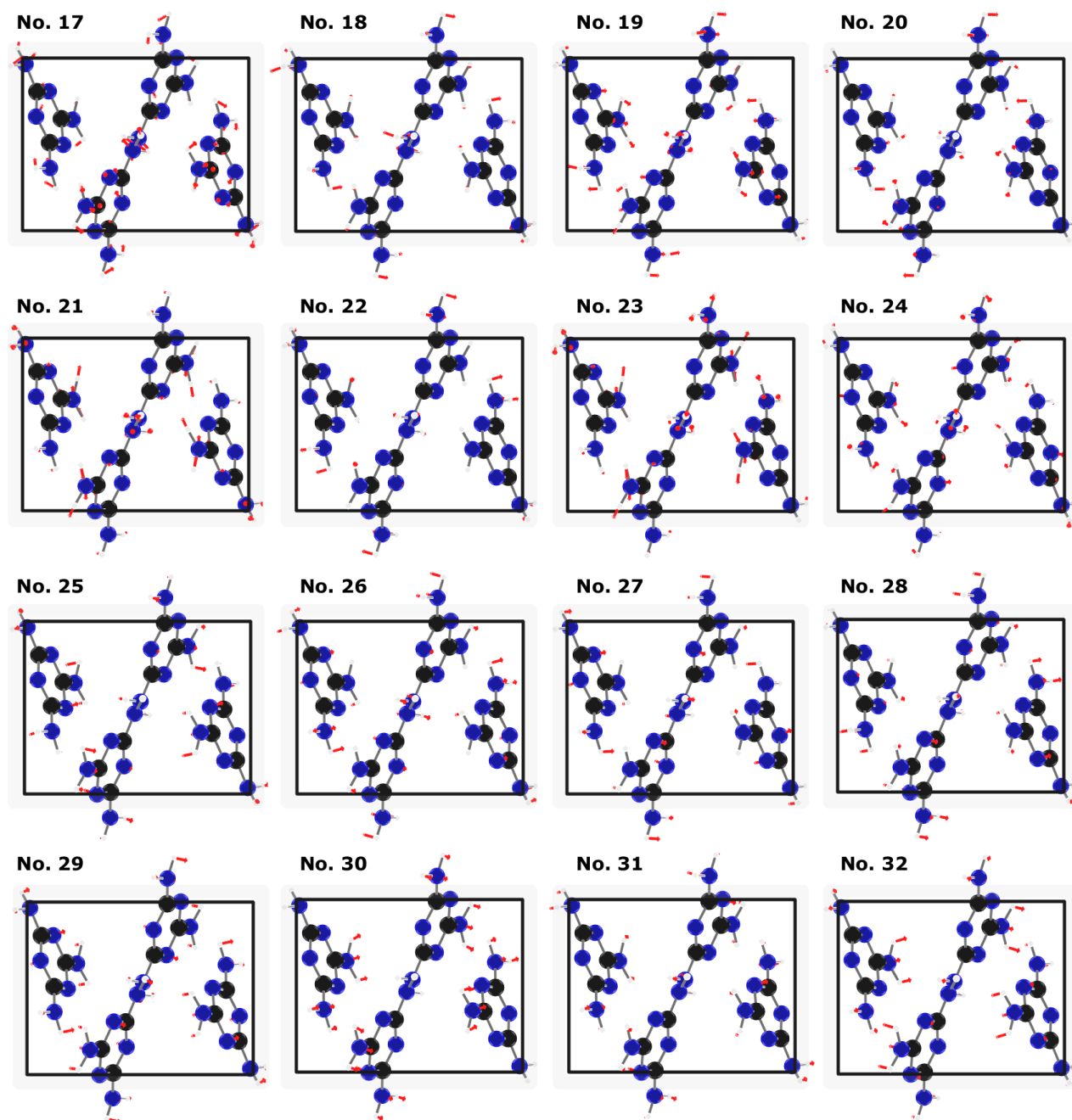


Figure S5. Schematic representation of the zone-centre modes eigenvectors (No. 17 - 32), according to harmonic lattice dynamics calculations (linear-response with PBE-TS). Atoms are shown as solid spheres: hydrogen (grey), carbon (black), and nitrogen (blue). Atomic displacements are shown as solid red vectors.

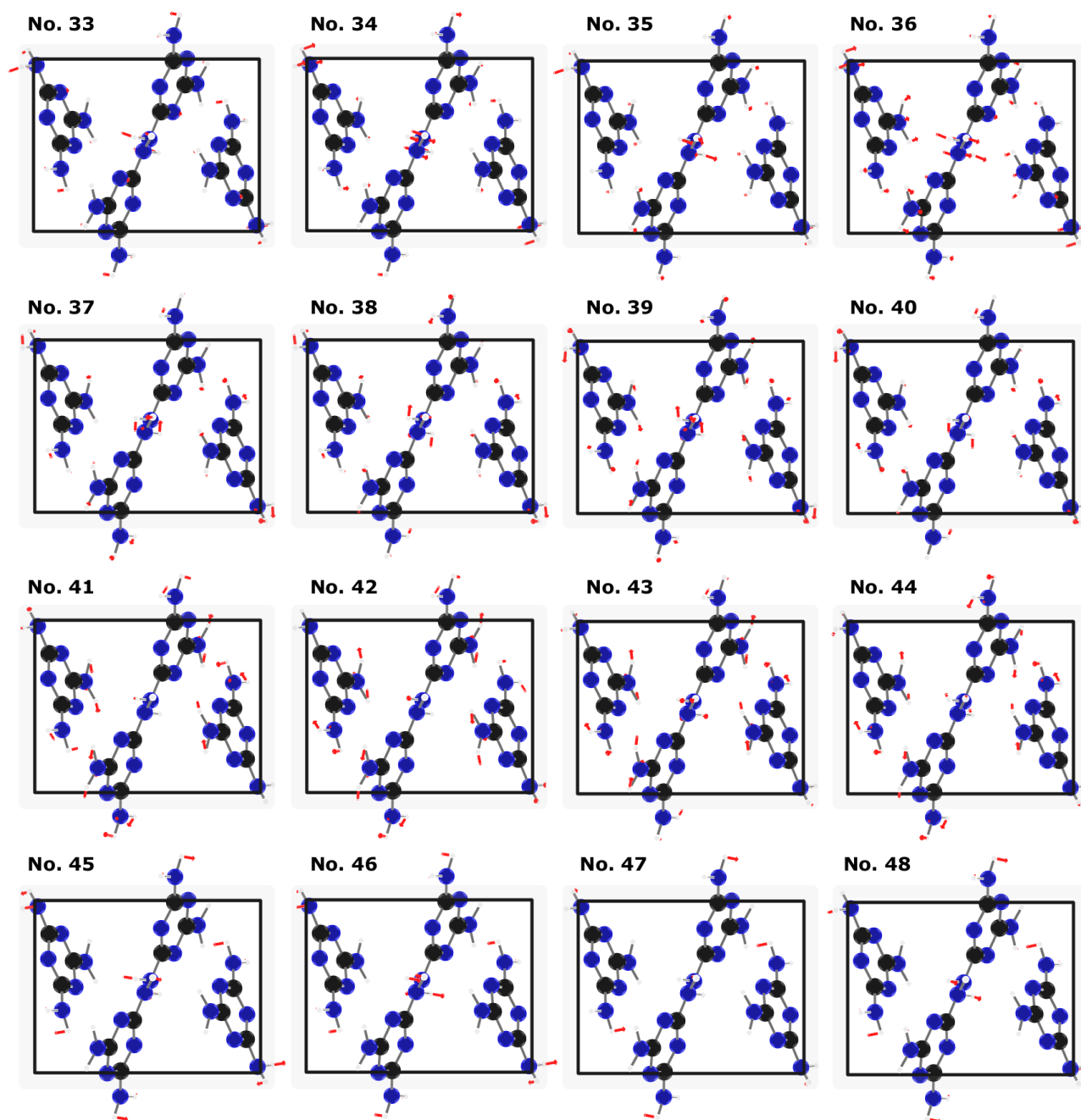


Figure S6. Schematic representation of the zone-centre modes eigenvectors (No. 33 - 48), according to harmonic lattice dynamics calculations (linear-response with PBE-TS). Atoms are shown as solid spheres: hydrogen (grey), carbon (black), and nitrogen (blue). Atomic displacements are shown as solid red vectors.

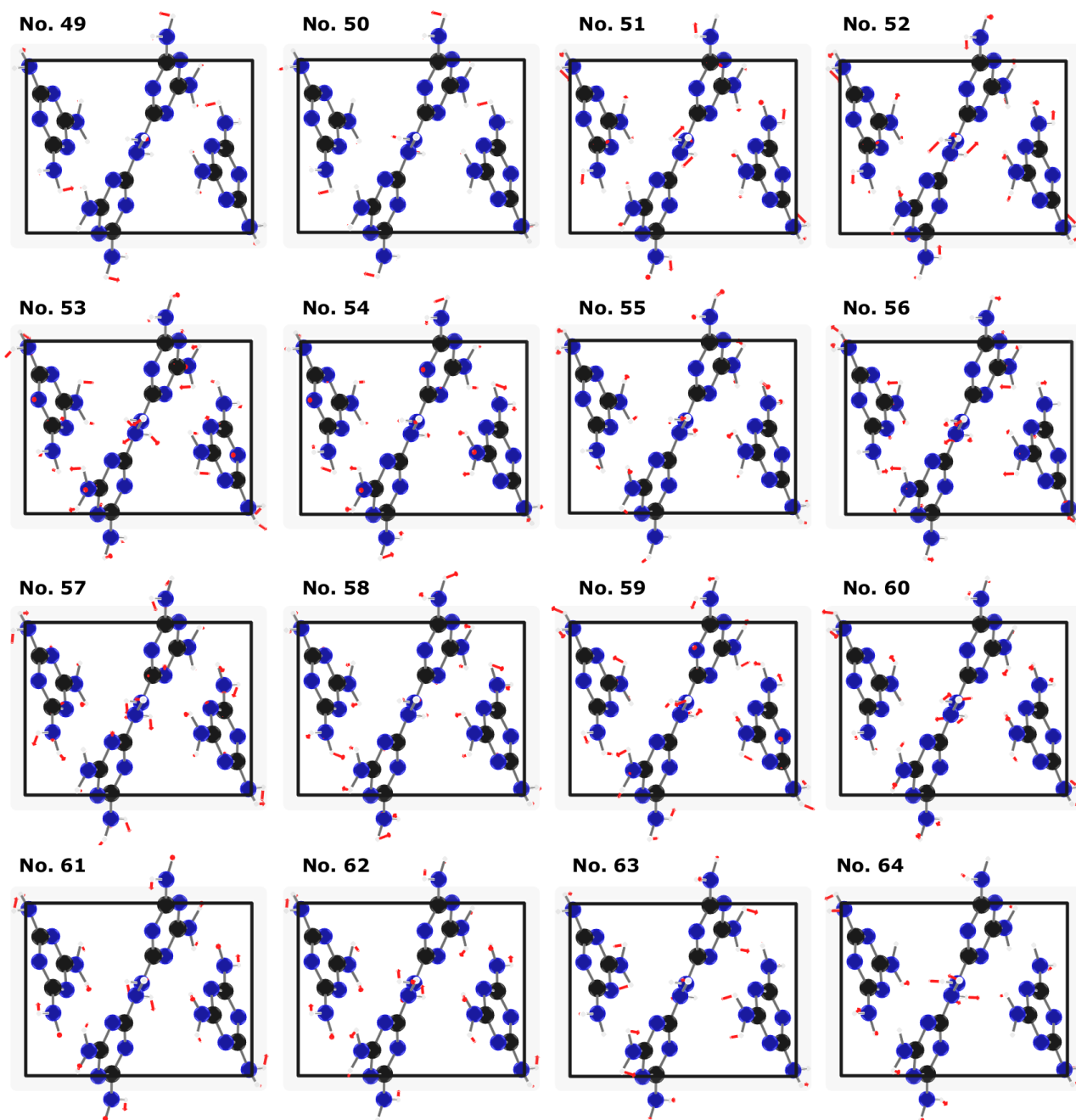


Figure S7. Schematic representation of the zone-centre modes eigenvectors (No. 49 - 64), according to harmonic lattice dynamics calculations (linear-response with PBE-TS). Atoms are shown as solid spheres: hydrogen (grey), carbon (black), and nitrogen (blue). Atomic displacements are shown as solid red vectors.

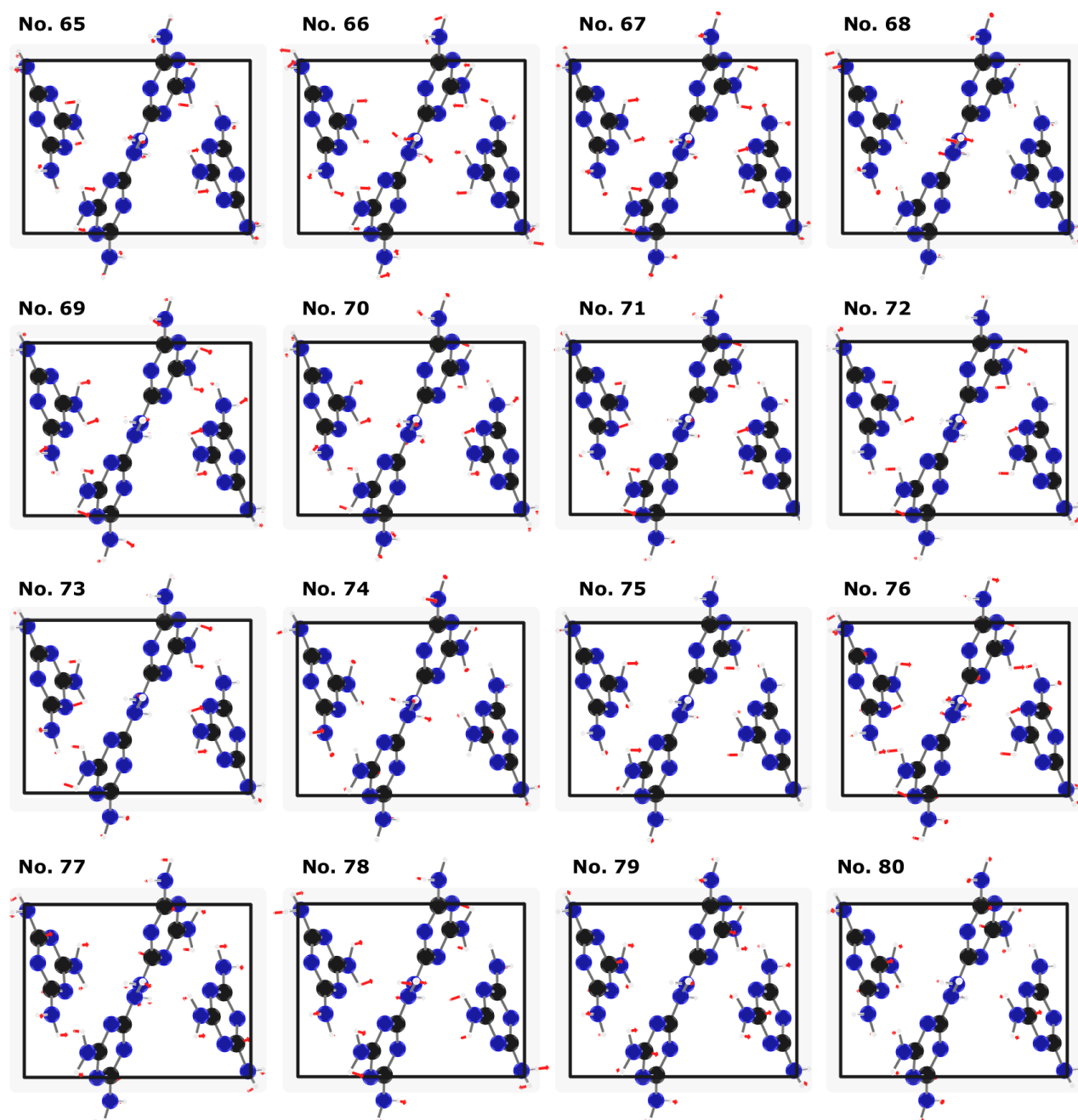


Figure S8. Schematic representation of the zone-centre modes eigenvectors (No. 65 - 80), according to harmonic lattice dynamics calculations (linear-response with PBE-TS). Atoms are shown as solid spheres: hydrogen (grey), carbon (black), and nitrogen (blue). Atomic displacements are shown as solid red vectors.

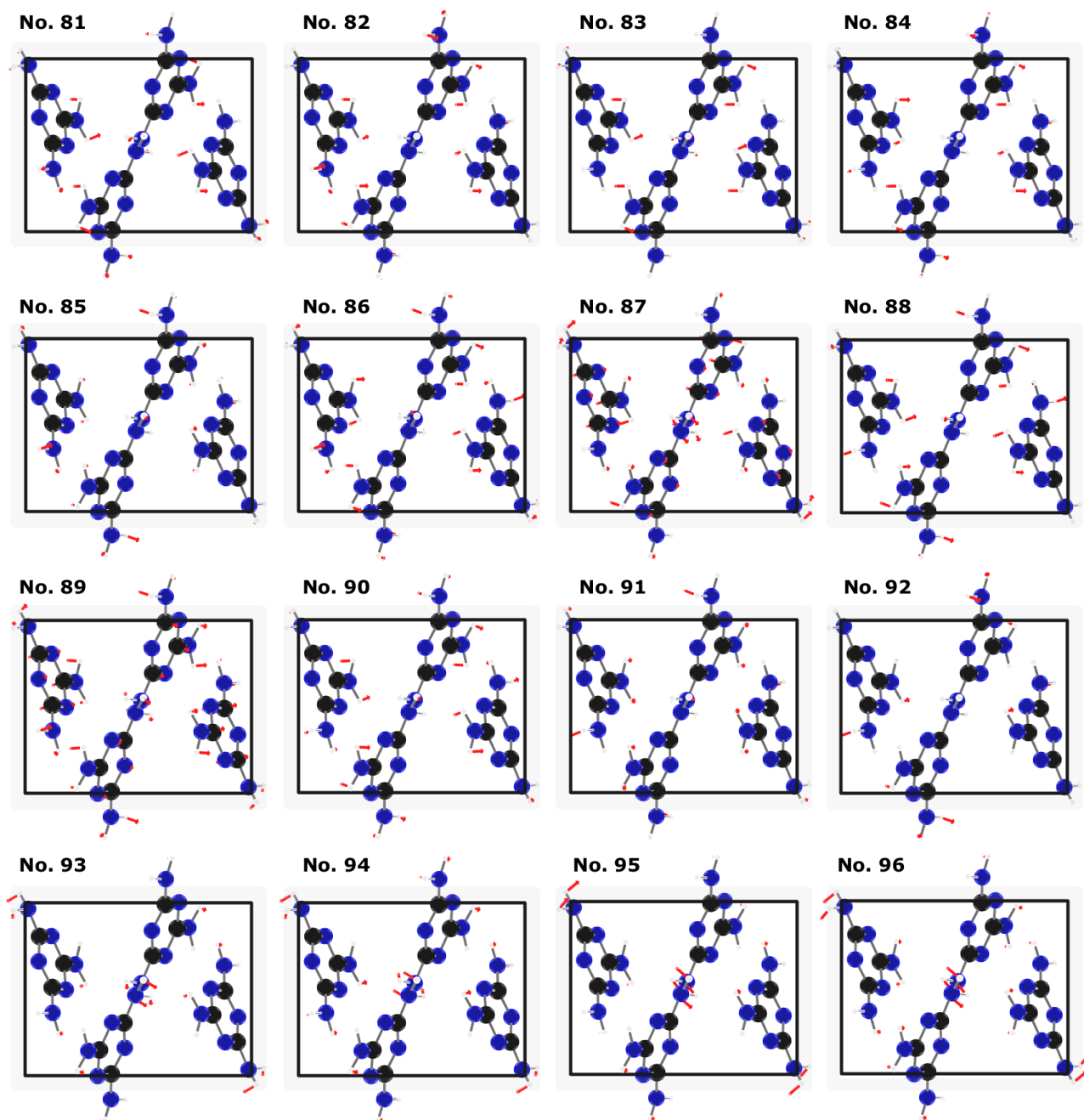


Figure S9. Schematic representation of the zone-centre modes eigenvectors (No. 81 - 96), according to harmonic lattice dynamics calculations (linear-response with PBE-TS). Atoms are shown as solid spheres: hydrogen (grey), carbon (black), and nitrogen (blue). Atomic displacements are shown as solid red vectors.

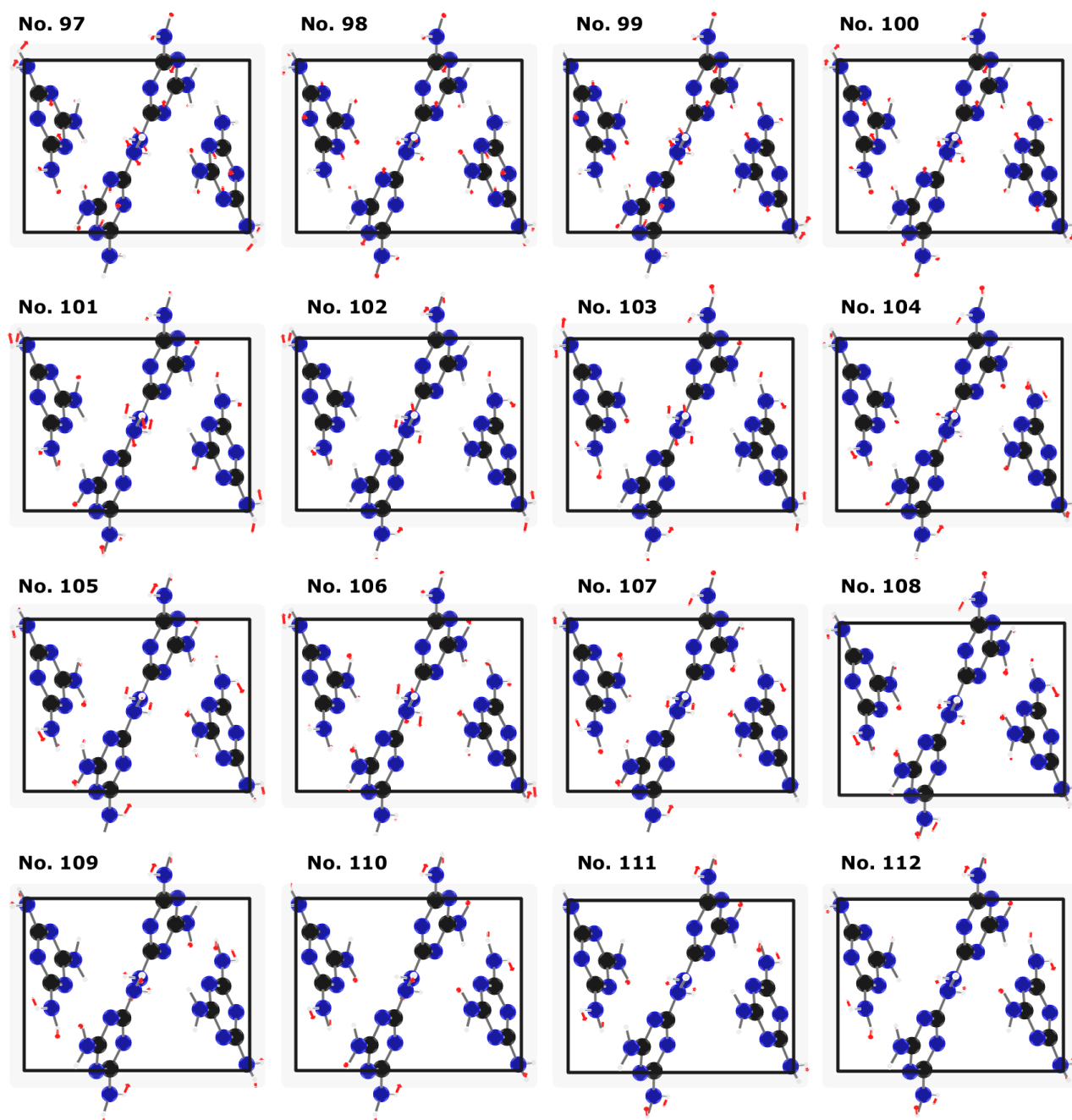


Figure S10. Schematic representation of the zone-centre modes eigenvectors (No. 97 - 112), according to harmonic lattice dynamics calculations (linear-response with PBE-TS). Atoms are shown as solid spheres: hydrogen (grey), carbon (black), and nitrogen (blue). Atomic displacements are shown as solid red vectors.

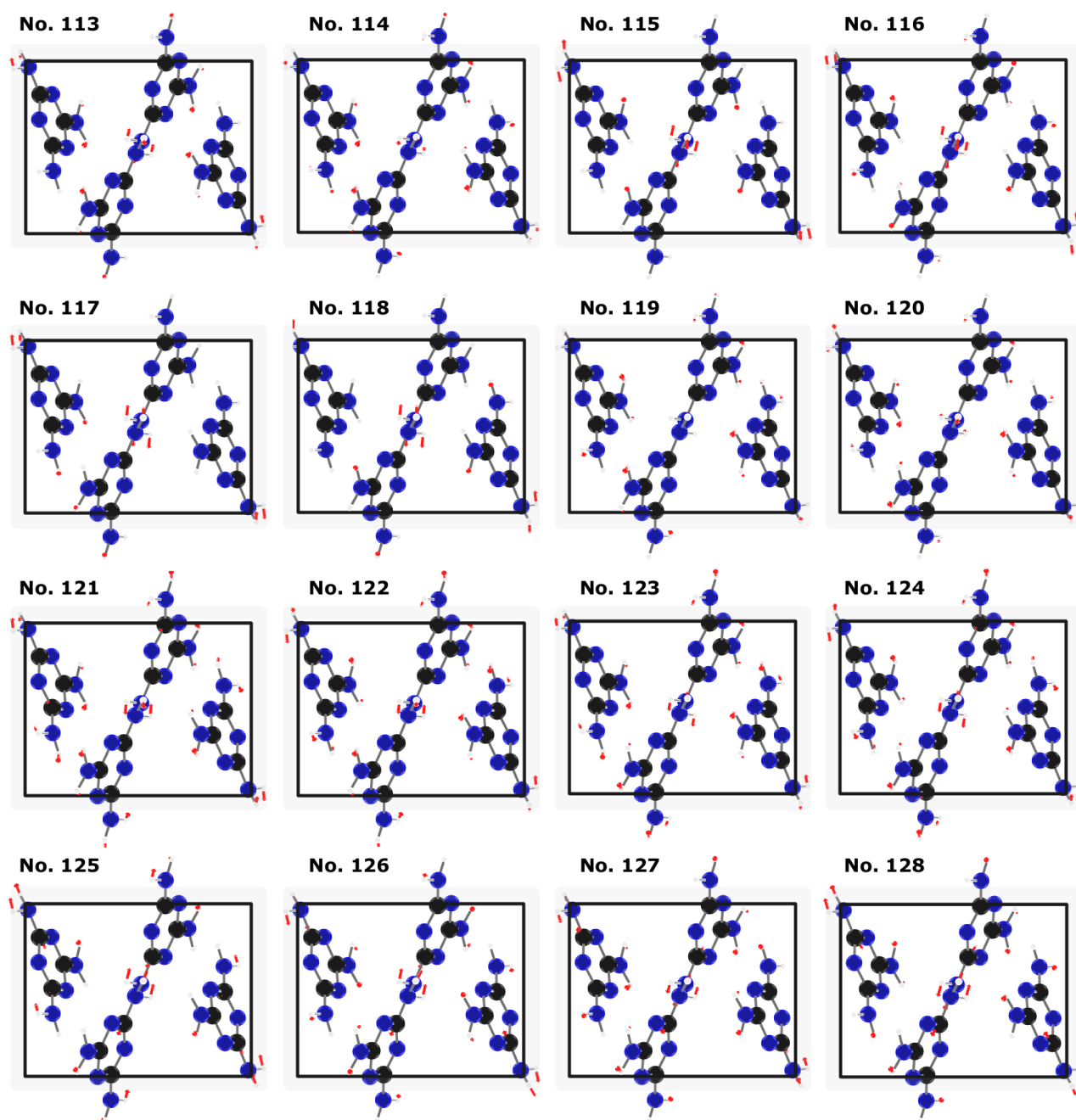


Figure S11. Schematic representation of the zone-centre modes eigenvectors (No. 113 - 128), according to harmonic lattice dynamics calculations (linear-response with PBE-TS). Atoms are shown as solid spheres: hydrogen (grey), carbon (black), and nitrogen (blue). Atomic displacements are shown as solid red vectors.

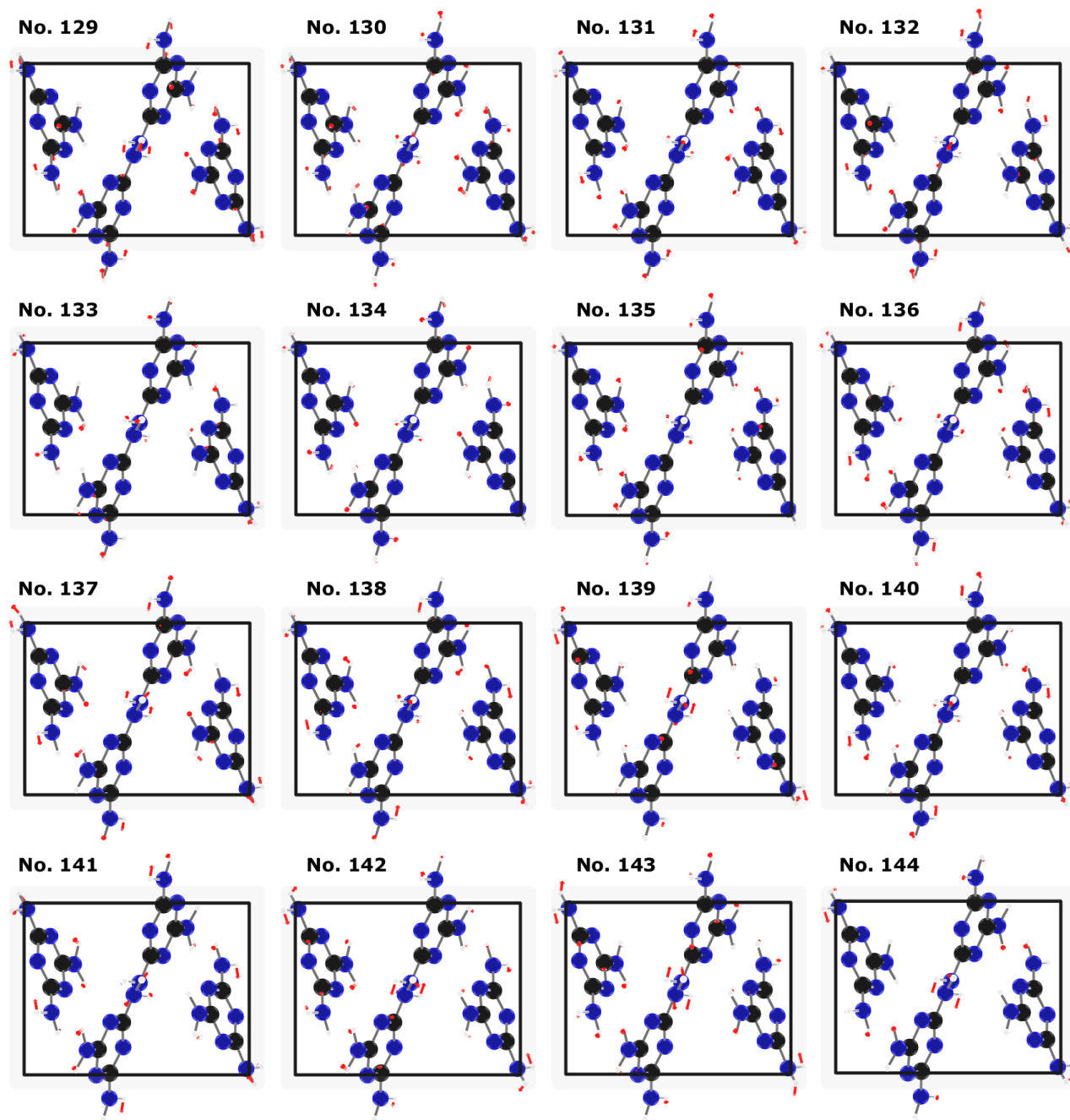


Figure S12. Schematic representation of the zone-centre modes eigenvectors (No. 129 - 144), according to harmonic lattice dynamics calculations (linear-response with PBE-TS). Atoms are shown as solid spheres: hydrogen (grey), carbon (black), and nitrogen (blue). Atomic displacements are shown as solid red vectors.

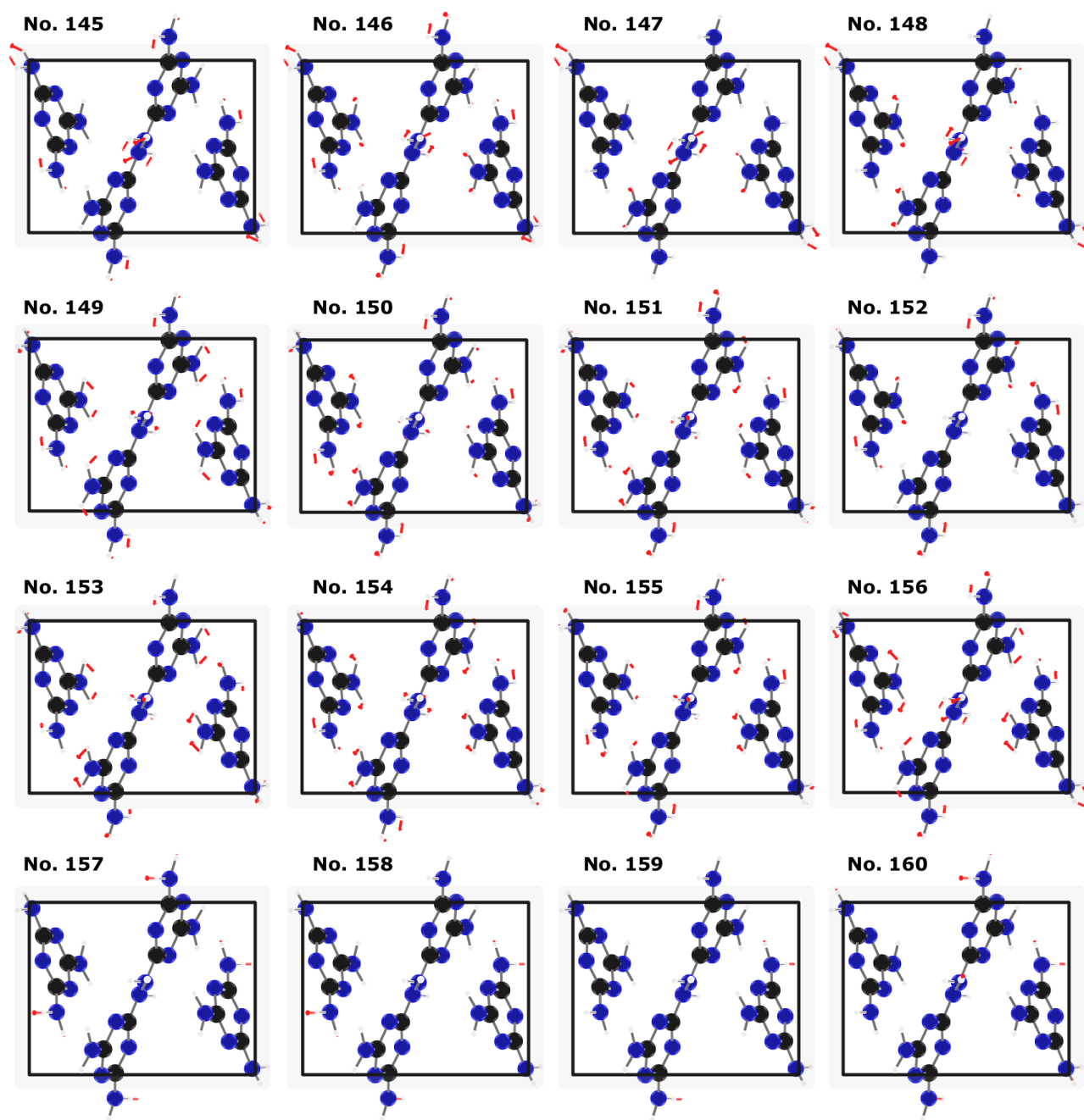


Figure S13. Schematic representation of the zone-centre modes eigenvectors (No. 145 - 160), according to harmonic lattice dynamics calculations (linear-response with PBE-TS). Atoms are shown as solid spheres: hydrogen (grey), carbon (black), and nitrogen (blue). Atomic displacements are shown as solid red vectors.

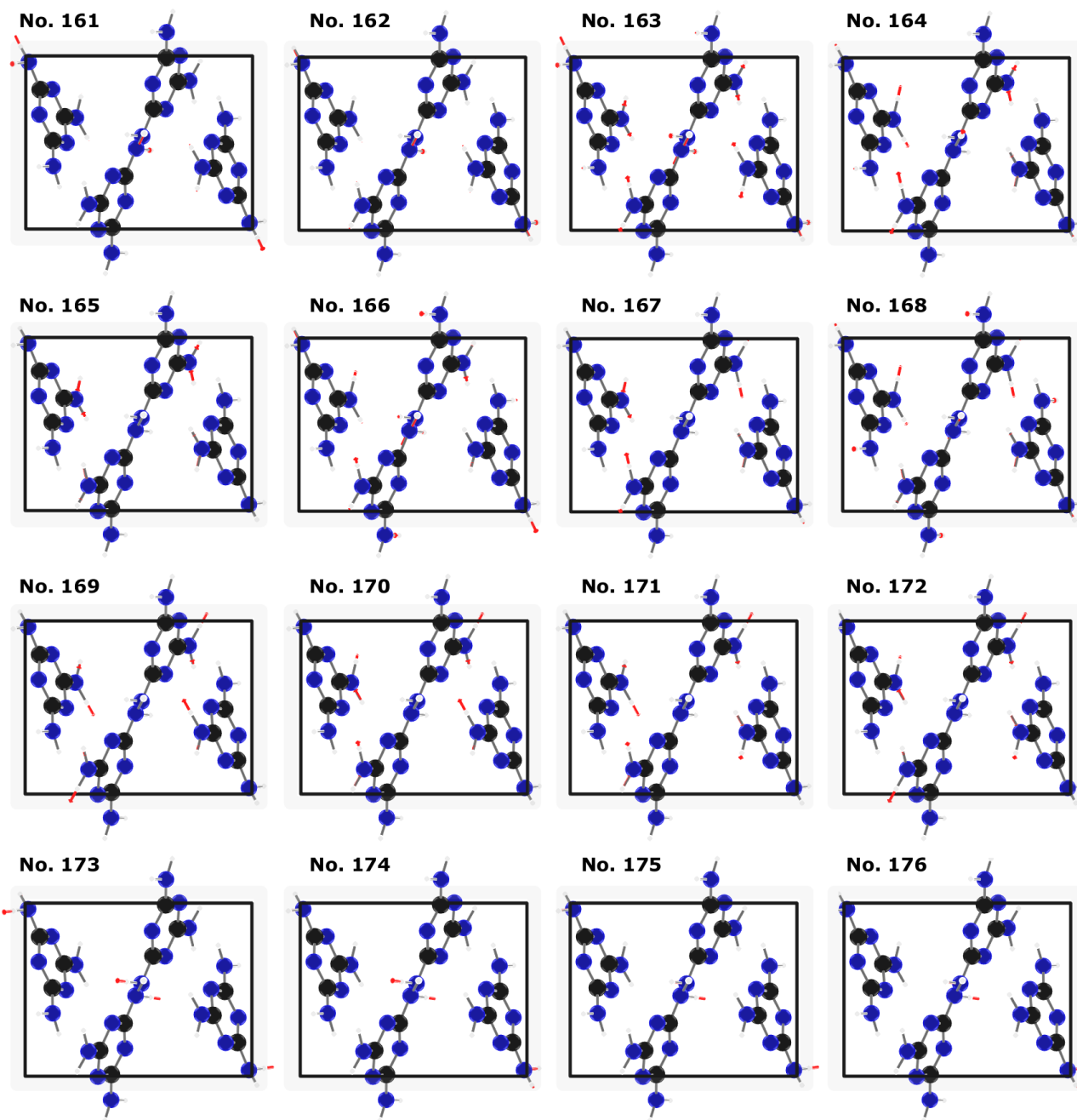


Figure S14. Schematic representation of the zone-centre modes eigenvectors (No. 161 - 176), according to harmonic lattice dynamics calculations (linear-response with PBE-TS). Atoms are shown as solid spheres: hydrogen (grey), carbon (black), and nitrogen (blue). Atomic displacements are shown as solid red vectors.

Mode no.	$\omega(q_1)$	$\omega(q_2)$	$\omega(q_3)$	$\omega(q_4)$	$\omega(q_5)$	$\omega(q_6)$	$\omega(q_7)$	$\omega(q_8)$	$\omega(q_9)$	$\omega(q_{10})$	$\omega(q_{11})$	$\omega(q_{12})$	$\omega(q_{13})$	$\omega(q_{14})$	$\omega(q_{15})$	$\omega(q_{16})$	$\omega(q_{17})$	$\omega(q_{18})$	$\omega(q_{19})$	$\omega(q_{20})$	$\omega(q_{21})$	$\omega(q_{22})$	$\omega(q_{23})$	$\omega(q_{24})$	$\omega(q_{25})$	$\omega(q_{26})$	$\omega(q_{27})$	$\omega(q_{28})$	$\omega(q_{29})$	
1	4.6283	4.7610	4.2365	3.0079	1.5548	0.0000	0.0000	0.0000	0.94166	2.4462	4.4672	4.9842	5.2780	5.0040	5.6177	6.2054	5.9698	4.9656	3.7270	4.6643	4.4411	2.9962	4.3952	4.4510	5.2693	6.3592	6.8328	6.7795	6.6790	6.6790
2	5.0573	5.3078	4.5254	3.7629	2.1313	0.0000	1.8560	3.7071	5.2049	4.4672	4.9842	5.2780	5.0040	5.6177	6.2054	5.9698	4.9656	5.7144	5.3586	4.4498	4.0555	4.3952	4.4510	5.2693	6.3592	6.8328	6.7795	6.6790	6.6790	
3	6.3083	5.4878	6.5724	5.8682	1.5111	0.091029	0.07018	7.5385	8.6615	6.7026	6.6046	6.4745	6.8092	7.5560	7.6411	7.2965	6.1843	6.1112	5.7219	5.5843	6.4013	6.0046	5.2557	5.9401	7.1254	8.2896	9.2405	9.4699	9.7340	
4	6.4621	6.7919	6.9072	7.7751	7.9003	6.9406	6.9406	7.9895	8.6839	8.1966	6.6046	6.4745	6.8092	7.3560	7.6411	7.2965	6.1843	6.1112	7.1849	7.4105	7.0237	7.0014	5.2557	5.9401	7.1254	8.2896	9.2405	9.4699	9.7340	
5	6.6418	7.2667	7.0721	8.2363	8.6367	7.9573	7.9536	8.3603	9.2616	9.8258	10.447	10.113	9.5778	9.4662	10.234	11.116	10.601	10.386	9.3596	8.2995	7.1465	7.0262	6.3540	8.0342	10.167	11.221	10.406	10.659	11.385	
6	6.8938	8.8760	9.8753	9.9981	8.8046	9.1091	9.1364	9.9373	9.4488	9.1038	10.447	10.113	9.5778	9.4662	10.234	11.116	10.601	10.386	11.240	11.118	9.3968	8.3441	6.8340	8.0342	10.167	11.221	10.406	10.659	11.385	
7	10.935	11.088	10.922	11.035	9.5443	10.245	10.245	10.257	10.389	11.015	11.663	11.407	10.845	10.404	10.730	11.920	13.142	13.266	12.671	11.703	10.722	8.7768	9.7910	10.420	11.641	12.436	13.353	13.018	12.671	
8	11.746	11.764	11.948	11.027	11.147	10.245	10.245	10.257	10.389	11.015	11.663	11.407	10.845	10.404	10.730	11.920	13.142	13.266	12.845	12.039	11.673	11.141	9.7910	10.420	11.641	12.436	13.353	13.018	12.671	
9	12.324	12.026	12.510	12.584	11.977	12.460	12.460	12.473	12.597	12.288	11.699	11.942	12.473	13.080	12.820	12.882	13.663	14.209	13.837	13.502	12.845	11.523	11.974	12.121	12.944	14.184	14.804	14.494	13.812	
10	12.994	13.564	13.328	12.746	13.142	13.242	13.242	12.908	12.733	12.309	11.699	11.942	12.473	13.080	12.820	12.882	13.663	14.209	14.568	14.023	12.907	12.473	11.974	12.121	12.944	14.184	14.804	14.494	13.812	
11	13.440	13.013	13.403	13.192	13.279	13.316	13.316	13.403	13.737	13.911	14.501	14.501	13.812	13.541	13.180	13.601	14.705	15.151	15.705	14.469	14.047	14.469	14.717	14.407	15.665	14.692	15.324	15.238	14.779	
12	14.432	14.072	14.816	14.407	14.494	14.444	14.444	14.271	14.581	14.680	14.531	14.295	13.812	13.341	13.180	13.601	14.705	15.151	15.647	15.101	15.089	14.866	14.717	14.407	15.665	14.692	15.324	15.238	14.779	
13	15.833	15.399	15.275	15.386	15.535	15.461	15.461	15.498	15.076	14.680	14.577	15.386	15.089	14.407	14.023	13.936	14.977	15.882	16.403	15.889	16.453	15.771	15.597	15.461	15.907	16.478	16.354	16.118	16.205	
14	15.907	16.031	15.647	15.572	15.833	15.882	15.845	15.696	15.461	15.473	15.386	15.089	14.407	14.023	13.936	14.977	15.882	16.403	16.589	16.453	15.771	15.597	15.461	15.907	16.478	16.354	16.118	16.205		
15	15.920	16.242	16.242	16.440	16.643	16.713	16.713	16.081	15.548	15.721	15.866	15.672	14.692	14.035	15.312	16.329	17.035	17.221	16.775	16.725	16.453	15.634	15.672	16.341	17.283	17.693	17.643	17.333	17.110	
16	16.478	16.543	16.552	16.527	16.673	16.874	16.874	16.465	16.192	16.490	16.081	15.672	14.692	14.035	15.312	16.329	17.035	17.221	17.544	17.234	17.445	16.601	15.672	16.341	17.283	17.693	17.643	17.333	17.110	
17	17.177	17.333	16.763	16.564	16.800	17.135	17.135	17.445	17.705	17.283	17.407	17.531	17.668	17.705	17.866	18.089	18.089	18.077	17.556	17.804	18.003	18.102	18.350	18.399	18.312	18.102	17.866	18.275	18.759	
18	17.177	17.631	17.581	17.866	18.005	17.990	17.990	17.866	17.990	17.693	17.407	17.531	17.668	17.705	17.866	18.089	18.089	18.077	18.151	18.399	18.077	18.374	18.350	18.399	18.312	18.102	17.866	18.275	18.759	
19	18.734	19.044	19.019	18.759	19.007	19.540	19.540	18.957	18.709	18.498	18.846	18.833	18.784	18.771	18.759	18.759	19.007	19.106	19.019	19.193	19.131	19.218	19.515	19.515	19.862	20.160	20.160	19.986	19.652	
20	18.957	19.230	19.701	19.726	19.577	19.540	19.540	19.763	20.185	19.515	19.391	18.846	18.833	18.784	18.771	18.759	18.796	19.007	19.106	19.713	19.825	19.751	19.937	19.515	19.862	20.160	20.160	19.986	19.652	
21	19.999	20.056	20.259	20.696	20.581	20.259	20.247	20.209	19.949	19.639	19.857	19.763	19.788	19.713	20.185	20.743	20.953	20.594	20.482	20.519	20.135	20.234	20.470	20.705	20.792	20.879	20.631	20.222		
22	20.705	20.743	20.941	21.152	21.139	21.127	21.127	20.867	20.346	20.172	19.887	19.880	19.763	19.788	19.713	20.185	20.743	20.953	21.090	21.090	20.991	20.457	20.234	20.470	20.705	20.792	20.879	20.631	20.222	
23	21.548	21.499	21.400	21.511	21.883	21.958	21.958	21.325	20.619	20.309	20.217	20.222	20.098	20.023	20.569	21.437	22.230	22.726	22.454	21.821	21.177	21.177	21.201	21.313	21.685	22.094	22.255	22.401	22.788	
24	22.652	22.553	22.280	21.995	21.920	22.044	22.044	21.734	21.189	20.656	20.271	20.222	20.098	20.023	20.569	21.437	22.230	22.726	22.652	22.255	21.710	21.201	21.313	21.685	22.094	22.255	22.401	22.788		
25	24.425	24.512	24.760	24.722	24.574	24.512	24.512	24.398	24.797	25.156	25.404	25.256	25.070	25.045	24.983	24.970	24.946	24.884	24.673	24.499	24.338	24.289	24.274	24.859	25.665	25.851	25.863	25.851		
26	25.256	25.156	25.403	25.426	25.326	25.351	25.351	25.578	25.137	25.256	25.404	25.256	25.070	25.045	24.983	24.970	24.946	24.884	24.673	24.499	24.338	24.289	24.274	24.859	25.665	25.851	25.863	25.851		
27	25.876	25.938	26.074	26.148	26.233	26.136	26.136	25.888	25.640	25.479	25.640	25.603	25.429	25.280	25.442	25.690	25.950	26.148	25.975	25.677	25.900	25.938	26.061	26.012	25.987	26.533	26.867	26.867	26.830	
28	26.334	26.297	26.235	26.334	26.433	26.272	26.272	26.533	26.495	26.123	25.640	25.603	25.429	25.280	25.442	25.690	25.950	26.148	26.099	25.975	25.938	26.198	26.061	26.012	25.987	26.533	26.867	26.867	26.830	
29	26.867	26.929	26.967	26.781	26.471	26.533	26.508	26.681	26.917	27.277	27.450	27.512	27.574	27.599	27.301	26.979	26.855	26.793	26.743	26.681	26.719	26.781	26.967	27.016	27.128	27.239	27.314	27.326	27.363	
30	27.289	27.289	27.227	27.153	27.023	26.991	26.979	27.115	27.401	27.487	27.450	27.512	27.574	27.599	27.301	26.979	26.855	26.793	26.818	26.805	26.743	26.843	26.967	27.016	27.128	27.239	27.314	27.326	27.363	
31	27.363	27.414	27.388	27.661	27.648	27.673	27.673	27.673	27.723	27.896	27.896	27.896	27.903	28.129	28.330	28.492	28.554	28.368	27.996	27.574	27.376	27.540	27.376	27.540	27.376	27.540	27.376	27.540	27.376	
32	27.463	27.537	27.648	27.696	28.008	28.144	28.144	28.132	28.132	28.070	27.896	27.896	27.896	27.909	28.120	28.330	28.492	28.554	28.504	28.268	27.983	27.673	27.301	27.376	27.540	27.376	27.540	27.376	27.540	
33	30.575	30.643	30.178	29.697	30.044	30.165	30.165	30.240	30.413	30.550	30.587	30.674	30.835	30.922	31.008	31.194	31.269	31.256	30.922	30.798	30.860	30.984	31.157	31.058	30.772	30.773	30.773	30.773	30.773	
34	31.827	31.752	31.604	31.504	30.946	30.562	30.562	30.357	30.624	30.587	30.674	30.835	30.922	31.008	31.194	31.269	31.256	31.554	31.480	31.343	31.157	31.058	30.772	30.773	30.773	30.773	30.773	30.773	30.773	
35	32.819	32.682	32.548	31.604	31.554	31.678	31.703	31.777	31.963	32.112	32.224	32.174	32.075	32.013	31.938	31.802	31.814	31.914	32.000	32.248	32.620	32.943	33.116	33.200	33.687	34.034	34.170	34.170	34.170	
36	33.426	33.339	33.104	32.732	32.335	32.075	32.075	32.038	32.013	32.162	32.224	32.174	32.075	32.013	31.938	31.802	31.814	31.914	32.000	32.248	32.620	32.943	33.116	33.200	33.687	34.034	34.170	34.170	34.170	
37	38.379	48.242	48.069	47.994	47.																									

Table S5. List of modes in melamine calculated from the mode dispersion HLD simulation in CASTEP software. Mode numbers 91 – 180. For details, please take a look at the main article text.

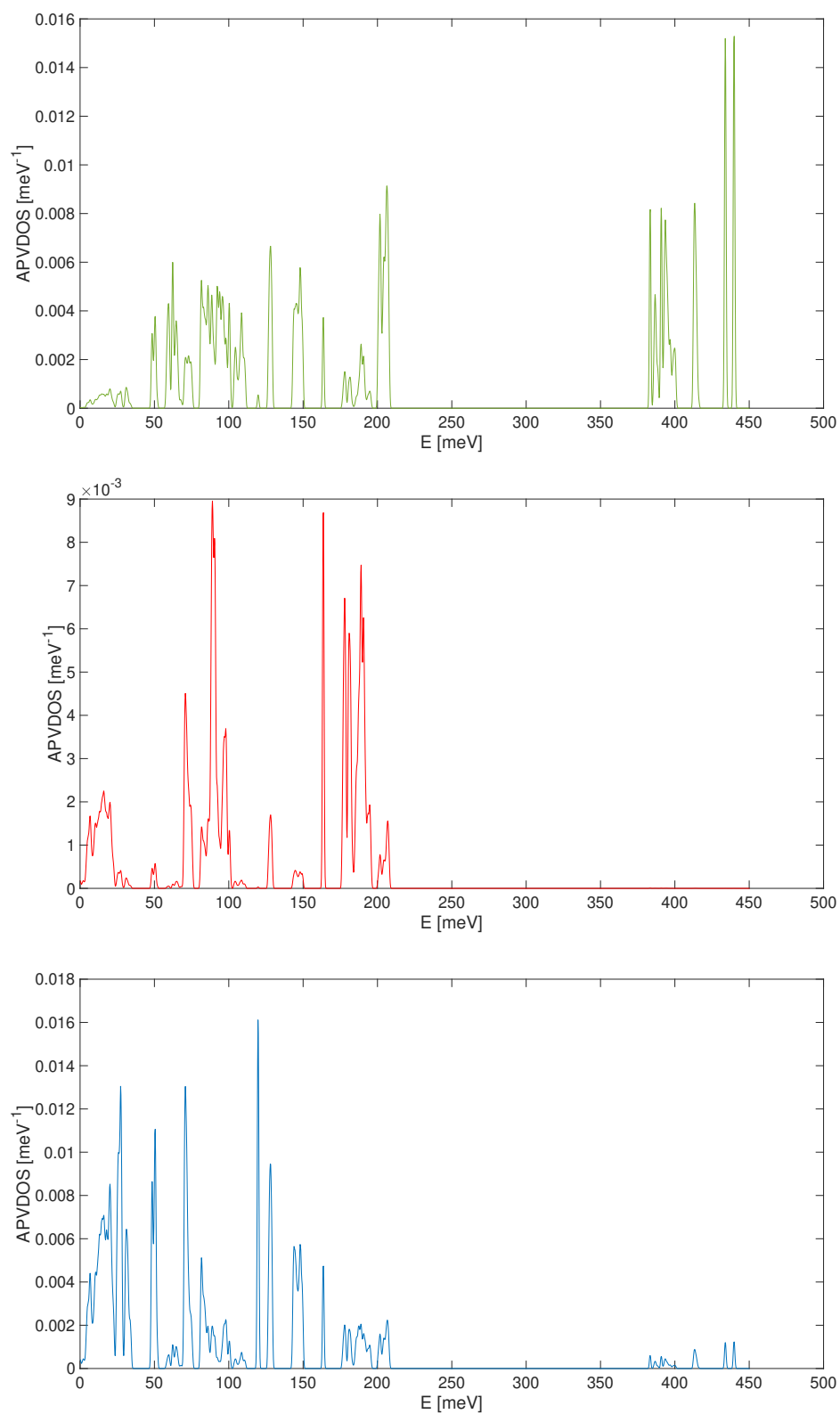


Figure S17. apVDoSs calculated from the mode dispersion HLD simulation in CASTEP software. apVDoS for hydrogen (top panel), carbon (middle panel), and nitrogen (bottom panel). For details, see the text of the main article.

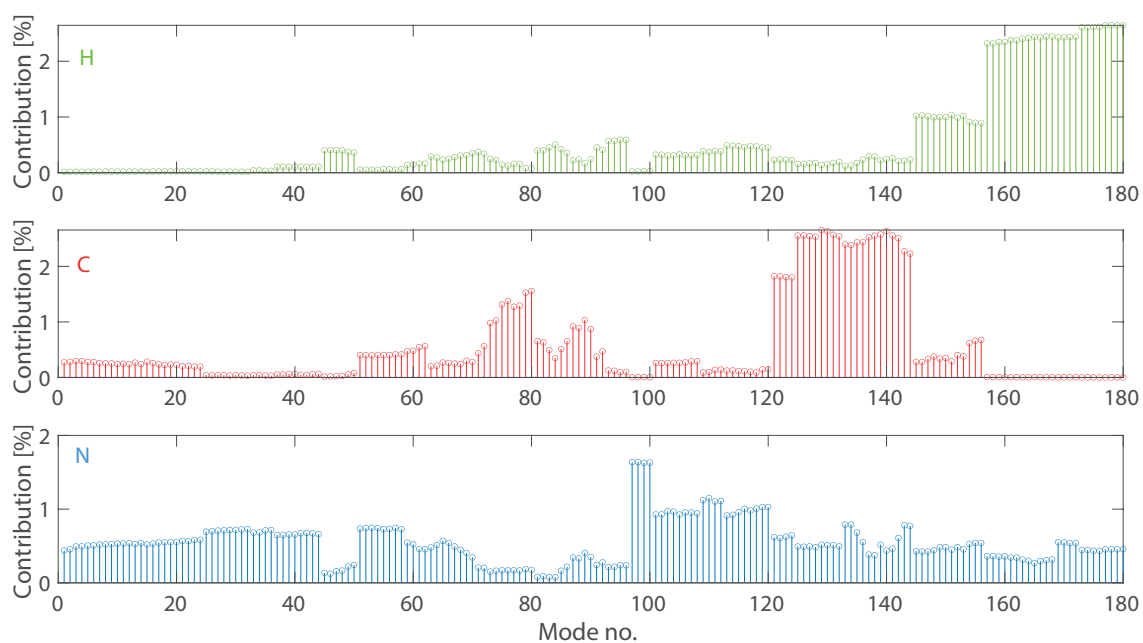


Figure S18. q-averaged individual mode contributions to the total kinetic energy of protons (top panel), carbon (middle panel), and nitrogen (bottom panel) in melamine. For details, see the text of the main article.

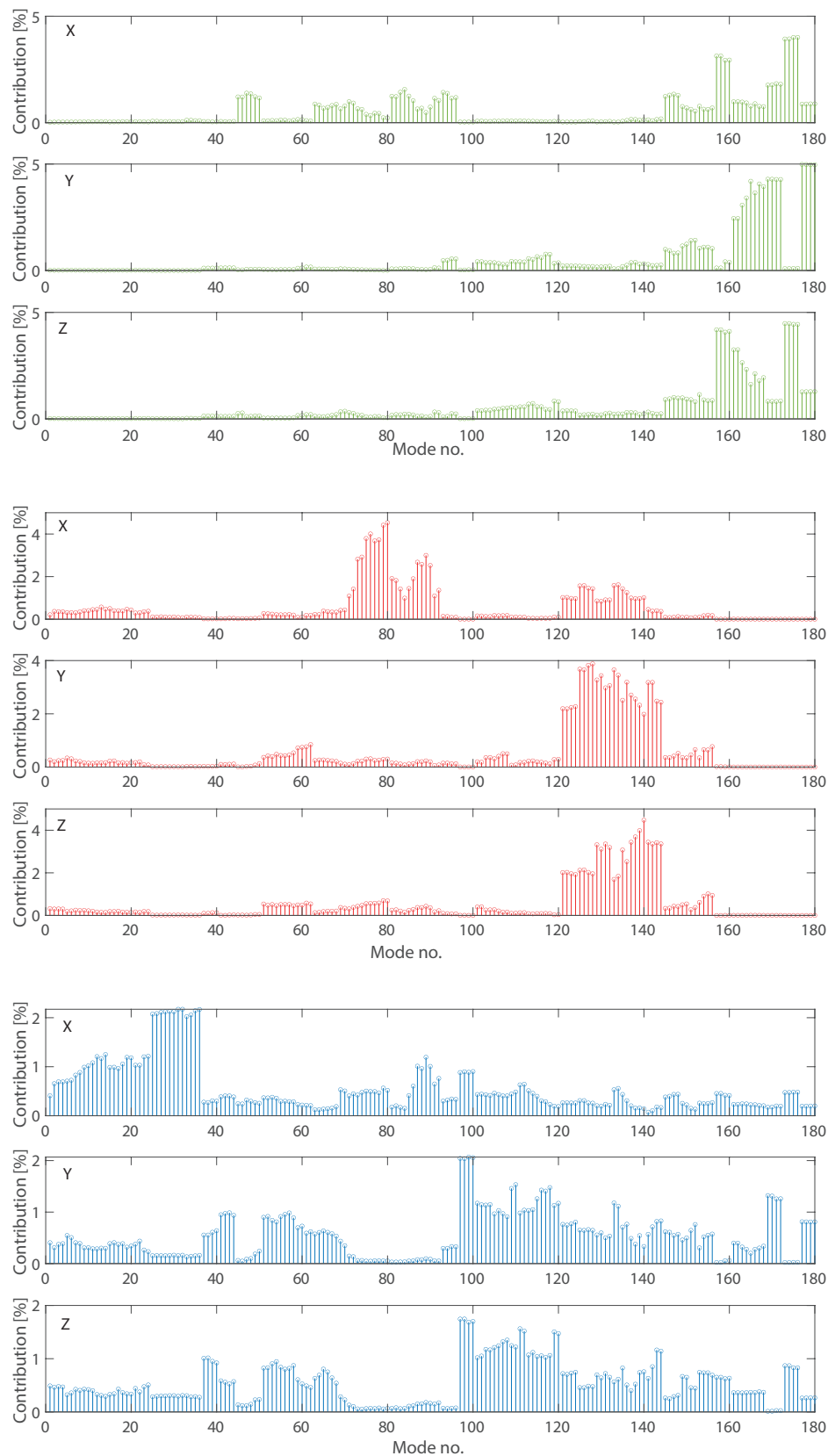


Figure S19. q-averaged individual mode contributions to the total kinetic energy of protons (top panel), carbon (middle panel), and nitrogen (bottom panel) in melamine along the X, Y, and Z crystallographic axes. For details, see the text of the main article.