Table 1S. Comparison of experimental and predicted[a] crystallographic parameters

Pressure (GPa)	Volume (Å^3)[b]	a (Å)[b]	b (Å)[b]	c (Å)[b]	α (deg.)[c]	β (deg.)[c]	γ (deg.)[c]
RDX							
0.0	1641.4	13.2	11.6	10.72	90.00	90.0	90.00
	1884.5 (14.8)	13.6876 (3.7)	11.9330 (2.9)	11.5378 (7.6)	90.00 (0.00)	90.0 (0.00)	90.00 (0.00)
0.73	1565.7	13.02	11.42	10.53	90.00	90.0	90.00
	1703.6 (8.8)	13.3848 (2.8)	11.5487 (1.1)	11.0208 (4.7)	90.00 (0.00)	90.0 (0.00)	90.00 (0.00)
2.75	1439.6	12.8	11.07	10.16	90.00	90.0	90.00
	1516.5 (5.3)	13.0063 (1.6)	11.1404 (0.6)	10.466 (3.0)	90.00 (0.00)	90.0 (0.00)	90.00 (0.00)
3.95	1389.0	12.67	10.93	10.03	90.00	90.0	90.00
	1455.8 (4.8)	12.8946 (1.8)	10.9916 (0.6)	10.2712 (2.4)	90.00 (0.00)	90.0 (0.00)	90.00 (0.00)
β-HMX							
0.0	519.4	6.54	11.03	8.71	90.00	124.4	90.00
	593.3 (14.2)	6.8600 (4.9)	11.5172 (4.4)	8.9288 (2.5)	90.00 (0.00)	122.8 (-1.60)	90.00 (0.00)
1.61	479.9	6.39	10.66	8.57	90.00	125.0	90.00
	507.6 (7.3)	6.5089 (1.9)	10.8589 (3.2)	8.6893 (2.4)	90.00 (0.00)	124.27 (-0.78)	90.00 (0.00)
2.47	466.9	6.35	10.5	8.54	90.00	125.2	90.00
	488.7 (4.6)	6.4517 (1.6)	10.64 (1.3)	8.6413 (1.2)	90.00 (0.00)	124.54 (-0.66)	90.00 (0.00)
3.24	457.6	6.3	10.41	8.51	90.00	125.4	90.00
	475.1 (3.8)	6.3849 (1.4)	10.5104 (1.0)	8.5911 (1.0)	90.00 (0.00)	124.51 (-0.89)	90.00 (0.00)
4.03	452.4	6.3	10.29	8.51	90.00	125.4	90.00
	463.8 (2.5)	6.3424 (0.7)	10.4031 (1.1)	8.5564 (0.6)	90.00 (0.00)	124.75 (-0.65)	90.00 (0.00)
4.82	444.6	6.26	10.19	8.51	90.00	125.5	90.00
	454.6 (2.3)	6.3083 (0.8)	10.2648 (0.7)	8.5396 (0.4)	90.00 (0.00)	124.69 (0.81)	90.00 (0.00)
5.42	440.4	6.24	10.16	8.48	90.00	125.4	90.00
	448.3 (1.8)	6.2849 (0.7)	10.1899 (0.3)	8.5232 (0.5)	90.00 (0.00)	124.79 (-0.61)	90.00 (0.00)
6.31	437.8	6.22	10.08	8.51	90.00	125.3	90.00
	439.9 (0.5)	6.2521 (0.5)	10.07 (-0.1)	8.5087 (0.0)	90.00 (0.00)	124.79 (-0.51)	90.00 (0.00)
6.74	434.7	6.22	10.01	8.51	90.00	125.3	90.00
	436.2 (0.3)	6.2283 (0.1)	10.0269 (0.2)	8.4944 (-0.2)	90.00 (0.00)	124.69 (-0.61)	90.00 (0.00)
7.47	429.5	6.21	9.98	8.49	90.00	125.7	90.00
	430.5 (0.2)	6.2024 (-0.1)	9.9597 (-0.2)	8.4715 (-0.2)	90.00 (0.00)	124.65 (-1.05)	90.00 (0.00)

ε-CL-20												
0.0	1423.0		8.8520		12.5560		13.3860		90.00		106.82		90.00	
	1645.5	(15.6)	9.2739	(4.8)	13.3231	(6.1)	13.9806	(4.4)	90.00	(0.00)	107.71	(0.89)	90.00	(0.00)
0.35	1392.1		8.783		12.453		13.281		90.00		106.61		90.00	
	1583.9	(13.8)	9.141	(4.1)	13.1717	(5.8)	13.7681	(3.7)	90.00	(0.00)	107.16	(0.55)	90.00	(0.00)
0.90	1356.5		8.7285		12.3091		13.1514		90.00		106.26		90.00	
	1480.6	(14.0)	8.9425	(2.4)	12.8058	(4.0)	13.5094	(2.7)	90.00	(0.00)	106.85	(0.59)	90.00	(0.00)
1.70	1299.0		8.5999		12.1114		12.9745		90.00		106.01		90.00	
	1444.4	(11.2)	8.8898	(3.4)	12.6031	(4.1)	13.4741	(3.8)	90.00	(0.00)	106.90	(0.89)	90.00	(0.00)
2.50	1263.1		8.544		11.937		12.839		90.00		105.28		90.00	
	1354.8	(7.3)	8.705	(1.9)	12.3231	(3.3)	13.1423	(2.4)	90.00	(0.00)	106.06	(0.78)	90.00	(0.00)
TATB														
0.0	442.5		9.01		9.028		6.812		108.6		91.8		120	
	530.5	(19.9)	9.3649	(3.9)	9.3691	(3.8)	7.5054	(10.2)	107.22	(-1.38)	91.85	(0.05)	120.18	(0.18)
1.41	411.1		8.958		8.976		6.461		109.5		91.9		120	
	447.8	(8.9)	9.0616	(1.2)	9.078	(1.1)	6.823	(5.6)	108.52	(-0.98)	91.88	(0.02)	120.07	(0.07)
2.69	391.6		8.877		8.895		6.289		109.9		91.9		120	
	417.7	(6.7)	8.9667	(1.0)	8.9849	(1.0)	6.5509	(4.2)	109.46	(-0.44)	91.94	(0.04)	120.02	(0.02)
3.56	384.8		8.846		8.864		6.205		110.1		92		120	
	404.5	(5.1)	8.9281	(0.9)	8.9373	(0.8)	6.4397	(3.8)	109.93	(-0.17)	91.95	(0.05)	120.08	(0.08)
6.17	363.5		8.752		8.77		6.039		110.4		92		120	
	377.5	(3.8)	8.8192	(0.8)	8.8361	(0.8)	6.2001	(2.7)	110.73	(0.33)	92.18	(0.18)	119.96	(-0.04)
7.02	351.5		8.678		8.695		5.951		110.6		92		120	
	371.0	(5.6)	8.7888	(1.3)	8.8124	(1.4)	6.1396	(3.2)	110.94	(0.34)	92.12	(0.12)	119.94	(-0.06)
PETN														
0.0	591.6		9.386		9.386		6.715		90.00		90.0		90.00	
	680.7	(15.1)	9.8749	(5.2)	9.8609	(5.1)	6.9908	(4.1)	90.02	(0.02)	89.84	(-0.16)	90.03	(0.03)
1.28	546.8		9.1926		9.1926		6.4706		90.00		90.0		90.00	
	582.0	(6.4)	9.3329	(1.5)	9.3435	(1.6)	6.6744	(3.2)	90.00	(0.00)	89.96	(-0.04)	90.06	(0.06)
2.25	530.8		9.1138		9.1138		6.3907		90.00		90.0		90.00	
	548.6	(3.3)	9.1461	(0.4)	9.1547	(0.4)	6.5516	(2.5)	90.16	(0.16)	89.96	(-0.04)	90.05	(0.05)
3.53	504.4		8.9514		8.9514		6.2953		90.00		90.0		90.00	
	522.0	(3.5)	8.9926	(0.5)	8.9904	(0.4)	6.4569	(2.6)	90.01	(0.01)	89.93	(-0.07)	90.03	(0.03)
4.90	493.3		8.9054		8.9054		6.2201		90.00		90.0		90.00	
	502.3	(1.8)	8.8613	(-0.5)	8.8654	(-0.4)	6.3939	(2.8)	90.01	(0.01)	89.96	(-0.04)	90.03	(0.03)

5.64	482.0		8.8294		8.8294		6.1832		90.00		90.0		90.00	
	492.8	(2.2)	8.8045	(-0.3)	8.8049	(-0.3)	6.3563	(2.8)	90.02	(0.02)	89.98	(-0.02)	90.03	(0.03)
6.73	469.6		8.7449		8.7449		6.1409		90.00		90.0		90.00	
	481.8	(2.6)	8.7243	(-0.2)	8.7279	(-0.2)	6.3269	(3.0)	90.02	(0.02)	89.99	(-0.01)	90.02	(0.02)
7.60	463.8		8.6952		8.6952		6.1342		90.00		90.0		90.00	
	473.9	(2.2)	8.6714	(-0.3)	8.6746	(-0.2)	6.3001	(2.7)	90.02	(0.02)	89.98	(-0.02)	90.02	(0.02)
8.40	453.8		8.6398		8.6398		6.0791		90.00		90.0		90.00	
	467.0	(2.9)	8.6266	(-0.2)	8.6296	(-0.1)	6.2732	(3.2)	90.01	(0.01)	89.96	(-0.04)	90.01	(0.01)
9.16	450.2		8.6257		8.6257		6.0502		90.00		90.0		90.00	
	461.1	(2.4)	8.5881	(-0.4)	8.5898	(-0.4)	6.25	(3.3)	90.00	(0.00)	89.96	(-0.04)	90.00	(0.00)

a. PW91 at 545 eV, given directly under experimental value
b. Percent difference given in parentheses
c. Difference given in parentheses

Table 2S. Crystallographic and molecular structural parameters for RDX

P (GPa)	Crystallographic structural parameters						Molecular parameters	
	sx	sy	sz	θ (°)	ϕ (°)	ψ (°)	rms (Å)	max deviation (Å)
				Molecule 1				
Expt.	-0.4183	-0.0948	-0.1479	101.42	32.44	-6.15		
0.73	-0.4171	-0.0929	-0.1482	100.69	32.20	-8.50	0.064	0.135
2.75	-0.4201	-0.0924	-0.1479	100.49	31.85	-5.87	0.048	0.128
3.95	-0.0781	0.0937	0.3525	80.37	31.50	5.01	0.057	0.171
				Molecule 2				
Expt.	-0.0817	0.0948	0.35	78.58	32.44	6.15		
0.73	-0.0829	0.0929	0.3518	79.31	32.20	8.50	0.064	0.135
2.75	-0.0799	0.0924	0.3521	79.51	31.85	5.87	0.048	0.128
3.95	-0.0781	0.0937	0.3525	80.37	31.50	5.01	0.057	0.171
				Molecule 3				
Expt.	0.4183	0.4052	-0.3521	78.58	-32.44	-6.15		
0.73	0.4171	0.4071	-0.3518	79.31	-32.20	-8.50	0.064	0.135
2.75	0.4201	0.4076	-0.3521	79.51	-31.85	-5.87	0.048	0.128
3.95	0.4220	0.4063	-0.3525	80.37	-31.50	-5.00	0.057	0.171
				Molecule 4				
Expt.	0.0817	-0.4052	0.1479	101.42	-32.44	6.15		
0.73	0.0829	-0.4071	0.1482	100.69	-32.20	8.50	0.064	0.135
2.75	0.0799	-0.4076	0.1479	100.49	-31.85	5.87	0.048	0.128
3.95	0.0781	-0.4063	0.1475	99.63	-31.50	5.00	0.057	0.171
				Molecule 5				
Expt.	0.4183	0.0948	0.1479	101.42	32.44	-6.15		
0.73	0.4171	0.0929	0.1482	100.69	32.20	-8.50	0.064	0.135
2.75	0.4201	0.0924	0.1479	100.49	31.85	-5.87	0.048	0.128
3.95	0.4220	0.0937	0.1475	99.63	31.50	-5.00	0.057	0.171
				Molecule 6				
Expt.	0.0817	-0.0948	-0.3521	78.58	32.44	6.15		
0.73	0.0829	-0.0929	-0.3518	79.31	32.20	8.50	0.064	0.135
2.75	0.0799	-0.0924	-0.3521	79.51	31.85	5.87	0.048	0.128
3.95	0.0781	-0.0937	-0.3525	80.37	31.50	5.00	0.057	0.171
				Molecule 7				
Expt.	-0.4183	-0.4052	0.3521	78.58	-32.44	-6.15		
0.73	-0.4171	-0.4071	0.3518	79.31	-32.20	-8.50	0.064	0.135
2.75	-0.4201	-0.4076	0.3521	79.51	-31.85	-5.87	0.048	0.128
3.95	-0.4220	-0.4063	0.3525	80.37	-31.50	-5.00	0.057	0.171
				Molecule 8				
Expt.	-0.0817	0.4052	-0.1479	101.42	-32.44	6.15		
0.73	-0.0829	0.4071	-0.1482	100.69	-32.20	8.50	0.064	0.135
2.75	-0.0799	0.4076	-0.1479	100.49	-31.85	5.87	0.048	0.128
3.95	-0.0781	0.4063	-0.1475	99.63	-31.50	5.00	0.057	0.171

Table 3S. Crystallographic and molecular structural parameters for β-HMX

P (GPa)	Crystallographic structural parameters						Molecular parameters	
	sx	sy	sz	θ (°)	ϕ (°)	ψ (°)	rms (Å)	max deviation (Å)
				Molecule 1				
Expt.	0.2269	0.2500	0.3026	164.34	22.36	13.95		
1.61	0.2279	0.2500	0.3025	164.09	23.70	15.14	0.034	0.063
2.47	0.2306	0.2500	0.3035	163.87	23.71	15.39	0.045	0.086
3.24	0.2320	0.2500	0.3034	163.60	23.02	15.06	0.055	0.110
4.03	0.2343	0.2500	0.3043	163.61	22.13	14.30	0.062	0.130
4.82	0.2351	0.2500	0.3041	163.47	22.19	14.87	0.075	0.163
5.42	0.2363	0.2500	0.3044	163.46	21.71	14.51	0.081	0.179
6.31	0.2376	0.2500	0.3044	163.19	21.11	14.37	0.092	0.201
6.74	0.2378	0.2500	0.3040	163.16	21.31	14.80	0.098	0.214
7.47	0.2380	0.2500	0.3039	163.07	21.23	14.98	0.106	0.229
				Molecule 2				
Expt.	-0.2269	-0.2500	-0.3026	15.66	-22.36	13.95		
1.61	-0.2279	-0.2500	-0.3025	15.91	-23.70	15.14	0.034	0.063
2.47	-0.2306	-0.2500	-0.3035	16.13	-23.71	15.39	0.045	0.086
3.24	-0.2320	-0.2500	-0.3034	16.40	-23.02	15.06	0.055	0.110
4.03	-0.2343	-0.2500	-0.3043	16.39	-22.13	14.30	0.062	0.130
4.82	-0.2351	-0.2500	-0.3041	16.53	-22.19	14.87	0.075	0.163
5.42	-0.2363	-0.2500	-0.3044	16.54	-21.71	14.51	0.081	0.179
6.31	-0.2376	-0.2500	-0.3044	16.81	-21.11	14.37	0.092	0.201
6.74	-0.2378	-0.2500	-0.3040	16.84	-21.31	14.80	0.098	0.214
7.47	-0.2380	-0.2500	-0.3039	16.93	-21.23	14.98	0.106	0.229

Table 4S. Crystallographic and molecular structural parameters for ε-CL20

P (GPa)	Crystallographic structural parameters						Molecular parameters	
	sx	sy	sz	θ (°)	ϕ (°)	ψ (°)	rms (Å)	max deviation (Å)
				Molecule 1				
Expt	0.0913	0.1355	0.2776	64.77	51.21	5.50		
0.35	0.0920	0.1367	0.2790	64.43	51.26	4.74	0.094	0.192
0.90	0.0922	0.1359	0.2794	65.75	51.40	4.87	0.081	0.184
1.70	0.0921	0.1355	0.2777	65.12	51.23	5.50	0.041	0.083
2.50	0.0891	0.1354	0.2779	67.40	51.50	5.24	0.079	0.175
				Molecule 2				
Expt	-0.2976	-0.3645	0.3447	64.77	128.79	-5.50		
0.35	-0.2954	-0.3633	0.3456	64.43	128.74	-4.74	0.094	0.192
0.90	-0.2985	-0.3641	0.3431	65.75	128.60	-4.87	0.081	0.184
1.70	-0.2964	-0.3645	0.3450	65.12	128.77	-5.50	0.041	0.083
2.50	-0.3059	-0.3646	0.3398	67.40	128.51	-5.24	0.079	0.175
				Molecule 3				
Expt	-0.0913	-0.1355	-0.2776	64.77	51.21	5.50		
0.35	-0.0920	-0.1367	-0.2790	64.43	51.26	4.74	0.094	0.192
0.90	-0.0922	-0.1359	-0.2794	65.75	51.40	4.87	0.081	0.184
1.70	-0.0921	-0.1355	-0.2777	65.12	51.23	5.50	0.041	0.083
2.50	-0.0891	-0.1354	-0.2779	67.39	51.49	5.24	0.079	0.175
				Molecule 4				
Expt	0.2976	0.3645	-0.3447	64.77	128.79	-5.50		
0.35	0.2954	0.3633	-0.3456	64.43	128.74	-4.74	0.094	0.192
0.90	0.2985	0.3641	-0.3431	65.75	128.60	-4.87	0.081	0.184
1.70	0.2964	0.3645	-0.3450	65.12	128.77	-5.50	0.041	0.083
2.50	0.3059	0.3646	-0.3398	67.40	128.51	-5.24	0.079	0.175

Table 5S. Crystallographic and molecular structural parameters for TATB

P (GPa)	Crystallographic structural parameters						Molecular parameters	
	sx	sy	sz	θ (°)	ϕ (°)	ψ (°)	rms (Å)	max deviation (Å)
				Molecule 1				
Expt	-0.2716	-0.3263	-0.1121	157.01	-33.11	-124.91		
0	-0.2780	-0.3333	-0.1216	156.84	-34.96	-111.16	0.104	0.280
1.41	-0.2704	-0.3251	-0.1122	156.97	-34.06	-76.60	0.102	0.279
2.69	-0.2661	-0.3210	-0.1068	156.58	-33.33	-80.20	0.103	0.279
3.56	-0.2650	-0.3186	-0.1039	156.56	-33.22	-69.24	0.104	0.280
6.17	-0.2602	-0.3154	-0.0989	156.73	-32.26	-71.28	0.107	0.290
7.02	-0.2593	-0.3146	-0.0975	156.72	-32.23	-75.87	0.107	0.290
				Molecule 2				
Expt	0.2716	0.3263	0.1121	157.01	-33.11	-124.91		
0	0.2780	0.3333	0.1216	156.84	-34.96	-111.27	0.104	0.280
1.41	0.2704	0.3251	0.1122	156.97	-34.06	-76.54	0.102	0.279
2.69	0.2661	0.3210	0.1068	156.58	-33.33	-80.16	0.103	0.279
3.56	0.2650	0.3186	0.1039	156.56	-33.22	-69.25	0.104	0.280
6.17	0.2602	0.3154	0.0989	156.73	-32.26	-71.27	0.107	0.290
7.02	0.2593	0.3146	0.0975	156.72	-32.23	-75.88	0.107	0.290

Table 6S. Crystallographic and molecular structural parameters for PETN

P (GPa)	Crystallographic structural parameters						Molecular parameters[a]	
	sx	sy	sz	θ (°)	ϕ (°)	ψ (°)	rms (Å)	max deviation (Å)
				Asymmetric Unit 1				
Expt.	0.4679	0.2462	0.0300	47.68	-131.76	111.84		
0.00	0.4566	0.2478	0.0197	47.87	-130.56	111.41	0.070	0.114
1.28	0.4672	0.2473	0.0324	48.75	-133.28	112.93	0.065	0.111
2.25	0.4710	0.2486	0.0372	48.96	-133.69	113.37	0.065	0.111
3.53	0.4723	0.2486	0.0420	49.13	-133.59	113.05	0.071	0.109
4.90	0.4740	0.2489	0.0444	49.25	-134.14	113.25	0.077	0.109
5.64	0.4747	0.2486	0.0465	49.31	-134.16	113.11	0.083	0.112
6.73	0.4754	0.2492	0.0479	49.49	-134.24	113.08	0.091	0.125
7.60	0.4757	0.2493	0.0492	49.53	-134.27	113.00	0.098	0.138
8.40	0.4758	0.2495	0.0507	49.64	-134.33	112.99	0.104	0.148
9.16	0.4761	0.2498	0.0518	49.68	-134.28	112.94	0.108	0.156
10.45	0.4679	0.2462	0.0300	47.68	-131.76	111.84	0.117	0.170
				Asymmetric Unit 2				
Expt.	-0.4679	-0.2538	-0.0300	132.32	131.76	111.84		
0.00	-0.4568	-0.2516	-0.0200	132.20	130.53	111.61	0.070	0.113
1.28	-0.4674	-0.2524	-0.0325	131.24	133.23	112.98	0.064	0.113
2.25	-0.4705	-0.2513	-0.0371	131.25	133.03	112.92	0.065	0.115
3.53	-0.4724	-0.2509	-0.0418	130.75	133.55	113.17	0.071	0.111
4.90	-0.4737	-0.2511	-0.0448	130.70	133.98	113.12	0.078	0.109
5.64	-0.4746	-0.2512	-0.0466	130.62	134.23	113.17	0.083	0.112
6.73	-0.4753	-0.2511	-0.0482	130.54	134.03	112.89	0.091	0.124
7.60	-0.4756	-0.2509	-0.0495	130.46	134.13	112.90	0.098	0.137
8.40	-0.4757	-0.2506	-0.0509	130.36	134.27	112.94	0.103	0.147
9.16	-0.4759	-0.2505	-0.0520	130.31	134.27	112.89	0.108	0.156
10.45	-0.4764	-0.2503	-0.0532	130.25	134.24	112.76	0.117	0.169
				Asymmetric Unit 3				
Expt.	0.0322	0.2538	0.0300	132.32	-131.76	-111.84		
0.00	0.0413	0.2524	0.0188	132.42	-130.27	-111.19		
1.28	0.0320	0.2525	0.0322	131.29	-133.29	-112.96		
2.25	0.0289	0.2515	0.0374	131.30	-133.04	-112.82		
3.53	0.0267	0.2511	0.0420	130.88	-133.57	-113.03		
4.90	0.0251	0.2511	0.0444	130.78	-134.09	-113.22		
5.64	0.0247	0.2514	0.0465	130.71	-134.12	-113.07		
6.73	0.0241	0.2509	0.0480	130.53	-134.17	-113.02		
7.60	0.0236	0.2508	0.0493	130.47	-134.20	-112.96		
8.40	0.0230	0.2505	0.0508	130.36	-134.29	-112.98		
9.16	0.0225	0.2503	0.0518	130.34	-134.30	-112.97		
10.45	0.0220	0.2501	0.0528	130.27	-134.34	-112.91		
				Asymmetric Unit 4				
Expt.	-0.0322	-0.2462	-0.0300	47.68	131.76	-111.84		
0.00	-0.0404	-0.2481	-0.0186	47.50	130.40	-111.49		
1.28	-0.0314	-0.2474	-0.0321	48.40	132.94	-112.81		
2.25	-0.0286	-0.2487	-0.0374	48.98	133.59	-113.23		
3.53	-0.0267	-0.2484	-0.0421	49.17	134.16	-113.30		
4.90	-0.0250	-0.2490	-0.0442	49.24	134.12	-113.26		
5.64	-0.0246	-0.2488	-0.0465	49.34	134.06	-113.08		
6.73	-0.0240	-0.2492	-0.0478	49.52	134.29	-113.13		

7.60	-0.0235	-0.2493	-0.0491	49.55	134.30	-113.05
8.40	-0.0227	-0.2496	-0.0507	49.61	134.32	-113.04
9.16	-0.0223	-0.2497	-0.0516	49.64	134.35	-113.01
			Asymmetric Unit 5			
Expt.	0.2462	0.0322	-0.5300	47.68	-41.76	-68.16
0.00	0.2478	0.0409	-0.5191	47.45	-40.54	-68.50
1.28	0.2474	0.0325	-0.5322	48.79	-43.36	-66.97
2.25	0.2488	0.0281	-0.5380	48.86	-43.34	-66.92
3.53	0.2490	0.0272	-0.5425	49.22	-43.52	-66.97
4.90	0.2490	0.0256	-0.5445	49.30	-44.13	-66.69
5.64	0.2489	0.0248	-0.5467	49.42	-44.27	-66.75
6.73	0.2493	0.0243	-0.5483	49.53	-44.22	-66.85
7.60	0.2494	0.0239	-0.5495	49.60	-44.27	-66.90
8.40	0.2498	0.0236	-0.5508	49.72	-44.32	-66.89
9.16	0.2499	0.0233	-0.5518	49.74	-44.30	-66.95
10.45	0.2501	0.0228	-0.5529	49.79	-44.34	-67.02
			Asymmetric Unit 6			
Expt.	-0.2462	-0.4679	0.5300	47.68	-138.24	68.16
0.00	-0.2481	-0.4583	0.5190	47.68	-139.36	68.45
1.28	-0.2477	-0.4674	0.5322	48.88	-136.61	66.94
2.25	-0.2493	-0.4701	0.5373	49.03	-136.27	66.49
3.53	-0.2462	-0.4679	0.5300	47.68	-138.24	68.16
4.90	-0.2492	-0.4744	0.5447	49.36	-135.72	66.60
5.64	-0.2489	-0.4749	0.5467	49.41	-135.83	66.82
6.73	-0.2462	-0.4679	0.5300	47.68	-138.24	68.16
7.60	-0.2495	-0.4759	0.5495	49.64	-135.67	66.89
8.40	-0.2499	-0.4763	0.5507	49.79	-135.54	66.81
9.16	-0.2500	-0.4769	0.5518	49.79	-135.56	66.86
10.45	-0.2462	-0.4679	0.5300	47.68	-138.24	68.16
			Asymmetric Unit 7			
Expt.	0.2462	0.0322	-0.5300	47.68	-41.76	-68.16
0.00	0.2478	0.0409	-0.5191	47.45	-40.54	-68.50
1.28	0.2474	0.0325	-0.5322	48.79	-43.36	-66.97
2.25	0.2488	0.0281	-0.5380	48.86	-43.34	-66.92
3.53	0.2490	0.0272	-0.5425	49.22	-43.52	-66.97
4.90	0.2490	0.0256	-0.5445	49.30	-44.13	-66.69
5.64	0.2489	0.0248	-0.5467	49.42	-44.27	-66.75
6.73	0.2493	0.0243	-0.5483	49.53	-44.22	-66.85
7.60	0.2494	0.0239	-0.5495	49.60	-44.27	-66.90
8.40	0.2498	0.0236	-0.5508	49.72	-44.32	-66.89
9.16	0.2499	0.0233	-0.5518	49.74	-44.30	-66.95
10.45	0.2501	0.0228	-0.5529	49.79	-44.34	-67.02
			Asymmetric Unit 8			
Expt.	-0.2462	-0.4679	0.5300	47.68	-138.24	68.16
0.00	-0.2481	-0.4583	0.5190	47.68	-139.36	68.45
1.28	-0.2477	-0.4674	0.5322	48.88	-136.61	66.94
2.25	-0.2493	-0.4701	0.5373	49.03	-136.27	66.49
3.53	-0.2462	-0.4679	0.5300	47.68	-138.24	68.16
4.90	-0.2492	-0.4744	0.5447	49.36	-135.72	66.60
5.64	-0.2489	-0.4749	0.5467	49.41	-135.83	66.82
6.73	-0.2462	-0.4679	0.5300	47.68	-138.24	68.16
7.60	-0.2495	-0.4759	0.5495	49.64	-135.67	66.89
8.40	-0.2499	-0.4763	0.5507	49.79	-135.54	66.81
9.16	-0.2500	-0.4769	0.5518	49.79	-135.56	66.86
10.45	-0.2502	-0.4774	0.5529	49.85	-135.53	66.92

a. RMS and maximum atomic displacements for the two full molecules (not symmetry-equivalent fragments) in the unit cell; see text.