Electronic Supplementary Material (ESI) for CrystEngComm.

The Rich Structural Phase Behaviour of 2,2,2-Trifluoroethanol

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1. Single Crystal Diffraction

Crystals of trifluoroethanol (CF_3CD_2OD, TFE) Form 4 were grown by compressing the diamond-anvil cell (DAC) beyond the Form 2 regime and then carefully cycling the temperature so that the polycrystalline material was partially melted each time with the objective that just a single crystallite would remain. The experiment was performed twice, using a 200 μm thick tungsten gasket that had been pre-indented to a thickness of ~100 μm, with a 200 μm diameter hole drilled through it, to produce Form 4 being at 1.54(5) GPa and 2.09(5) GPa. No images were taken of the sample in the cell for either experiment.

Crystals of Forms 5, 2 and 3 were grown in sequence from one DAC loading. This loading was not further pressurised to produce Form 4.
A steel gasket, with an initial thickness of 200 μm and gasket hole diameter of 400 μm, filled with perdeuterated TFE, was used for the characterisation.

The bolts were tightened to seal the diamond-anvil cell, and then just tweaked a fraction more until the sample was no longer fully liquid.

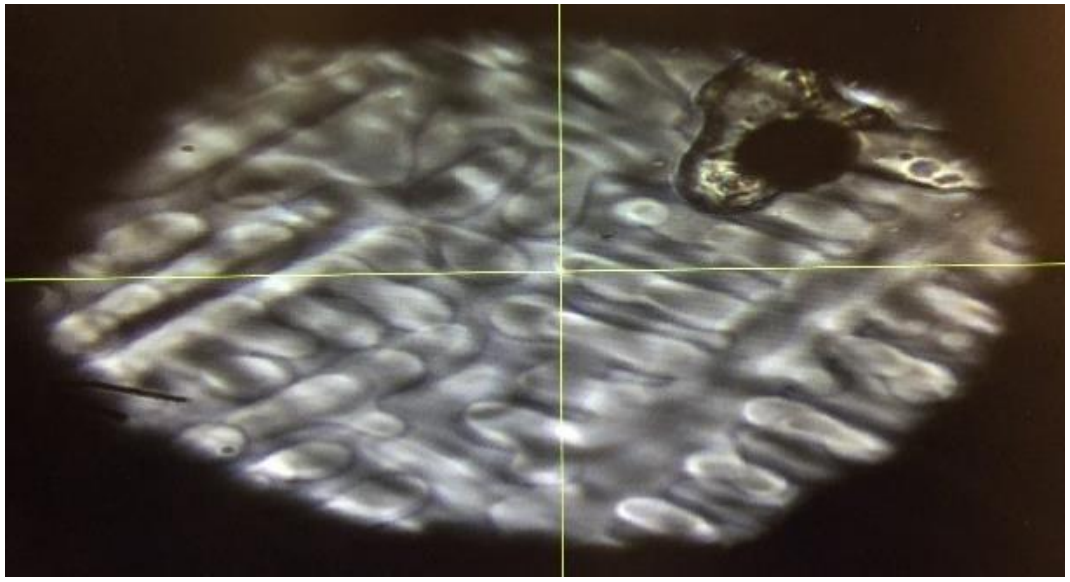


Figure S1.1: Image of initial DAC contents after the application of pressure to TFE - the liquid sample crystallised to produce many, relatively large, grains with ill-defined facets. Sample pressure found to be 0.60(5) GPa.

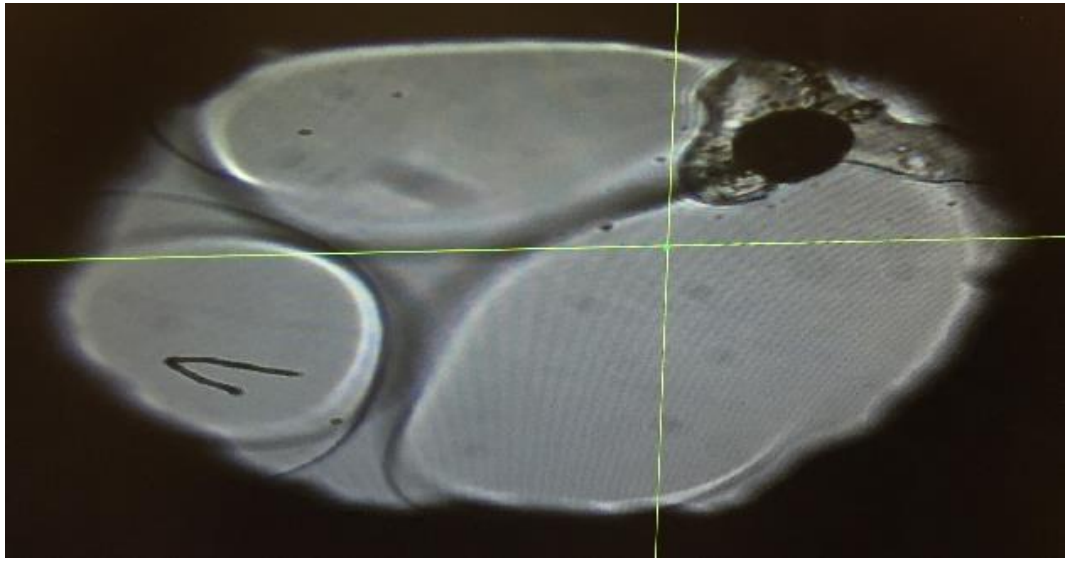


Figure S1.2: Image of TFE within the DAC after leaving it, at room temperature, for 2 days – the grains coalesced to form three crystals. Sample pressure found to be 0.60(5) GPa.

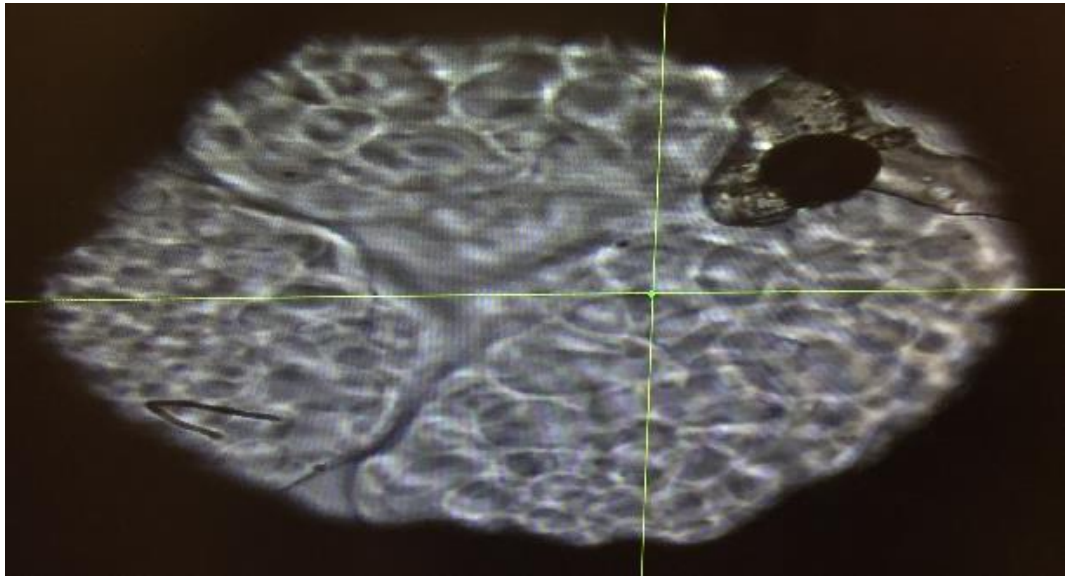


Figure S1.3: Image of TFE within the DAC after collecting data on Form 5. Sample pressure found to be 0.63(5) GPa.

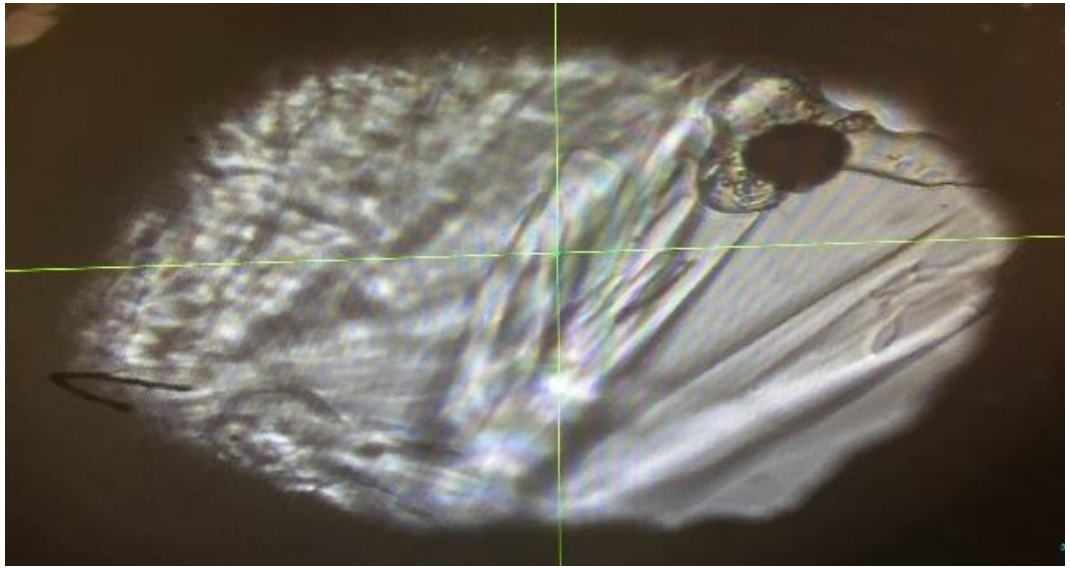


Figure S1.4: Pressure in the DAC backed off very slightly and the TFE crystal form changed to laths. Sample pressure found to be 0.55(5) GPa.

The cell was temperature cycled to produce a single crystallite which was allowed to grow for ~30 minutes. Sample pressure found to be 0.60(5) GPa
The cell was then left for a further 20 minutes and, although there was not much change in crystal growth during this time, there was a pressure drop to 0.55(5) GPa

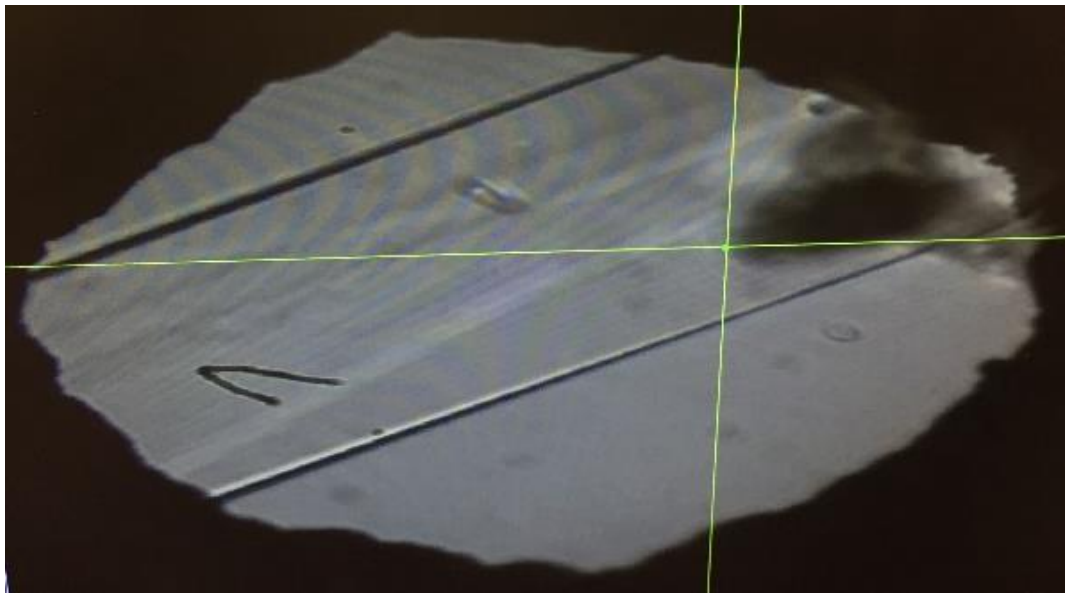


Figure S1.5: Image of the DAC with one crystal of TFE Form 2 sitting within the liquid TFE. Sample pressure found to be 0.55(5) GPa.

Figure S1.6: Image of TFE Form 2 within the DAC, after 1st pressure increase. Sample pressure found to be 0.60(5) GPa

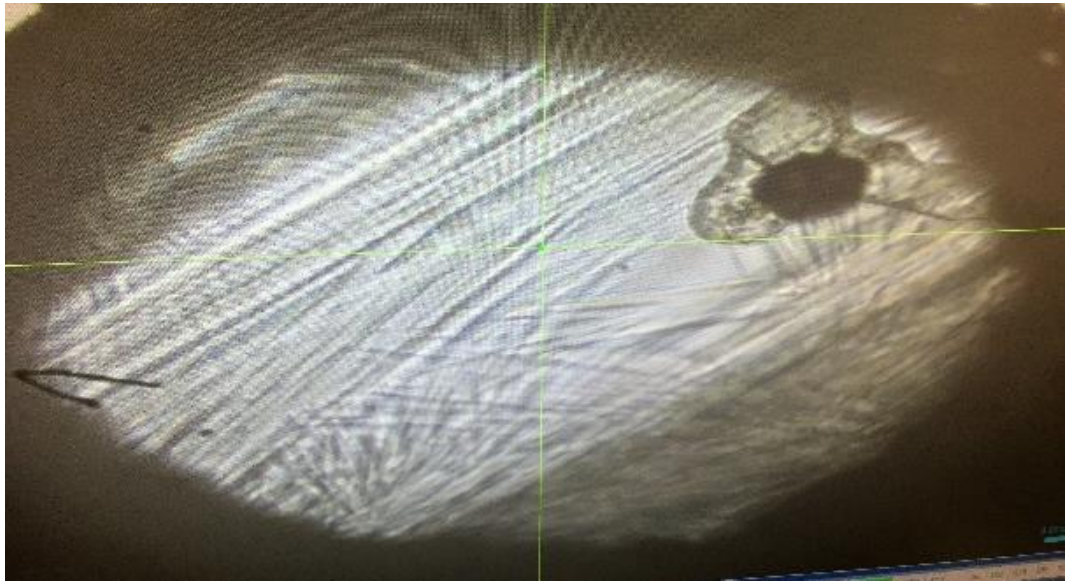


Figure S1.7: Image of TFE within the DAC after 2nd pressure increase, the TFE crystal form changed to needles. Sample pressure found to be 0.71(5) GPa

The DAC was temperature cycled in an attempt to isolate just one crystal but the sample repeatedly crash-melted, so data was collected on the cell containing a mass of needles.

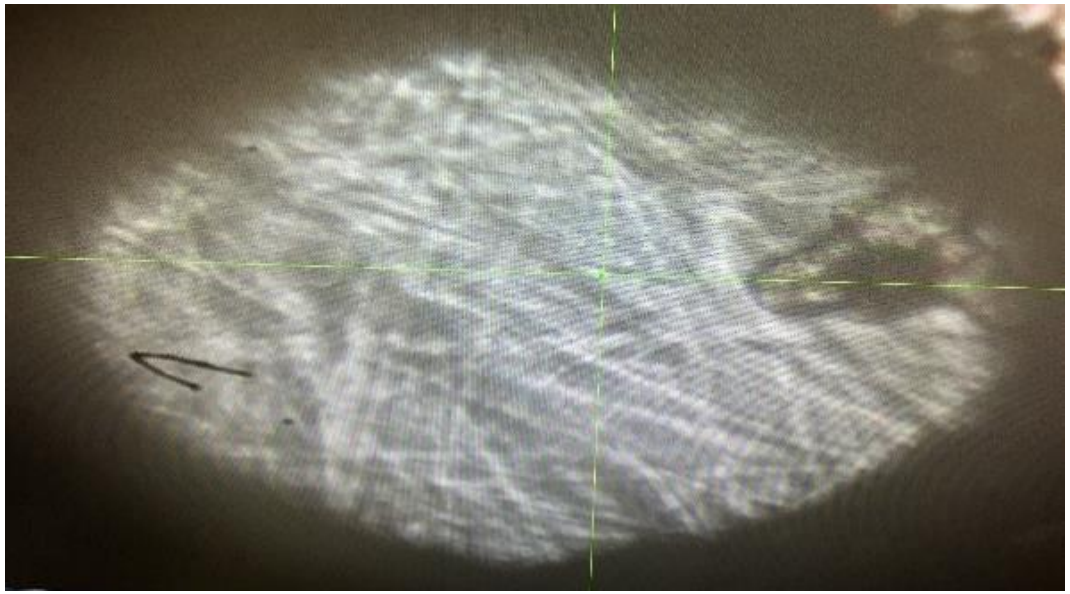


Figure S1.8: Image of the cell containing Form 3 after a number melt-cool cycles. Sample pressure was found to be 0.71(5) GPa.

2. Powder Neutron Data

Table S2.1: Crystallographic data for the high-pressure neutron powder studies of TFE at 295 K on PEARL

Load (T)	Pressure (GPa) *	wR	Form	Space Group	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	V (Å^3)	Density (g/cm^3)	Z / Z'	VpM (Å^3) **
12	0.44(7)	0.09254	2	*P*-1	4.9130(11)	8.875(6)	9.190(8)	111.617(16)	103.073(7)	90.948(5)	360.66(4)	1.8980	4 / 2	90.165(4)
14	0.83(5)	0.08295	3	$P2_1/c$	4.8281(5)	32.746(4)	8.8002(11)	90	91.543(9)	90	1390.84(18)	1.9687	16 / 4	86.93(18)
16	0.99(4)	0.07284	3	$P2_1/c$	4.8122(4)	32.660(3)	8.7638(9)	90	91.538(7)	90	1376.88(14)	1.9886	16 / 4	86.06(14)
18	1.23(4)	0.07536	3	$P2_1/c$	4.7947(4)	32.565(3)	8.7261(9)	90	91.538(7)	90	1362.03(14)	2.0103	16 / 4	85.13(14)
20	1.40(4)	0.07322	3	$P2_1/c$	4.7715(6)	32.446(5)	8.6890(13)	90	91.506(11)	90	1344.7(2)	2.0362	16 / 4	84.1(2)
20	1.40(4)	0.07322	4	$P2_1/c$	4.7312(12)	16.284(5)	8.670(3)	90	91.96(2)	90	667.5(2)	2.0509	8 / 2	83.4(2)
22	1.46(3)	0.07949	3	$P2_1/c$	4.7504(15)	32.331(13)	8.672(3)	90	91.55(2)	90	1331.3(5)	2.0567	16 / 4	83.2(5)
22	1.46(3)	0.07949	4	$P2_1/c$	4.7074(5)	16.232(2)	8.6440(10)	90	91.847(9)	90	660.15(9)	2.0738	8 / 2	82.52(9)
24	1.60(6)	0.06835	4	$P2_1/c$	4.6902(4)	16.1700(14)	8.6078(8)	90	91.847(6)	90	652.48(6)	2.0982	8 / 2	81.56(6)
26	1.89(7)	0.08448	4	$P2_1/c$	4.6707(4)	16.1199(17)	8.5772(9)	90	91.858(8)	90	645.45(7)	2.1211	8 / 2	80.68(7)
28	2.19(7)	0.08452	4	$P2_1/c$	4.6484(5)	16.0630(17)	8.5406(9)	90	91.867(8)	90	637.36(7)	2.1480	8 / 2	79.67(7)
30	2.72(9)	0.09239	4	$P2_1/c$	4.6208(5)	15.986(2)	8.4957(11)	90	91.913(10)	90	627.21(8)	2.1828	8 / 2	78.40(8)
36	2.91(9)	0.09506	4	$P2_1/c$	4.5930(6)	15.902(2)	8.4542(13)	90	91.954(11)	90	617.10(9)	2.2185	8 / 2	77.14(9)
40	3.30(9)	0.09466	4	$P2_1/c$	4.5636(8)	15.816(3)	8.3995(15)	90	92.054(14)	90	605.86(11)	2.2594	8 / 2	75.73(11)
44	3.73(10)	0.09743	4	$P2_1/c$	4.5366(8)	15.745(3)	8.3437(15)	90	92.089(14)	90	595.58(11)	2.2987	8 / 2	74.45(11)
48	4.36(12)	0.10133	4	$P2_1/c$	4.5127(9)	15.662(3)	8.3145(18)	90	92.126(17)	90	587.25(13)	2.3313	8 / 2	73.41(13)
52	4.88(14)	0.11097	4	$P2_1/c$	4.4867(11)	15.568(4)	8.283(2)	90	92.18(2)	90	578.17(15)	2.3679	8 / 2	72.27(15)
56	5.42(15)	0.11741	4	$P2_1/c$	4.4561(14)	15.495(5)	8.256(3)	90	92.31(3)	90	569.58(18)	2.4036	8 / 2	71.20(18)
60	6.14(21)	0.10830	4	$P2_1/c$	4.4333(18)	15.383(6)	8.247(3)	90	92.36(3)	90	562.0(2)	2.4362	8 / 2	70.3(2)

* Pressure calculated using the refined value for the Pb *a*-axis[1]

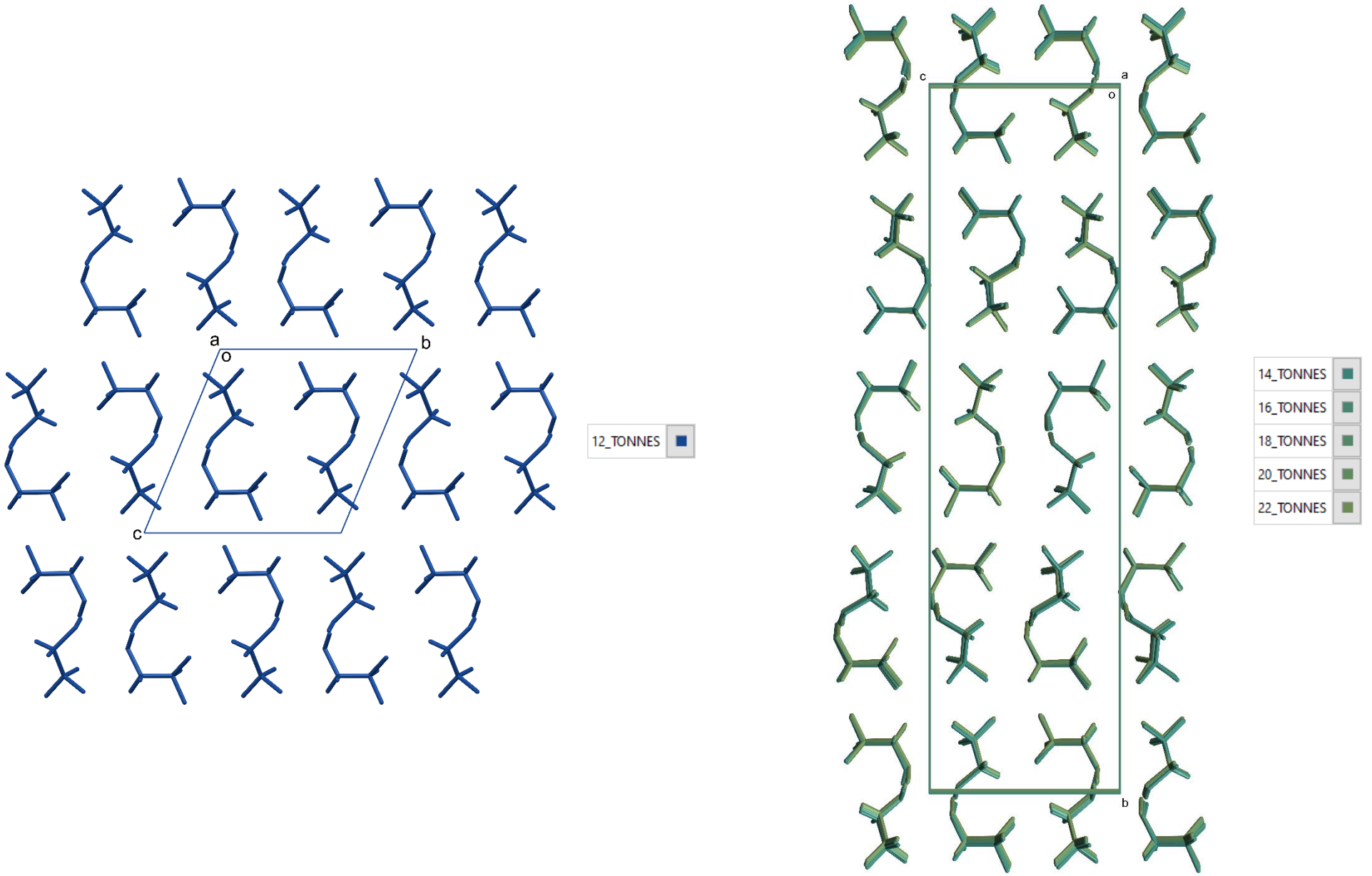
** VpM: volume per molecule calculated by dividing the unit cell volume by Z and used for Figure 9 of the main text (volume per formula unit)

Table S2.2a: Atomic positions for the structures refined from the high-pressure neutron powder-diffraction studies at 295 K on PEARL (Forms 2 and 3)

Form 2		12T	Form 3		14T	16T	18T	20T	22T
Atom		0.44 GPa	Atom		0.83 GPa	0.99 GPa	1.23 GPa	1.40 GPa	1.46 GPa
C1	x	0.95483	C1	x	0.44601	0.45046	0.45435	0.45412	0.45382
	y	0.21494		y	0.53562	0.53404	0.53366	0.53355	0.53355
	z	0.36562		z	0.23111	0.23052	0.23003	0.22988	0.22977
D1A		1.12883	D1A		0.24881	0.25226	0.25547	0.25441	0.25306
		0.22824			0.53904	0.53837	0.53797	0.53788	0.53789
		0.33509			0.20703	0.20999	0.20907	0.20885	0.20868
D1B		0.88692	D1B		0.53876	0.53483	0.53965	0.53978	0.53988
		0.31825			0.52524	0.52251	0.52212	0.52192	0.52193
		0.40866			0.14484	0.14305	0.14234	0.14188	0.14153
O1		1.01130	O1		0.47517	0.48113	0.48470	0.48461	0.48453
		0.14885			0.50771	0.50678	0.50633	0.50601	0.50603
		0.48410			0.35021	0.35239	0.35244	0.35273	0.35295
D1		0.89080	D1		0.62402	0.62531	0.63201	0.63254	0.63323
		0.14311			0.49609	0.49354	0.49382	0.49341	0.49343
		0.53137			0.36515	0.36297	0.36546	0.36580	0.36605
C2		0.74558	C2		0.56155	0.57879	0.58255	0.58287	0.58326
		0.10533			0.57575	0.57392	0.57368	0.57386	0.57385
		0.22030			0.27492	0.26807	0.26797	0.26796	0.26795
F1		0.85056	F1		0.40780	0.44193	0.44138	0.44110	0.44080
		-0.02448			0.59509	0.59420	0.59434	0.59467	0.59465
		0.13568			0.37347	0.37229	0.37020	0.37056	0.37082
F2		0.52760	F2		0.81317	0.83760	0.84021	0.84161	0.84338
		0.05322			0.57228	0.56960	0.56935	0.56950	0.56949
		0.25791			0.33672	0.32016	0.32352	0.32371	0.32385
F3		0.60111	F3		0.62371	0.63269	0.64139	0.64195	0.64259
		0.15423			0.60340	0.60109	0.60067	0.60104	0.60103
		0.11335			0.17694	0.16602	0.16534	0.16496	0.16468
C3		0.61270	C3		0.04479	0.05131	0.05126	0.05158	0.05201
		0.28589			0.42867	0.43037	0.43030	0.43026	0.43026
		0.77892			0.31222	0.30894	0.31013	0.31036	0.31053
D3A		0.74961	D3A		-0.06085	-0.03870	-0.04123	-0.04129	-0.04132
		0.26451			0.40829	0.40828	0.40816	0.40796	0.40797
		0.86223			0.36719	0.36410	0.36455	0.36497	0.36529
D3B		0.43185	D3B		0.23757	0.24792	0.24810	0.24926	0.25072
		0.28913			0.42220	0.42644	0.42587	0.42580	0.42580
		0.80123			0.31793	0.31106	0.31163	0.31187	0.31204
O2		0.59710	O2		0.00389	-0.00865	-0.00420	-0.00411	-0.00394
		0.15976			0.46666	0.46733	0.46724	0.46748	0.46746
		0.63038			0.37980	0.38071	0.38429	0.38478	0.38516

D2	0.47361 0.15343 0.55086	D2	0.11077 0.48548 0.36264	0.10160 0.48644 0.37622	0.10946 0.48605 0.38143	0.11003 0.48642 0.38191	0.11080 0.48640 0.38227
C4	0.70702 0.44392 0.77765	C4	-0.05470 0.42883 0.15233	-0.05708 0.43017 0.14993	-0.05858 0.43095 0.15067	-0.05872 0.43092 0.15032	-0.05894 0.43092 0.15006
F4	0.75725 0.56110 0.92321	F4	-0.04497 0.39193 0.09169	-0.04549 0.39318 0.08901	-0.03210 0.39478 0.08375	-0.03213 0.39448 0.08316	-0.03225 0.39449 0.08272
F5	0.52082 0.49066 0.67942	F5	0.09135 0.45327 0.06638	0.08115 0.45508 0.06106	0.06875 0.45818 0.06523	0.06914 0.45834 0.06458	0.06955 0.45833 0.06409
F6	0.94429 0.47230 0.74918	F6	-0.30899 0.43632 0.11242	-0.31502 0.43690 0.11399	-0.32006 0.43572 0.11594	-0.32131 0.43572 0.11547	-0.32292 0.43572 0.11511
		C5	0.94018 0.72373 0.30113	0.95169 0.72385 0.31819	0.95635 0.72327 0.31937	0.95596 0.72337 0.31929	0.95546 0.72337 0.31922
		D5A	1.02939 0.73987 0.22306	1.02727 0.74020 0.23580	1.03565 0.73987 0.23823	1.03559 0.74010 0.23785	1.03547 0.74009 0.23757
		D5B	0.75016 0.71919 0.27343	0.75949 0.71832 0.29785	0.76333 0.71821 0.29733	0.76212 0.71828 0.29716	0.76061 0.71828 0.29704
		O3	0.95462 0.74547 0.43742	0.97848 0.74612 0.45363	0.98237 0.74493 0.45692	0.98209 0.74520 0.45733	0.98180 0.74519 0.45764
		D3	1.10092 0.75633 0.46461	1.11965 0.75962 0.47092	1.10204 0.76283 0.46666	1.10227 0.76323 0.46711	1.10260 0.76321 0.46744
		C6	1.08713 0.68439 0.31582	1.10907 0.68516 0.32879	1.11035 0.68410 0.32856	1.11060 0.68392 0.32851	1.11092 0.68393 0.32847
		F7	1.33547 0.68822 0.38033	1.34876 0.68930 0.40368	1.35236 0.68762 0.40280	1.35364 0.68746 0.40301	1.35526 0.68747 0.40317
		F8	0.94753 0.65800 0.39788	0.96719 0.65637 0.39878	0.96599 0.65546 0.39892	0.96564 0.65506 0.39912	0.96524 0.65508 0.39927
		F9	1.12444 0.66027 0.20211	1.16773 0.66344 0.21082	1.16521 0.66235 0.20938	1.16570 0.66201 0.20890	1.16624 0.66202 0.20854

		C7	0.59760 0.81853 0.42267	0.56580 0.81874 0.42158	0.55032 0.81939 0.41801	0.55045 0.81945 0.41827	0.55065 0.81945 0.41846
		D7A	0.79850 0.82151 0.43225	0.76607 0.82304 0.43260	0.75062 0.82436 0.42918	0.75159 0.82446 0.42948	0.75284 0.82445 0.42970
		D7B	0.50849 0.84037 0.47401	0.46856 0.84038 0.47021	0.44928 0.84115 0.46439	0.44899 0.84137 0.46481	0.44868 0.84136 0.46513
		O4	0.52325 0.78164 0.48957	0.49996 0.78177 0.49167	0.48860 0.78264 0.49190	0.48847 0.78242 0.49242	0.48838 0.78243 0.49281
		D4	0.62495 0.76170 0.48220	0.59890 0.76165 0.47909	0.59482 0.76301 0.48496	0.59514 0.76265 0.48545	0.59561 0.76266 0.48582
		C8	0.51821 0.81906 0.25971	0.49099 0.81771 0.25732	0.47702 0.81698 0.25305	0.47683 0.81702 0.25271	0.47657 0.81702 0.25245
		F10	0.54572 0.85091 0.17499	0.50862 0.84936 0.16982	0.49920 0.84783 0.16120	0.49912 0.84810 0.16053	0.49892 0.84808 0.16002
		F11	0.24715 0.81541 0.23831	0.22151 0.81164 0.23388	0.20614 0.81135 0.22930	0.20482 0.81135 0.22887	0.20312 0.81135 0.22855
		F12	0.63558 0.78939 0.18319	0.62252 0.78860 0.18402	0.60667 0.78679 0.18378	0.60704 0.78660 0.18320	0.60741 0.78661 0.18275



(a) (b)

Figure S2.1: Packing of the TFE structures refined from the neutron powder-diffraction data from PEARL at 295 K (a) Form 2 at 0.44(7) GPa and (b) overlay of Form 3 at pressures from 0.83(5) GPa to 1.46(3) GPa. Form 3 progression from 0.83 GPa (14T, cyan) to 1.46 GPa (22T, green) is shown by successively greener shading.

Table S2.2b: Atomic positions for the structures refined from the high-pressure neutron powder-diffraction studies at 295 K on PEARL (Form 4)

Form 4	20T	22T	24T	26T	28T	30T	36T	40T	44T	48T	52T	56T	60T
Atom	1.40 GPa	1.46 GPa	1.60 GPa	1.89 GPa	2.19 GPa	2.71 GPa	2.91 GPa	3.30 GPa	3.73 GPa	4.36 GPa	4.88 GPa	5.42 GPa	6.14 GPa
C1 x	0.80267	0.80267	0.79891	0.80737	0.81699	0.81955	0.81765	0.81621	0.81333	0.81321	0.80577	0.80154	0.77687
y	0.30889	0.30889	0.30866	0.30805	0.30851	0.30890	0.30916	0.30875	0.30917	0.30865	0.30725	0.30736	0.30714
z	0.49603	0.49603	0.49530	0.49996	0.50416	0.50640	0.50493	0.49079	0.49293	0.49547	0.49426	0.49635	0.49469
D1A	1.00329	1.00329	1.00043	1.01003	1.01872	1.02244	1.02169	1.02632	1.02193	1.02180	1.01535	1.00978	0.99459
	0.31767	0.31767	0.31692	0.31626	0.31811	0.31868	0.31891	0.31424	0.31490	0.31470	0.31338	0.31501	0.31261
	0.52505	0.52505	0.52284	0.52698	0.53413	0.53651	0.53562	0.51451	0.52403	0.52899	0.52839	0.53495	0.51562
D1B	0.71128	0.71128	0.70849	0.71753	0.72521	0.72776	0.72493	0.72623	0.71521	0.71315	0.70494	0.69709	0.69040
	0.27837	0.27837	0.27853	0.27762	0.27747	0.27750	0.27736	0.27731	0.27560	0.27379	0.27189	0.27181	0.27311
	0.57523	0.57523	0.57537	0.58036	0.58370	0.58623	0.58466	0.57283	0.56991	0.57038	0.56887	0.56985	0.57766
O1	0.78755	0.78755	0.77895	0.78561	0.80540	0.80801	0.80659	0.77659	0.79114	0.79721	0.79077	0.80016	0.72634
	0.26356	0.26356	0.26314	0.26276	0.26278	0.26315	0.26360	0.26551	0.26863	0.26945	0.26826	0.26695	0.26561
	0.35812	0.35812	0.35769	0.36149	0.36522	0.36648	0.36383	0.34687	0.34431	0.34473	0.34253	0.34535	0.34560
D1	0.63633	0.63633	0.62724	0.62860	0.64875	0.65078	0.64841	0.62898	0.64430	0.64719	0.63991	0.65487	0.58288
	0.24185	0.24185	0.24106	0.24563	0.25197	0.25367	0.25369	0.23666	0.24019	0.24300	0.24183	0.23772	0.23225
	0.33012	0.33012	0.33176	0.33017	0.32297	0.32231	0.31968	0.33089	0.32072	0.31642	0.31337	0.31514	0.33293
C2	0.66535	0.66535	0.66386	0.67164	0.67500	0.67581	0.67314	0.68841	0.68211	0.67854	0.66975	0.65883	0.64393
	0.39039	0.39039	0.39050	0.39021	0.39001	0.39070	0.39145	0.39428	0.39480	0.39441	0.39347	0.39311	0.39491
	0.47552	0.47552	0.47533	0.48115	0.48281	0.48542	0.48449	0.47995	0.48400	0.48838	0.48777	0.48427	0.49191
F1	0.40732	0.40732	0.40459	0.41033	0.41330	0.41154	0.40589	0.41265	0.40474	0.40062	0.39060	0.37952	0.35306
	0.38368	0.38368	0.38444	0.38428	0.38212	0.38257	0.38338	0.39221	0.39234	0.39160	0.39065	0.38797	0.39301
	0.41019	0.41019	0.41132	0.41804	0.41911	0.42267	0.42311	0.42604	0.42961	0.43222	0.43069	0.42459	0.44878
F2	0.81283	0.81283	0.81137	0.81840	0.81954	0.81917	0.81556	0.83284	0.82579	0.82291	0.81524	0.80439	0.77652
	0.44069	0.44069	0.44035	0.44037	0.44054	0.44149	0.44235	0.44445	0.44622	0.44733	0.44710	0.44653	0.44740
	0.38817	0.38817	0.38709	0.39225	0.39250	0.39375	0.39129	0.38491	0.38956	0.39600	0.39601	0.39100	0.39045
F3	0.59100	0.59100	0.59298	0.60243	0.60149	0.60367	0.60355	0.64193	0.63401	0.62650	0.61620	0.59817	0.61572
	0.43574	0.43574	0.43613	0.43574	0.43613	0.43708	0.43823	0.44027	0.44002	0.43862	0.43751	0.43878	0.44094
	0.59085	0.59085	0.59100	0.59791	0.59871	0.60221	0.60220	0.60353	0.60947	0.61532	0.61553	0.60960	0.62133
C3	0.21611	0.21611	0.21329	0.21584	0.22068	0.21842	0.21937	0.19734	0.20277	0.20720	0.20473	0.20786	0.24535
	0.11053	0.11053	0.11114	0.10941	0.10813	0.10761	0.10595	0.10772	0.10595	0.10502	0.10430	0.10390	0.09623
	0.38243	0.38243	0.38159	0.37949	0.37960	0.37803	0.37876	0.37895	0.37382	0.37186	0.37226	0.37313	0.35373
D3A	0.32444	0.32444	0.32063	0.32560	0.32725	0.32222	0.32497	0.29696	0.30971	0.31178	0.30569	0.30482	0.36993
	0.06665	0.06665	0.06741	0.06513	0.06223	0.06059	0.05897	0.06070	0.05942	0.05803	0.05683	0.05541	0.05437
	0.33348	0.33348	0.33154	0.33185	0.33405	0.33311	0.33341	0.32853	0.32495	0.32173	0.32011	0.32079	0.29795
D3B	0.01698	0.01698	0.01430	0.01585	0.01859	0.01448	0.01440	-0.00922	-0.00412	-0.00116	-0.00524	-0.00478	0.04306
	0.09839	0.09839	0.09867	0.09747	0.09871	0.09941	0.09670	0.09803	0.09472	0.09427	0.09425	0.09607	0.07526
	0.37508	0.37508	0.37644	0.37030	0.36650	0.36463	0.36733	0.37665	0.36834	0.36797	0.37059	0.36927	0.35804
O2	0.26641	0.26641	0.25918	0.26997	0.29150	0.29569	0.29028	0.25394	0.25768	0.26229	0.25999	0.27579	0.24364
	0.18446	0.18446	0.18510	0.18328	0.18135	0.18033	0.17904	0.18136	0.18023	0.17965	0.17948	0.17922	0.17394
	0.30439	0.30439	0.30274	0.30099	0.30186	0.29893	0.29734	0.29396	0.28883	0.28642	0.28681	0.28960	0.26682

D2	0.14297	0.14297	0.13469	0.15367	0.18260	0.18881	0.18211	0.11669	0.12008	0.12607	0.12531	0.14396	0.11716
	0.22044	0.22044	0.22078	0.22137	0.22150	0.22130	0.22004	0.20982	0.21167	0.21308	0.21449	0.21525	0.21119
	0.30101	0.30101	0.30026	0.30370	0.30443	0.30028	0.30042	0.25782	0.26236	0.26588	0.27098	0.27089	0.28524
C4	0.31163	0.31163	0.31467	0.30661	0.30191	0.29981	0.30641	0.31048	0.30747	0.31743	0.32256	0.32246	0.37625
	0.11629	0.11629	0.11720	0.11554	0.11344	0.11318	0.11268	0.11462	0.11382	0.11248	0.11080	0.10833	0.10869
	0.54698	0.54698	0.54516	0.54538	0.54768	0.54705	0.54782	0.54512	0.54258	0.54049	0.54047	0.54298	0.51957
F4	0.22633	0.22633	0.24343	0.22363	0.19828	0.19564	0.20161	0.25222	0.24202	0.25119	0.25470	0.23015	0.32000
	0.05298	0.05298	0.05225	0.05132	0.05121	0.05072	0.05097	0.04711	0.04679	0.04529	0.04341	0.04319	0.04305
	0.63013	0.63013	0.62805	0.62778	0.62928	0.62926	0.63316	0.63050	0.62909	0.62770	0.62822	0.63091	0.61643
F5	0.59289	0.59289	0.59543	0.58839	0.58458	0.58413	0.59297	0.59801	0.59679	0.60887	0.61636	0.61940	0.67297
	0.11964	0.11964	0.12436	0.12075	0.11332	0.11317	0.11187	0.12543	0.12402	0.12169	0.11837	0.10826	0.11827
	0.56199	0.56199	0.55679	0.56289	0.57093	0.57069	0.56927	0.55261	0.55477	0.55048	0.54735	0.55315	0.51971
F6	0.26248	0.26248	0.25884	0.24971	0.25369	0.25089	0.26230	0.24933	0.24260	0.25751	0.27040	0.28749	0.32466
	0.18005	0.18005	0.17965	0.17898	0.17855	0.17870	0.17941	0.17741	0.17770	0.17687	0.17572	0.17521	0.17672
	0.63239	0.63239	0.63259	0.63090	0.63153	0.63100	0.63069	0.63639	0.63169	0.63061	0.63218	0.63358	0.60564

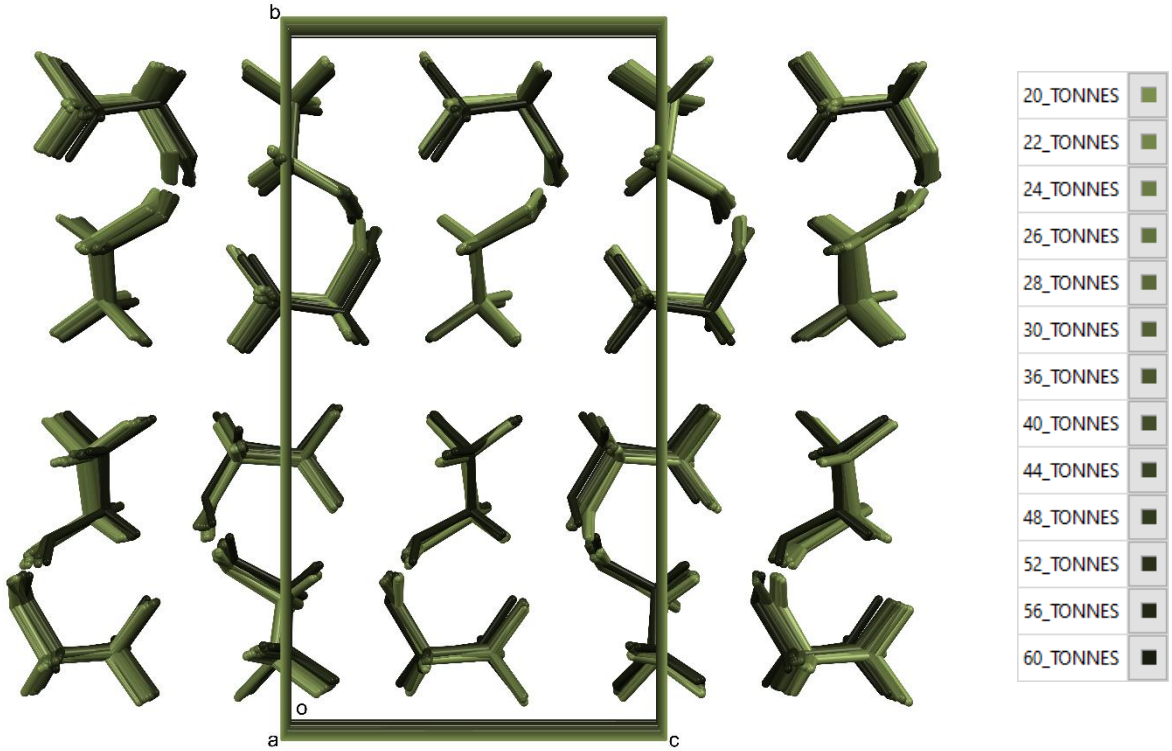


Figure S2.2: Packing of the TFE structures refined from the neutron powder-diffraction data from PEARL at 295 K showing an overlay of Form 4 at pressures from 1.40(4) GPa to 6.14(21) GPa. Progression from 1.40 GPa (20T, green) to 6.14 GPa (60T, black) is show by successively darker shading.

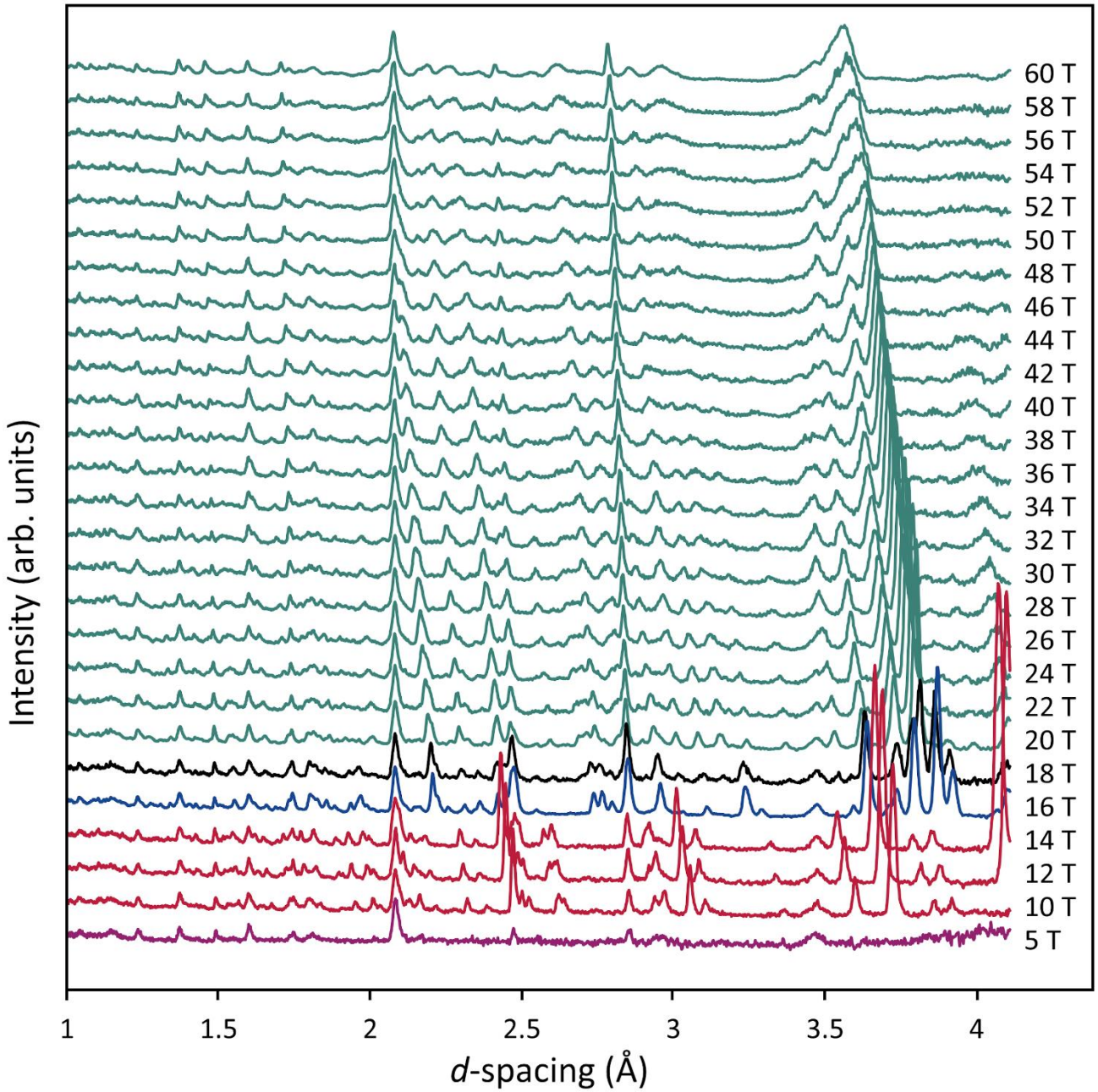


Figure S2.3: Neutron powder-diffraction patterns of TFE obtained from PEARL, collected at 245 K, shown with increasing pressure (liquid – purple; Form 1 – red; Form 2 – blue; Form 3 – cyan; mixed phase of Forms 2 and 3 – black).

Table S2.3: Crystallographic data for the high-pressure neutron powder studies of TFE at 245 K on PEARL

Load (T)	Pressure (GPa) *	wR	Form	Space Group	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	V (Å^3)	Density (g/cm^3)	Z / Z'	VpM (Å^3) **
10	0.003(37) ^	0.08343	1	*Pca*2$_1$	8.5113(8)	9.9903(11)	9.0888(8)	90	90	90	772.83(9)	1.7887	8 / 2	96.60(9)
12	0.25(3)	0.08378	1	*Pca*2$_1$	8.4210(6)	9.9339(9)	8.9988(7)	90	90	90	752.78(7)	1.8363	8 / 2	94.10(7)
14	0.48(2)	0.08115	1	*Pca*2$_1$	8.3612(6)	9.8952(9)	8.9318(5)	90	90	90	738.98(6)	1.8706	8 / 2	92.37(6)
16	0.52(2)	0.05911	2	*P*-1	4.8936(7)	8.876(4)	9.198(5)	111.615(10)	102.907(5)	91.077(3)	359.80(3)	1.9025	4 / 2	89.95(3)
18	0.46(3)	0.08545	2	*P*-1	4.8812(17)	8.851(8)	9.182(11)	111.67(2)	102.903(11)	91.117(7)	357.07(6)	1.9170	4 / 2	89.27(6)
18	0.46(3)	0.08545	3	*P*2$_1$/*c*	4.8399(10)	32.887(8)	8.856(2)	90	91.667(17)	90	1409.1(4)	1.9431	16 / 4	88.1(4)
20	0.72(2)	0.05546	3	*P*2$_1$/*c*	4.8238(3)	32.824(3)	8.8291(7)	90	91.649(5)	90	1397.41(11)	1.9594	16 / 4	87.34(11)
22	0.82(2)	0.06978	3	*P*2$_1$/*c*	4.8086(4)	32.735(3)	8.7939(8)	90	91.667(7)	90	1383.65(14)	1.9789	16 / 4	86.48(14)
24	0.98(2)	0.06000	3	*P*2$_1$/*c*	4.7899(4)	32.612(3)	8.7541(7)	90	91.646(6)	90	1366.91(12)	2.0031	16 / 4	85.43(12)
26	1.10(2)	0.06299	3	*P*2$_1$/*c*	4.7740(4)	32.516(3)	8.7218(8)	90	91.652(7)	90	1353.36(13)	2.0232	16 / 4	84.59(13)
28	1.28(2)	0.06344	3	*P*2$_1$/*c*	4.7561(4)	32.419(3)	8.6874(8)	90	91.636(7)	90	1338.98(14)	2.0449	16 / 4	83.69(14)
30	1.44(2)	0.06836	3	*P*2$_1$/*c*	4.7368(4)	32.321(3)	8.6503(10)	90	91.636(8)	90	1323.79(15)	2.0684	16 / 4	82.74(15)
32	1.57(2)	0.06846	3	*P*2$_1$/*c*	4.7240(5)	32.245(4)	8.6265(10)	90	91.640(8)	90	1313.49(16)	2.0846	16 / 4	82.09(16)
34	1.72(2)	0.06841	3	*P*2$_1$/*c*	4.7073(5)	32.165(4)	8.5957(11)	90	91.638(9)	90	1300.94(16)	2.1047	16 / 4	81.31(16)
36	1.86(2)	0.06815	3	*P*2$_1$/*c*	4.6916(5)	32.098(4)	8.5689(12)	90	91.645(9)	90	1289.86(17)	2.1228	16 / 4	80.62(17)
38	2.01(2)	0.06796	3	*P*2$_1$/*c*	4.6756(5)	32.039(4)	8.5426(13)	90	91.663(10)	90	1279.18(18)	2.1405	16 / 4	79.95(18)
40	2.21(2)	0.06887	3	*P*2$_1$/*c*	4.6612(6)	31.966(4)	8.5147(13)	90	91.660(10)	90	1268.13(19)	2.1591	16 / 4	79.26(19)
42	2.36(2)	0.06804	3	*P*2$_1$/*c*	4.6464(6)	31.910(4)	8.4922(14)	90	91.659(11)	90	1258.6(2)	2.1755	16 / 4	78.7(2)
44	2.55(3)	0.06881	3	*P*2$_1$/*c*	4.6322(7)	31.851(5)	8.4693(15)	90	91.660(12)	90	1249.0(2)	2.1922	16 / 4	78.1(2)
46	2.72(3)	0.06855	3	*P*2$_1$/*c*	4.6179(7)	31.793(5)	8.4499(16)	90	91.641(13)	90	1240.1(2)	2.2080	16 / 4	77.5(2)
48	2.90(3)	0.06610	3	*P*2$_1$/*c*	4.6025(8)	31.748(5)	8.4346(17)	90	91.589(14)	90	1232.0(3)	2.2225	16 / 4	77.0(3)
50 ^^	3.09(3)	0.07031	3	*P*2$_1$/*c*	4.5860(10)	31.720(7)	8.412(2)	90	91.506(17)	90	1223.2(3)	2.2385	16 / 4	76.5(3)

* Pressure calculated using the refined value for the Pb *a*-axis[1]

** VpM: volume per molecule calculated by dividing the unit cell volume by Z and used for Figure 9 of the main text (volume per formula unit)

^ The pressure calculated within the measuring uncertainty of the Pb pressure marker; the fact the sample has crystallised clearly indicates the pressure within the cell is greater than atmospheric, when it was still liquid

^^ Although data was collected up to 60T, the refinements beyond 50T (3.09 GPa) are not included due to the significant pressure broadening which began to be observed in the powder-diffraction patterns at this point

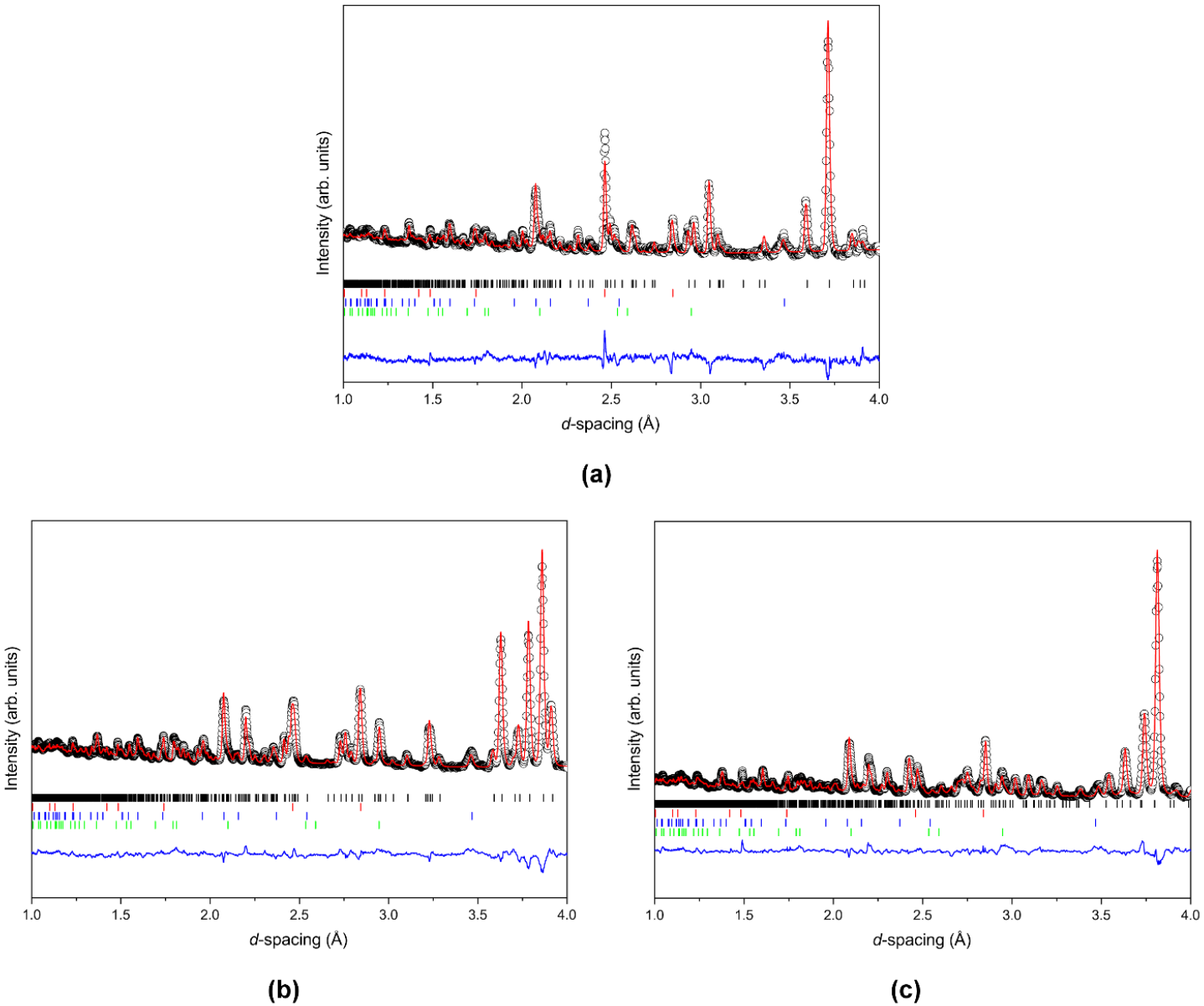
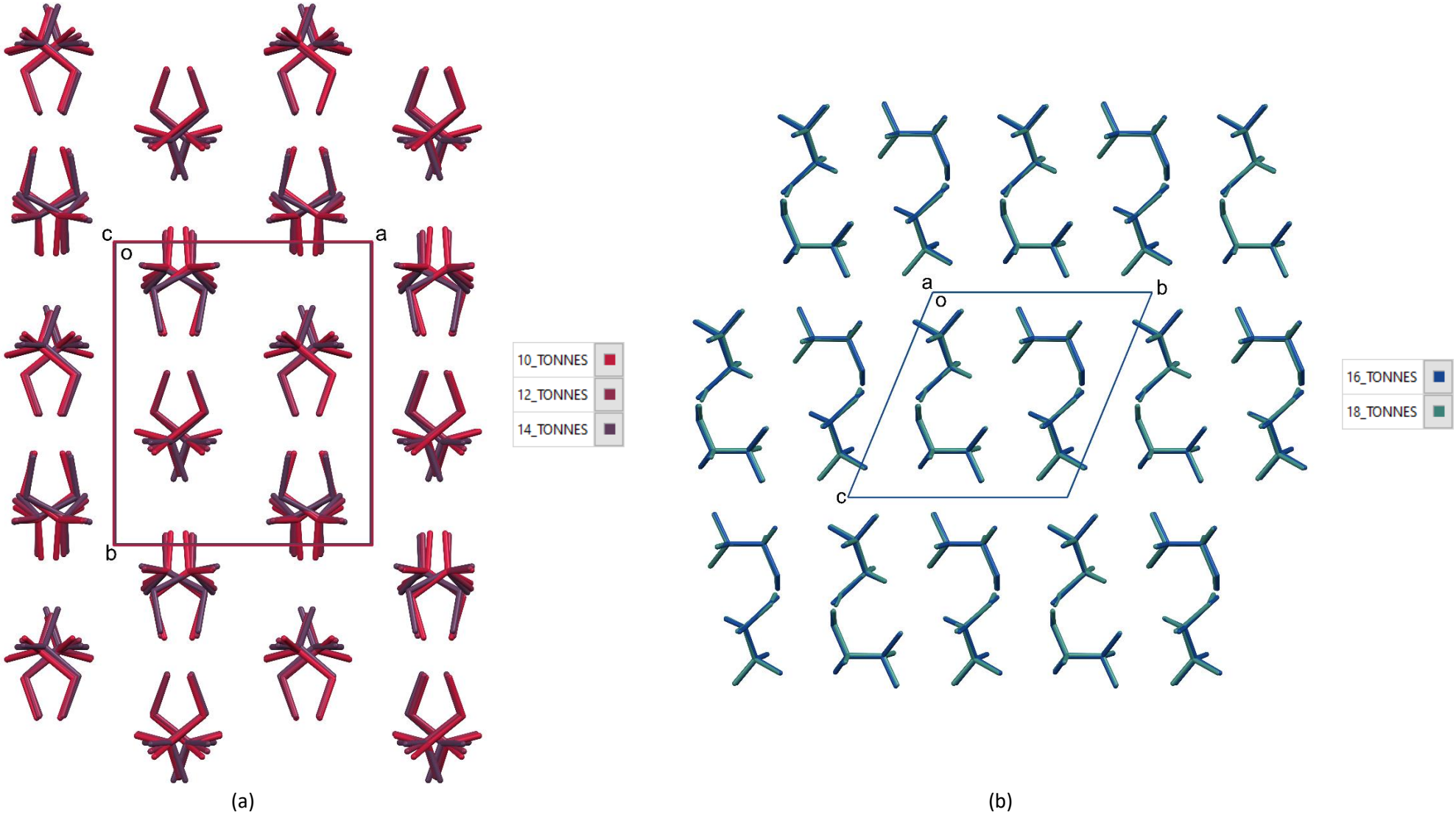


Figure S2.4: Selected Rietveld refinements of the neutron powder-diffraction PEARL data collected on TFE at 245 K for (a) Form 1 [0.003(37) GPa], (b) Form 2 [0.52(2) GPa] and (c) Form 3 [0.72(2) GPa] – representative refinements are shown for the patterns recorded at the lowest pressure exhibiting a single phase (black circle – observed data; red line – calculated patterns; black tick marks – TFE; green tick marks – Al_2O_3; red tick marks – Pb; blue tick marks – ZrO_2; blue line – difference between observed and calculated data)

Table S2.4a: Atomic positions for the structures refined from the high-pressure neutron powder-diffraction studies at 245 K on PEARL (Forms 1 and 2)

Form 1		10T	12T	14T	Form 2		16T	18T
Atom		0.003 GPa	0.25 GPa	0.48 GPa	Atom		0.52 GPa	0.46 GPa
C1	x	0.15097	0.14940	0.14951	C1	x	0.98354	0.98230
	y	0.17069	0.16435	0.15642		y	0.22262	0.22668
	z	0.44780	0.44537	0.44070		z	0.36694	0.36528
D1A		0.08645	0.08086	0.07892	D1A		1.16582	1.16456
		0.16824	0.15346	0.15844			0.24064	0.25022
		0.53365	0.52898	0.52465			0.34595	0.34648
D1B		0.09216	0.09807	0.10117	D1B		0.90794	0.90157
		0.13838	0.13004	0.10547			0.32390	0.32587
		0.36271	0.35578	0.35877			0.40744	0.40900
O1		0.19606	0.18030	0.17627	O1		1.02340	1.02591
		0.30276	0.30114	0.28846			0.15338	0.15095
		0.42116	0.42543	0.39200			0.48282	0.47633
D1		0.21394	0.20541	0.19651	D1		0.88820	0.90435
		0.35290	0.34758	0.34776			0.13246	0.14822
		0.49070	0.49710	0.45337			0.51396	0.52456
C2		0.28941	0.29791	0.30109	C2		0.79136	0.79415
		0.08390	0.08851	0.09006			0.11255	0.11850
		0.46803	0.46861	0.48223			0.21431	0.20949
F1		0.27905	0.30108	0.30685	F1		0.89719	0.89708
		-0.03975	-0.03120	-0.02413			-0.02381	-0.02012
		0.50833	0.52447	0.55201			0.14557	0.14286
F2		0.38080	0.38404	0.39773	F2		0.54711	0.54256
		0.08095	0.07918	0.07388			0.07176	0.08094
		0.35093	0.34666	0.36695			0.23652	0.22620
F3		0.37657	0.38788	0.37982	F3		0.68624	0.70222
		0.12374	0.14519	0.16022			0.15782	0.16528
		0.58023	0.57155	0.58445			0.09711	0.09146
C3		0.84720	0.84535	0.85427	C3		0.61516	0.61163
		0.43935	0.43958	0.43811			0.29484	0.29882
		0.20264	0.19982	0.22321			0.77457	0.77129
D3A		0.91872	0.91656	0.92875	D3A		0.76677	0.76398
		0.40629	0.40387	0.41190			0.27296	0.27419
		0.13039	0.12732	0.14761			0.85078	0.84539
D3B		0.89987	0.89940	0.90673	D3B		0.44170	0.43975
		0.44736	0.44897	0.43994			0.29283	0.29917
		0.29765	0.29522	0.32082			0.80529	0.80455
O2		0.79543	0.79497	0.79822	O2		0.58692	0.57473
		0.56606	0.56672	0.56775			0.17336	0.17760
		0.16003	0.15379	0.19130			0.62186	0.61703

D2	0.71634	0.72524	0.71104	D2	0.43222	0.41602
	0.59791	0.60589	0.59198		0.14702	0.14947
	0.19794	0.20058	0.22389		0.55686	0.55576
C4	0.71396	0.70910	0.72123	C4	0.68977	0.69175
	0.34624	0.34807	0.34044		0.45681	0.46091
	0.21928	0.21980	0.22998		0.77509	0.77262
F4	0.75418	0.75220	0.77317	F4	0.70875	0.70773
	0.23840	0.23404	0.21640		0.57370	0.57846
	0.29482	0.28403	0.25591		0.91794	0.91525
F5	0.65782	0.63976	0.63734	F5	0.50403	0.51092
	0.30534	0.31679	0.33683		0.49285	0.49764
	0.09174	0.09303	0.10502		0.66818	0.66382
F6	0.59071	0.59278	0.61490	F6	0.93128	0.93699
	0.37442	0.37395	0.34163		0.49988	0.50290
	0.29605	0.30884	0.33482		0.75904	0.75942



(a) (b)

Figure S2.5: Packing of the TFE structures refined from the neutron powder-diffraction data from PEARL at 245 K (a) overlay of Form 1 at pressures from 0.003(37) GPa to 0.48(2) GPa and (b) overlay of Form 2 at pressures from 0.52(2) GPa to 0.46(3) GPa. Form 1 progression from 0.003 GPa (10T, red) to 0.48 GPa (14T, purple) is shown by successively bluer shading; Form 2 progression from 0.52 GPa (16T, blue) to 0.48 GPa (18T, cyan) is shown by successively greener shading.

Table S2.4b: Atomic positions for the structures refined from the high-pressure neutron powder-diffraction studies at 245 K on PEARL (Form 3)

Form 3	18T	20T	22T	24T	26T	28T	30T	32T	34T	36T	38T	40T	42T	44T	46T	48T	50T
Atom	0.46 GPa	0.72 GPa	0.82 GPa	0.98 GPa	1.10 GPa	1.28 GPa	1.44 GPa	1.57 GPa	1.72 GPa	1.86 GPa	2.01 GPa	2.21 GPa	2.36 GPa	2.55 GPa	2.72 GPa	2.90 GPa	3.09 GPa
C1 x	0.45158	0.45158	0.44052	0.43776	0.44900	0.45015	0.46309	0.45621	0.46432	0.46303	0.47316	0.47834	0.48312	0.47629	0.47809	0.46666	0.46667
y	0.53492	0.53492	0.53573	0.53486	0.53372	0.53407	0.53304	0.53301	0.53230	0.53240	0.53140	0.53252	0.53259	0.53227	0.53234	0.53221	0.53221
z	0.22615	0.22615	0.22710	0.22643	0.22681	0.23142	0.23052	0.23181	0.22932	0.22793	0.23216	0.23583	0.23181	0.22641	0.22469	0.21995	0.21997
D1A	0.26019	0.26019	0.25009	0.24714	0.25854	0.25675	0.26847	0.26194	0.26883	0.26634	0.27075	0.27314	0.27770	0.27315	0.27396	0.26420	0.26420
	0.54145	0.54145	0.54240	0.54152	0.54107	0.54120	0.54017	0.54021	0.53946	0.54001	0.53697	0.53747	0.53713	0.53707	0.53697	0.53692	0.53692
	0.19653	0.19653	0.19456	0.19255	0.19358	0.20163	0.20144	0.20096	0.19928	0.20087	0.21004	0.21867	0.21117	0.19820	0.19690	0.18717	0.18720
D1B	0.54607	0.54607	0.53775	0.53668	0.54531	0.54240	0.55459	0.54931	0.55766	0.55177	0.56008	0.55911	0.57051	0.57318	0.57488	0.57035	0.57039
	0.52391	0.52391	0.52398	0.52281	0.52136	0.52187	0.52085	0.52032	0.52008	0.52039	0.52035	0.52152	0.52177	0.52041	0.52041	0.51993	0.51992
	0.14193	0.14193	0.14474	0.14464	0.14419	0.14655	0.14483	0.14729	0.14344	0.13973	0.14133	0.14275	0.13994	0.13902	0.13704	0.13508	0.13513
O1	0.44870	0.44870	0.43098	0.42585	0.43402	0.44427	0.45910	0.44839	0.45874	0.46049	0.49518	0.51479	0.51567	0.49188	0.49583	0.47325	0.47322
	0.50587	0.50587	0.50739	0.50673	0.50547	0.50564	0.50447	0.50492	0.50355	0.50306	0.50203	0.50339	0.50343	0.50412	0.50434	0.50453	0.50453
	0.34142	0.34142	0.34528	0.34611	0.34667	0.35180	0.35132	0.35461	0.35068	0.34801	0.35247	0.35676	0.35343	0.35258	0.35171	0.34850	0.34847
D1	0.59482	0.59482	0.57082	0.56202	0.57264	0.57982	0.59843	0.58444	0.60133	0.60606	0.64473	0.66893	0.67088	0.64515	0.64790	0.62753	0.62751
	0.49548	0.49548	0.49422	0.49228	0.49180	0.49044	0.49001	0.48966	0.48981	0.48992	0.48896	0.49122	0.49157	0.49227	0.49174	0.49360	0.49359
	0.37159	0.37159	0.36901	0.36686	0.37131	0.36819	0.36974	0.37248	0.37243	0.37038	0.36628	0.36859	0.36789	0.37455	0.37087	0.37707	0.37702
C2	0.58938	0.58938	0.57965	0.57704	0.59528	0.59750	0.61138	0.60553	0.61274	0.61709	0.61277	0.61640	0.61544	0.60830	0.60949	0.59666	0.59667
	0.57265	0.57265	0.57368	0.57304	0.57150	0.57213	0.57122	0.57134	0.57067	0.57037	0.57095	0.57265	0.57303	0.57290	0.57319	0.57314	0.57314
	0.27888	0.27888	0.27821	0.27706	0.27759	0.28007	0.27896	0.27899	0.27886	0.27804	0.27886	0.27804	0.27655	0.27058	0.26777	0.26446	0.26446
F1	0.44794	0.44794	0.44667	0.44296	0.46661	0.47335	0.48558	0.48132	0.48750	0.48970	0.46943	0.47689	0.46993	0.46097	0.45789	0.45042	0.45038
	0.59191	0.59191	0.59218	0.59178	0.59045	0.59099	0.59045	0.59074	0.58951	0.59017	0.59145	0.59326	0.59303	0.59313	0.59400	0.59276	0.59277
	0.38253	0.38253	0.38770	0.38647	0.38921	0.39418	0.39248	0.39318	0.39462	0.39147	0.38505	0.38612	0.38440	0.37764	0.37201	0.37461	0.37457
F2	0.83922	0.83922	0.83627	0.83456	0.85394	0.85986	0.87401	0.86966	0.87814	0.87974	0.87401	0.88231	0.88147	0.87452	0.87435	0.86705	0.86707
	0.56524	0.56524	0.56662	0.56606	0.56365	0.56455	0.56355	0.56374	0.56308	0.56183	0.56462	0.56714	0.56810	0.56809	0.56855	0.56878	0.56878
	0.33808	0.33808	0.32969	0.32922	0.32748	0.32608	0.32651	0.32542	0.32493	0.32827	0.33755	0.33251	0.33313	0.32836	0.32893	0.31916	0.31914
F3	0.66528	0.66528	0.64327	0.64113	0.66081	0.65680	0.67306	0.66554	0.67171	0.68647	0.68296	0.67741	0.67586	0.66999	0.67572	0.65167	0.65171
	0.60106	0.60106	0.60273	0.60206	0.60061	0.60139	0.60035	0.60043	0.60029	0.59947	0.59921	0.60075	0.60160	0.60133	0.60116	0.60210	0.60211
	0.18779	0.18779	0.18622	0.18406	0.18453	0.18554	0.18351	0.18246	0.18370	0.18224	0.17929	0.17534	0.17505	0.16822	0.16410	0.16206	0.16210
C3	0.04495	0.04495	0.05669	0.06889	0.07249	0.05955	0.05850	0.05800	0.04695	0.03355	0.01936	0.04669	0.05377	0.06078	0.06130	0.07595	0.07594
	0.43054	0.43054	0.43200	0.43088	0.43143	0.43216	0.43296	0.43298	0.43405	0.43571	0.43544	0.43409	0.43406	0.43492	0.43257	0.43133	0.43133
	0.31434	0.31434	0.31433	0.31828	0.32127	0.32317	0.32283	0.32316	0.32125	0.32298	0.32415	0.31878	0.31964	0.32132	0.32602	0.32627	0.32625
D3A	-0.05048	-0.05048	-0.03140	-0.01536	-0.00759	-0.03333	-0.03478	-0.03132	-0.05354	-0.08404	-0.09271	-0.04325	-0.03772	-0.03388	-0.02623	-0.00638	-0.00642
	0.40883	0.40883	0.40966	0.40792	0.40794	0.40952	0.41061	0.40993	0.41186	0.41501	0.41476	0.41136	0.41182	0.41354	0.41009	0.40794	0.40793
	0.36754	0.36754	0.36845	0.37166	0.37419	0.37558	0.37749	0.37641	0.37428	0.37430	0.37965	0.37598	0.37920	0.38420	0.38715	0.38520	0.38515
D3B	0.24093	0.24093	0.25426	0.26765	0.27218	0.25882	0.25867	0.25917	0.24737	0.23060	0.21807	0.24950	0.25680	0.26360	0.26620	0.28149	0.28150
	0.42699	0.42699	0.43002	0.42941	0.43044	0.42972	0.43017	0.43092	0.43026	0.42892	0.42874	0.43003	0.42960	0.42971	0.42881	0.42807	0.42807
	0.32482	0.32482	0.32547	0.32798	0.32907	0.33611	0.33380	0.33388	0.33398	0.33751	0.33302	0.31763	0.31811	0.31986	0.32395	0.32029	0.32026
O2	-0.02695	-0.02695	-0.02957	-0.02097	-0.01975	-0.02628	-0.02198	-0.02934	-0.02773	-0.01684	-0.02505	-0.01054	0.00058	0.01422	0.00201	0.01694	0.01690
	0.46773	0.46773	0.46885	0.46727	0.46737	0.46922	0.47052	0.46994	0.47194	0.47449	0.47440	0.47163	0.47222	0.47401	0.47087	0.46866	0.46867
	0.37881	0.37881	0.37725	0.38472	0.39112	0.38855	0.38775	0.39096	0.38764	0.39029	0.39224	0.39535	0.39348	0.39041	0.39886	0.40646	0.40641

D2	0.08179	0.08179	0.07286	0.07531	0.07484	0.08391	0.09386	0.08410	0.09637	0.11807	0.11285	0.11836	0.13104	0.14902	0.11941	0.11578	0.11575
	0.48693	0.48693	0.48887	0.48799	0.48838	0.48867	0.48929	0.48901	0.48902	0.48980	0.48907	0.48884	0.48940	0.49057	0.49017	0.48967	0.48968
	0.37632	0.37632	0.37476	0.37895	0.38642	0.39468	0.39739	0.40321	0.40999	0.41319	0.41698	0.40914	0.40448	0.40128	0.39440	0.39046	0.39041
C4	-0.04209	-0.04209	-0.02853	-0.02007	-0.02151	-0.02171	-0.02916	-0.02986	-0.03662	-0.04510	-0.07620	-0.07420	-0.06943	-0.06439	-0.06422	-0.05844	-0.05842
	0.42897	0.42897	0.42932	0.42879	0.42985	0.43039	0.43081	0.43135	0.43280	0.43597	0.43538	0.43444	0.43368	0.43342	0.43129	0.43165	0.43165
	0.15297	0.15297	0.15219	0.15578	0.15881	0.15821	0.15805	0.15785	0.15467	0.15511	0.15811	0.15681	0.15763	0.15931	0.16361	0.16542	0.16546
F4	0.03318	0.03318	0.04928	0.07260	0.07569	0.10022	0.09045	0.09265	0.08320	0.07475	-0.00474	-0.03159	-0.01921	-0.00378	-0.01067	-0.01806	-0.01801
	0.39441	0.39441	0.39432	0.39513	0.39688	0.39912	0.39926	0.40025	0.40123	0.40472	0.40036	0.39839	0.39774	0.39764	0.39506	0.39550	0.39549
	0.08913	0.08913	0.09154	0.08992	0.08928	0.08865	0.08785	0.08565	0.08301	0.08074	0.08726	0.08495	0.08595	0.08833	0.09340	0.09131	0.09138
F5	0.06361	0.06361	0.07725	0.06929	0.05939	0.04565	0.03583	0.03237	0.03386	0.03092	0.03338	0.03784	0.03497	0.02986	0.03673	0.04596	0.04603
	0.45892	0.45892	0.45891	0.46026	0.46222	0.46424	0.46458	0.46563	0.46698	0.47068	0.46648	0.46403	0.46378	0.46406	0.46137	0.46170	0.46171
	0.07353	0.07353	0.07018	0.07624	0.08049	0.08366	0.08129	0.08280	0.08034	0.08524	0.07842	0.06980	0.06952	0.06963	0.07298	0.07535	0.07543
F6	-0.29889	-0.29889	-0.28557	-0.27778	-0.28035	-0.27446	-0.28459	-0.28531	-0.29306	-0.30155	-0.34269	-0.34638	-0.34313	-0.33915	-0.33988	-0.33603	-0.33602
	0.42742	0.42742	0.42725	0.42446	0.42465	0.42215	0.42247	0.42270	0.42509	0.42909	0.43474	0.43652	0.43440	0.43230	0.43131	0.43332	0.43332
	0.10790	0.10790	0.10613	0.11127	0.11626	0.10938	0.11207	0.11130	0.10563	0.10269	0.11407	0.12498	0.12668	0.12926	0.13339	0.13959	0.13964
C5	0.93995	0.93995	0.93620	0.92309	0.91965	0.92325	0.91890	0.92242	0.92177	0.92117	0.91597	0.94985	0.95966	0.97334	0.96797	0.96051	0.96051
	0.72327	0.72327	0.72354	0.72375	0.72363	0.72229	0.72140	0.72110	0.72054	0.72047	0.72041	0.72029	0.72040	0.72050	0.71937	0.71867	0.71867
	0.29886	0.29886	0.29541	0.29453	0.29506	0.29775	0.29857	0.29827	0.29747	0.29917	0.30156	0.29809	0.29997	0.29455	0.28799	0.28636	0.28637
D5A	1.02312	1.02312	1.03031	1.00974	1.00450	1.01257	1.00621	1.00646	1.00521	1.01051	1.01162	1.05383	1.05718	1.06923	1.06086	1.04528	1.04532
	0.73842	0.73842	0.73886	0.73985	0.73952	0.73823	0.73746	0.73721	0.73687	0.73660	0.73688	0.73639	0.73633	0.73569	0.73414	0.73381	0.73381
	0.21659	0.21659	0.21674	0.21473	0.21357	0.21729	0.21716	0.21555	0.21465	0.21729	0.22244	0.22070	0.21916	0.21077	0.20177	0.19812	0.19817
D5B	0.74549	0.74549	0.74390	0.72961	0.72538	0.72910	0.72407	0.72638	0.72514	0.72391	0.71917	0.75271	0.75967	0.77208	0.76588	0.75619	0.75618
	0.72013	0.72013	0.72033	0.71967	0.71928	0.71806	0.71676	0.71635	0.71565	0.71626	0.71664	0.71776	0.71780	0.71779	0.71613	0.71538	0.71539
	0.27937	0.27937	0.26807	0.26996	0.27166	0.27164	0.27310	0.27493	0.27417	0.27366	0.27216	0.26597	0.27281	0.26925	0.26434	0.26808	0.26810
O3	0.98132	0.98132	0.95920	0.94854	0.94664	0.94479	0.94018	0.94836	0.94750	0.94568	0.93392	0.96786	0.98966	1.00767	1.00350	1.00820	1.00816
	0.74522	0.74522	0.74544	0.74534	0.74586	0.74451	0.74389	0.74370	0.74304	0.74279	0.74198	0.74143	0.74194	0.74331	0.74327	0.74214	0.74215
	0.43290	0.43290	0.43129	0.43178	0.43148	0.43511	0.43607	0.43585	0.43591	0.43859	0.44338	0.44135	0.44244	0.43447	0.42566	0.42451	0.42447
D3	1.12776	1.12776	1.10211	1.09026	1.08985	1.08428	1.07986	1.08447	1.08887	1.09045	1.07991	1.10279	1.13287	1.16174	1.16679	1.16911	1.16908
	0.75747	0.75747	0.75827	0.75877	0.75916	0.75879	0.75833	0.75919	0.75745	0.75641	0.75503	0.75735	0.75646	0.75511	0.75027	0.75239	0.75240
	0.44825	0.44825	0.45160	0.45071	0.44973	0.45320	0.45387	0.45007	0.45284	0.45798	0.46700	0.45983	0.45984	0.45488	0.45615	0.44345	0.44340
C6	1.07447	1.07447	1.07054	1.06761	1.06641	1.06899	1.06888	1.07420	1.07558	1.06856	1.06025	1.08239	1.09355	1.10704	1.10610	1.10128	1.10129
	0.68299	0.68299	0.68320	0.68389	0.68382	0.68227	0.68155	0.68124	0.68068	0.67999	0.67957	0.67849	0.67857	0.67863	0.67779	0.67704	0.67704
	0.30942	0.30942	0.31085	0.30592	0.30802	0.31238	0.31347	0.31171	0.31010	0.31283	0.31468	0.31133	0.31143	0.31013	0.30696	0.29949	0.29949
F7	1.34086	1.34086	1.33095	1.33089	1.32755	1.32986	1.33176	1.33786	1.34066	1.33522	1.32710	1.34967	1.36249	1.37843	1.37904	1.37873	1.37875
	0.68546	0.68546	0.68571	0.68753	0.68771	0.68604	0.68591	0.68569	0.68531	0.68374	0.68273	0.67996	0.68004	0.68042	0.68041	0.67965	0.67964
	0.34607	0.34607	0.36123	0.35226	0.35934	0.36607	0.36523	0.36341	0.36093	0.36374	0.36763	0.36622	0.36519	0.36113	0.35618	0.34168	0.34167
F8	0.95810	0.95810	0.93720	0.94472	0.93874	0.93727	0.94126	0.94753	0.95067	0.93879	0.92584	0.93818	0.95094	0.96676	0.96961	0.97425	0.97422
	0.65966	0.65966	0.65935	0.65900	0.65849	0.65703	0.65622	0.65553	0.65477	0.65468	0.65419	0.65381	0.65360	0.65459	0.65418	0.65294	0.65293
	0.41186	0.41186	0.40579	0.40250	0.40191	0.40572	0.40913	0.40697	0.40606	0.40972	0.40999	0.40551	0.40591	0.40954	0.40990	0.40504	0.40501
F9	1.06195	1.06195	1.07759	1.07421	1.08141	1.08652	1.08567	1.09139	1.09213	1.08075	1.07276	1.08996	1.09966	1.10870	1.10790	1.09378	1.09383
	0.65662	0.65662	0.65716	0.65817	0.65826	0.65655	0.65551	0.65543	0.65487	0.65385	0.65366	0.65259	0.65286	0.65179	0.65013	0.64976	0.64975
	0.20094	0.20094	0.20074	0.19396	0.19523	0.19958	0.20089	0.19795	0.19569	0.19867	0.19930	0.19519	0.19418	0.19587	0.19511	0.18590	0.18595

C7	0.58066	0.58066	0.59347	0.58980	0.58349	0.58584	0.58657	0.58764	0.58994	0.57669	0.56487	0.55571	0.54802	0.53888	0.53436	0.52838	0.52836
	0.81794	0.81794	0.81818	0.81874	0.81954	0.82140	0.82264	0.82374	0.82366	0.82561	0.82620	0.82442	0.82308	0.82132	0.82202	0.82297	0.82297
	0.43087	0.43087	0.42648	0.42518	0.42600	0.42536	0.42612	0.42775	0.42505	0.42109	0.41653	0.41935	0.41809	0.41771	0.41678	0.42054	0.42051
D7A	0.78080	0.78080	0.79512	0.79115	0.78555	0.78960	0.79074	0.79137	0.79412	0.78103	0.76919	0.75866	0.75148	0.74320	0.74010	0.73485	0.73484
	0.82210	0.82210	0.82094	0.82198	0.82289	0.82442	0.82647	0.82838	0.82860	0.83110	0.83228	0.83164	0.83008	0.82801	0.82851	0.82960	0.82960
	0.44004	0.44004	0.43794	0.44121	0.44126	0.43662	0.43574	0.43927	0.43617	0.43116	0.42624	0.43137	0.43314	0.43414	0.43075	0.43301	0.43298
D7B	0.48622	0.48622	0.50364	0.49325	0.48695	0.49412	0.49183	0.48702	0.48780	0.47210	0.45720	0.44062	0.43149	0.42262	0.42087	0.41529	0.41524
	0.83880	0.83880	0.83983	0.84017	0.84128	0.84368	0.84485	0.84590	0.84581	0.84801	0.84845	0.84560	0.84406	0.84223	0.84296	0.84361	0.84362
	0.48428	0.48428	0.47868	0.47587	0.47563	0.47532	0.47563	0.47464	0.47178	0.46515	0.46012	0.46523	0.46477	0.46566	0.46705	0.47326	0.47321
O4	0.51784	0.51784	0.51568	0.51112	0.50552	0.50845	0.51711	0.52172	0.52663	0.51758	0.51068	0.50982	0.49768	0.48508	0.48183	0.47937	0.47932
	0.78027	0.78027	0.78101	0.78115	0.78214	0.78443	0.78558	0.78674	0.78658	0.78907	0.78961	0.78666	0.78477	0.78262	0.78315	0.78370	0.78369
	0.49448	0.49448	0.49009	0.48659	0.49059	0.49458	0.49845	0.50232	0.50080	0.50220	0.49913	0.49681	0.49152	0.48817	0.48697	0.48900	0.48894
D4	0.62487	0.62487	0.61749	0.61654	0.60469	0.59985	0.59749	0.58716	0.58879	0.55173	0.54074	0.52113	0.51307	0.49464	0.47297	0.46169	0.46166
	0.76108	0.76108	0.76104	0.76140	0.76180	0.76344	0.76413	0.76480	0.76454	0.76641	0.76690	0.76456	0.76293	0.76105	0.76191	0.76283	0.76282
	0.48488	0.48488	0.48244	0.48125	0.47972	0.47913	0.47439	0.47103	0.46785	0.46249	0.45836	0.44838	0.44147	0.43558	0.43187	0.43212	0.43209
C8	0.49856	0.49856	0.51769	0.52574	0.51765	0.50946	0.50598	0.51305	0.51431	0.50022	0.48800	0.48364	0.48204	0.47488	0.46265	0.45135	0.45137
	0.81906	0.81906	0.81962	0.82025	0.82018	0.82126	0.82152	0.82147	0.82103	0.82121	0.82122	0.82065	0.82050	0.81973	0.82085	0.82247	0.82247
	0.26874	0.26874	0.26287	0.25948	0.25976	0.25964	0.26023	0.26080	0.25768	0.25377	0.24892	0.25017	0.24745	0.24622	0.24561	0.24958	0.24962
F10	0.49658	0.49658	0.53753	0.56224	0.55953	0.54204	0.52608	0.54134	0.54233	0.52878	0.50753	0.50880	0.52561	0.53885	0.55261	0.56029	0.56036
	0.85217	0.85217	0.85238	0.85271	0.85200	0.85297	0.85328	0.85245	0.85189	0.85106	0.85120	0.85131	0.85118	0.84989	0.84884	0.84852	0.84852
	0.18972	0.18972	0.18210	0.17799	0.17485	0.17196	0.17063	0.16767	0.16325	0.15440	0.14875	0.15278	0.15193	0.15150	0.14776	0.14975	0.14983
F11	0.23244	0.23244	0.24742	0.25452	0.24477	0.23452	0.23087	0.23720	0.23738	0.22221	0.21042	0.20533	0.20190	0.19365	0.18308	0.17700	0.17701
	0.81055	0.81055	0.81433	0.81682	0.81769	0.81794	0.81620	0.81684	0.81636	0.81646	0.81482	0.81483	0.81741	0.82024	0.82717	0.83331	0.83332
	0.24706	0.24706	0.23851	0.22948	0.23084	0.23586	0.23857	0.23643	0.23373	0.23074	0.22652	0.22447	0.21763	0.21462	0.21675	0.22261	0.22265
F12	0.63954	0.63954	0.64651	0.65111	0.63683	0.62830	0.63330	0.63920	0.64048	0.62582	0.62228	0.61806	0.60562	0.58022	0.53056	0.48877	0.48882
	0.79299	0.79299	0.79147	0.79087	0.78969	0.79073	0.79156	0.79042	0.78974	0.78904	0.78971	0.78930	0.78806	0.78584	0.78467	0.78514	0.78514
	0.18740	0.18740	0.18402	0.18394	0.18628	0.18515	0.18573	0.19116	0.18855	0.18910	0.18420	0.18364	0.18092	0.17942	0.18008	0.18474	0.18480

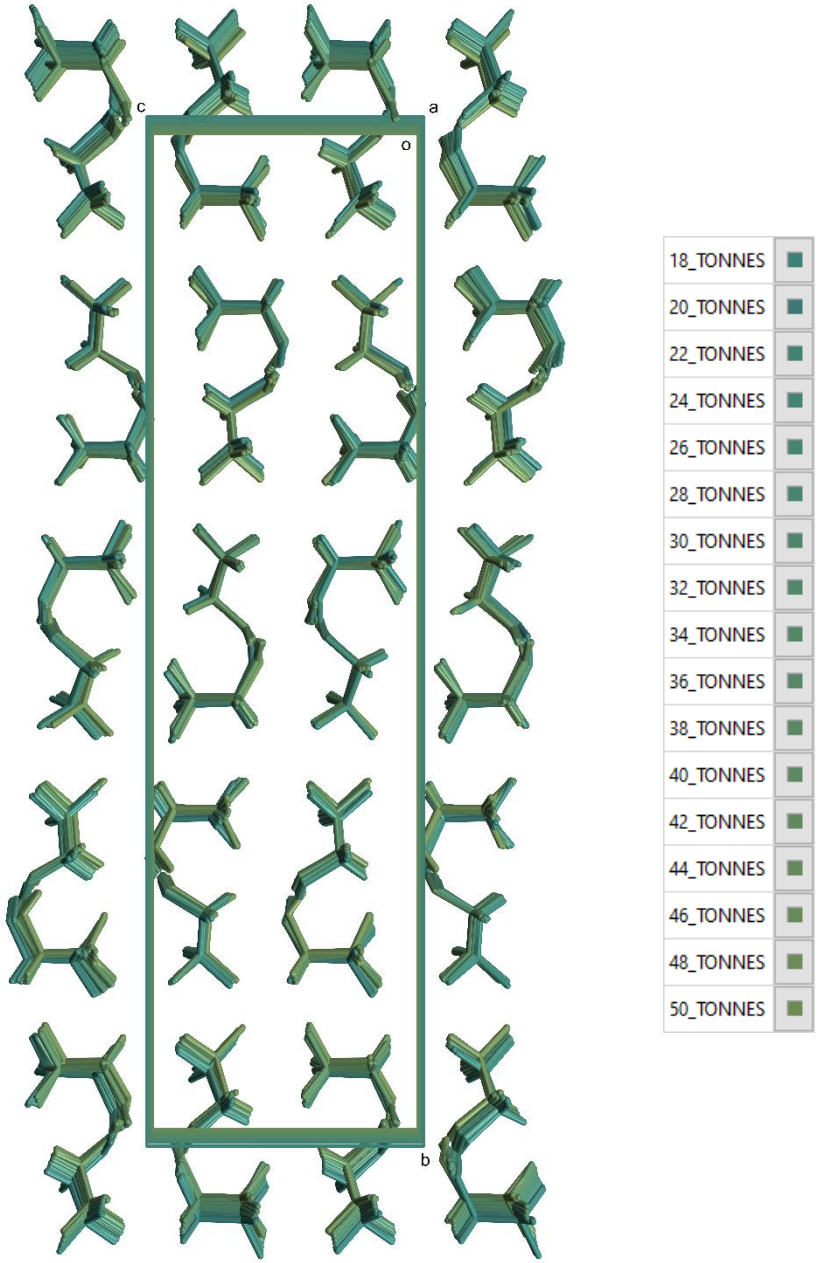


Figure S2.6: Packing of the TFE structures refined from the neutron powder-diffraction data from PEARL at 245 K showing an overlay of Form 3 at pressures from 0.46(3) GPa to 3.09(3) GPa. Progression from 0.46 GPa (18T, cyan) to 3.09 GPa (50T, green) is show by successively greener shading.

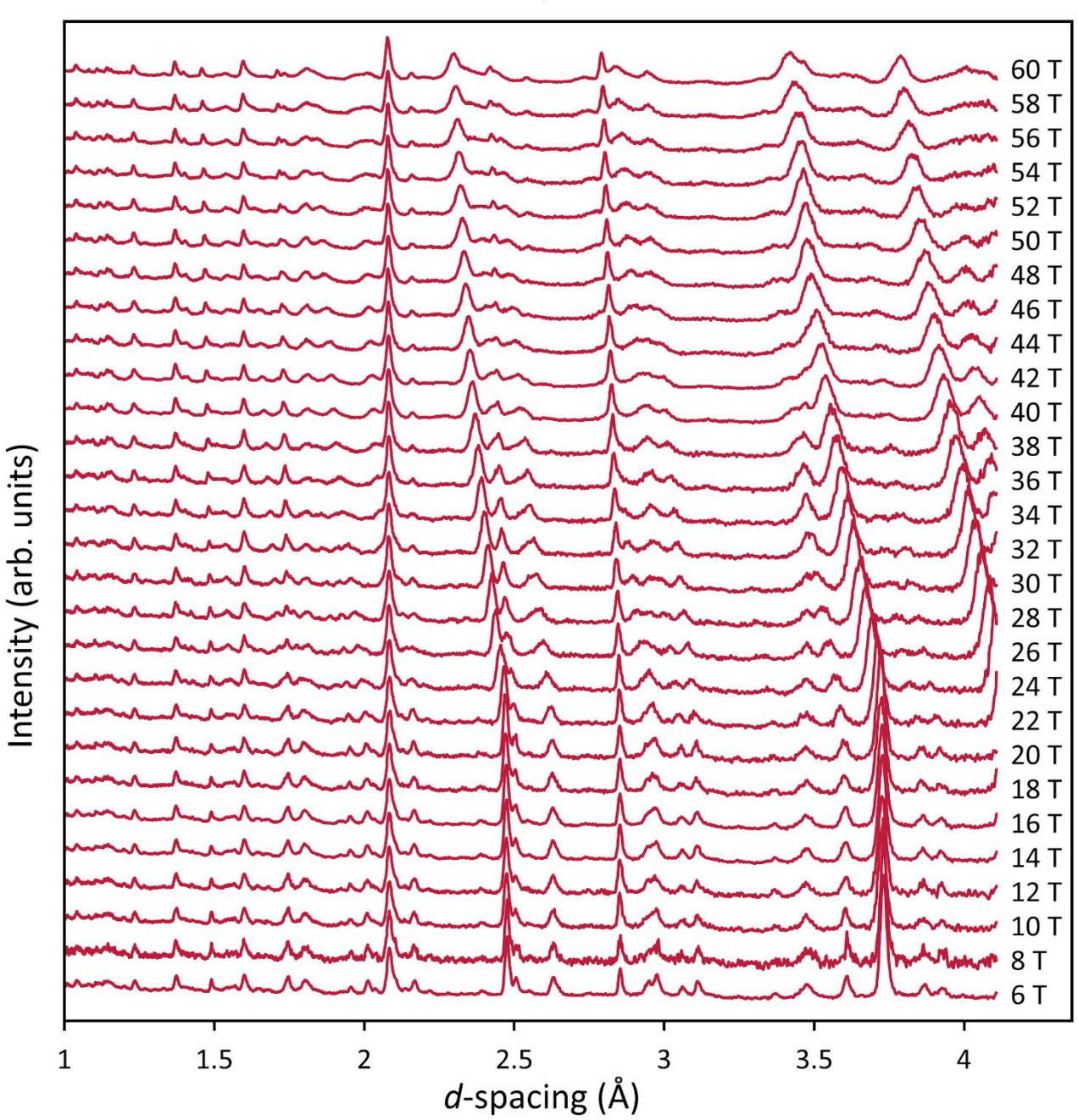


Figure S2.7: Neutron powder-diffraction patterns of TFE obtained from PEARL, collected at 200 K, shown with increasing pressure (Form 1 – red).

Table S2.5: Crystallographic data for the high-pressure neutron powder studies of TFE at 200 K on PEARL

Load (T)	Pressure (GPa) *	wR	Form	Space Group	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	V (Å^3)	Density (g/cm^3)	Z / Z'	VpM (Å^3) **
18	0.10(3)	0.08208	1	*Pca*2$_1$	8.5133(15)	9.9969(21)	9.0796(15)	90	90	90	772.74(17)	1.7889	8 / 2	96.59(17)
20	0.10(3)	0.08578	1	*Pca*2$_1$	8.5104(15)	9.9962(19)	9.0779(14)	90	90	90	772.28(15)	1.7899	8 / 2	96.54(15)
22	0.19(3)	0.08452	1	*Pca*2$_1$	8.4824(16)	9.980(2)	9.0581(16)	90	90	90	766.83(17)	1.8026	8 / 2	95.85(17)
24	0.24(3)	0.08398	1	*Pca*2$_1$	8.4360(19)	9.947(3)	9.0161(19)	90	90	90	756.6(2)	1.8271	8 / 2	94.6(2)
26	0.34(3)	0.08411	1	*Pca*2$_1$	8.3801(17)	9.904(3)	8.9544(19)	90	90	90	743.2(2)	1.8600	8 / 2	92.9(2)
28	0.46(3)	0.08850	1	*Pca*2$_1$	8.327(2)	9.870(3)	8.9025(16)	90	90	90	731.7(2)	1.8891	8 / 2	91.5(2)
30	0.61(3)	0.08619	1	*Pca*2$_1$	8.277(2)	9.837(3)	8.8472(16)	90	90	90	720.3(2)	1.9191	8 / 2	90.0(2)
32	0.80(3)	0.08574	1	*Pca*2$_1$	8.233(2)	9.804(3)	8.7961(17)	90	90	90	710.0(2)	1.9469	8 / 2	88.8(2)
34	0.99(3)	0.08045	1	*Pca*2$_1$	8.2009(18)	9.766(3)	8.7407(16)	90	90	90	700.0(2)	1.9748	8 / 2	87.5(2)
36	1.17(3)	0.07944	1	*Pca*2$_1$	8.1618(17)	9.742(3)	8.6942(16)	90	90	90	691.3(2)	1.9997	8 / 2	86.4(2)
38	1.39(3)	0.07788	1	*Pca*2$_1$	8.1288(18)	9.712(3)	8.6541(17)	90	90	90	683.2(2)	2.0234	8 / 2	85.4(2)
40 ^^	1.59(3)	0.07450	1	*Pca*2$_1$	8.0932(18)	9.680(3)	8.5999(17)	90	90	90	673.7(2)	2.0518	8 / 2	84.2(2)

* Pressure calculated using the refined value for the Pb *a*-axis[1]

** VpM: volume per molecule calculated by dividing the unit cell volume by Z and used for Figure 9 of the main text (volume per formula unit)

^^ Although data was collected up to 60T, Rietveld refinements were not performed on the data collected beyond 40T (1.60 GPa) due to the onset of non-hydrostatic conditions, as indicated by peak broadening

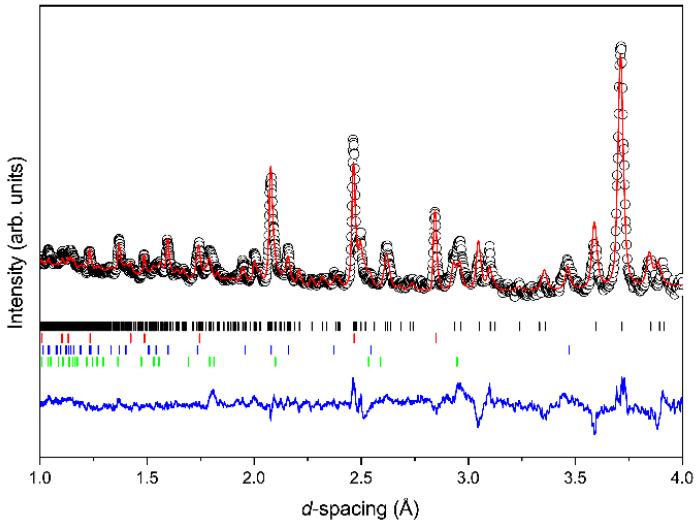


Figure 2.8: Rietveld refinement of the 200 K data at 0.10(3) GPa, corresponding to the powder neutron diffraction pattern collected at 20T (black circle – observed data; red line – calculated patterns; black tick marks – TFE; green tick marks – Al_2O_3; red tick marks – Pb; blue tick marks – ZrO_2; blue line – difference between observed and calculated data). The poor fit for Form 1 is likely to be due to the formation of coarse crystalline grains on initial freezing.

Table S2.6: Atomic positions for the structures refined from the high-pressure neutron powder-diffraction studies at 200 K on PEARL (Form 1)

Form 1	18T	20T	22T	24T	26T	28T	30T	32T	34T	36T	38T	40T
Atom	0.10 GPa	0.10 GPa	0.19 GPa	0.24 GPa	0.34 GPa	0.46 GPa	0.61 GPa	0.80 GPa	0.99 GPa	1.17 GPa	1.39 GPa	1.59 GPa
C1 x	0.14118	0.14372	0.14413	0.14078	0.13802	0.14888	0.15491	0.17532	0.16679	0.16553	0.16552	0.16656
y	0.16923	0.17096	0.16732	0.16470	0.16077	0.17181	0.17859	0.18546	0.17886	0.17532	0.17347	0.17368
z	0.45039	0.44572	0.44552	0.44627	0.44753	0.44962	0.45109	0.45034	0.45212	0.45264	0.45284	0.45233
D1A	0.07867	0.07426	0.07441	0.07110	0.06887	0.08137	0.08762	0.10898	0.10889	0.10786	0.10821	0.10904
	0.16112	0.16014	0.15723	0.15255	0.14493	0.14940	0.15228	0.15994	0.14483	0.13941	0.13677	0.13896
	0.53723	0.52742	0.52748	0.52860	0.53039	0.53266	0.53366	0.53467	0.53887	0.53925	0.53986	0.54099
D1B	0.08172	0.09149	0.09166	0.08789	0.08466	0.09488	0.09990	0.12116	0.11605	0.11392	0.11382	0.11605
	0.13926	0.14389	0.13957	0.13831	0.13618	0.14999	0.16120	0.16211	0.14609	0.14454	0.14248	0.13867
	0.36458	0.35472	0.35461	0.35448	0.35452	0.35533	0.35542	0.35511	0.35798	0.35741	0.35715	0.35709
O1	0.18081	0.18479	0.18564	0.18127	0.17560	0.17999	0.18644	0.19963	0.16037	0.15932	0.15768	0.15575
	0.30336	0.30562	0.30205	0.30034	0.29788	0.31059	0.31756	0.32622	0.32160	0.31840	0.31685	0.31750
	0.43030	0.43385	0.43236	0.43608	0.44206	0.45218	0.46149	0.45380	0.45304	0.45743	0.45818	0.45158
D1	0.24374	0.24433	0.23699	0.24040	0.23940	0.27122	0.27719	0.28008	0.23297	0.23364	0.23230	0.22596
	0.33902	0.33893	0.33809	0.33365	0.32939	0.33762	0.34364	0.35740	0.36527	0.36127	0.36033	0.36338
	0.48641	0.49476	0.49807	0.49832	0.50218	0.47024	0.48504	0.49652	0.49540	0.49904	0.49938	0.49711
C2	0.28317	0.28431	0.28504	0.28330	0.28344	0.29950	0.30624	0.33146	0.33701	0.33646	0.33773	0.34045
	0.08557	0.08665	0.08281	0.08045	0.07800	0.09340	0.09949	0.11198	0.13020	0.12631	0.12568	0.12825
	0.46333	0.46555	0.46619	0.46455	0.46186	0.45717	0.45314	0.45634	0.45544	0.45372	0.45341	0.45606
F1	0.27819	0.27769	0.27792	0.27676	0.28034	0.30294	0.31041	0.34238	0.37534	0.37481	0.37763	0.38308
	-0.04335	-0.04201	-0.04579	-0.04793	-0.05213	-0.03499	-0.02933	-0.01580	0.00272	-0.00224	-0.00296	0.00013
	0.46974	0.47629	0.48025	0.48462	0.46982	0.48432	0.48077	0.49031	0.47094	0.44882	0.45599	0.46763
F2	0.38729	0.39199	0.39210	0.38568	0.38902	0.38878	0.39061	0.41582	0.42154	0.42596	0.42433	0.42637
	0.11113	0.10845	0.10216	0.09590	0.10398	0.10795	0.11351	0.12430	0.17114	0.18299	0.17741	0.17488
	0.35953	0.36389	0.36282	0.35535	0.35654	0.33584	0.32767	0.32964	0.33554	0.34459	0.33837	0.33682
F3	0.35382	0.35106	0.35350	0.35851	0.35462	0.38826	0.40066	0.42403	0.41459	0.40919	0.41363	0.41600
	0.10310	0.10736	0.10599	0.10819	0.09767	0.12976	0.13606	0.15653	0.17377	0.15259	0.15935	0.17023
	0.59163	0.59513	0.59485	0.58956	0.59186	0.57362	0.56666	0.56872	0.57880	0.58640	0.58320	0.58396
C3	0.86612	0.86547	0.86996	0.86750	0.86836	0.86050	0.86121	0.85327	0.84428	0.84266	0.84074	0.84293
	0.43262	0.43317	0.43538	0.43681	0.43437	0.43028	0.42030	0.42227	0.42584	0.42677	0.42839	0.42639
	0.19572	0.19452	0.20085	0.19783	0.20710	0.21750	0.21215	0.23718	0.26114	0.26252	0.26590	0.27422
D3A	0.93012	0.92825	0.92659	0.93036	0.93391	0.92444	0.91938	0.91103	0.91120	0.90696	0.90749	0.91164
	0.39595	0.40150	0.41099	0.40563	0.40230	0.37813	0.36876	0.37218	0.37030	0.36938	0.37188	0.36974
	0.11942	0.11466	0.11386	0.11680	0.12749	0.14984	0.13872	0.16146	0.19687	0.19714	0.20101	0.21043
D3B	0.92494	0.92656	0.93717	0.92925	0.92715	0.91950	0.92511	0.92243	0.90332	0.90614	0.90132	0.90005
	0.43628	0.43301	0.42511	0.43470	0.43146	0.44651	0.42933	0.43728	0.45017	0.45362	0.45365	0.44929
	0.28794	0.28554	0.28759	0.28937	0.30116	0.31056	0.30435	0.32576	0.35420	0.35279	0.35909	0.37082
O2	0.82309	0.81880	0.82506	0.82206	0.82592	0.82612	0.83196	0.80952	0.80488	0.79942	0.80036	0.80853
	0.56254	0.56420	0.56950	0.56933	0.56803	0.55500	0.54995	0.54889	0.54609	0.54524	0.54860	0.54889
	0.15692	0.16489	0.19011	0.17048	0.17828	0.15134	0.15449	0.17758	0.18333	0.18198	0.18625	0.19515

D2	0.74658	0.73735	0.73113	0.73714	0.73800	0.77677	0.77752	0.80930	0.78073	0.76090	0.77500	0.76792
	0.59743	0.59318	0.58893	0.59702	0.59579	0.61252	0.60398	0.61628	0.61506	0.61100	0.61803	0.61427
	0.19626	0.20125	0.18660	0.20271	0.20435	0.19928	0.20348	0.23290	0.23192	0.22861	0.23474	0.24235
C4	0.72630	0.72800	0.73114	0.72769	0.72559	0.71150	0.70857	0.70867	0.69584	0.69580	0.69135	0.68937
	0.34808	0.34535	0.34795	0.34954	0.34844	0.35660	0.35108	0.34523	0.35018	0.35213	0.35292	0.35221
	0.21868	0.21513	0.21902	0.21711	0.22207	0.25448	0.25043	0.28631	0.30505	0.31510	0.31253	0.31357
F4	0.75659	0.76156	0.76323	0.75737	0.75034	0.73893	0.73084	0.74500	0.72889	0.73469	0.72667	0.71846
	0.24698	0.24210	0.24322	0.24901	0.24722	0.25608	0.25517	0.25491	0.25042	0.24742	0.24851	0.24544
	0.30820	0.30060	0.30324	0.30897	0.31554	0.34921	0.35306	0.39266	0.40253	0.40479	0.40483	0.40550
F5	0.67187	0.67391	0.67761	0.67858	0.67995	0.64144	0.64020	0.63916	0.62132	0.60825	0.60972	0.61178
	0.29721	0.29733	0.30183	0.29673	0.29587	0.30444	0.29337	0.27852	0.29464	0.30306	0.30277	0.30509
	0.09475	0.08967	0.09214	0.09108	0.09369	0.13488	0.13208	0.17357	0.18666	0.20011	0.19347	0.18961
F6	0.60258	0.60376	0.60613	0.59940	0.59490	0.59516	0.59095	0.58915	0.57969	0.58890	0.57905	0.57388
	0.38940	0.38220	0.38464	0.38928	0.38999	0.41036	0.41108	0.40078	0.40438	0.40537	0.40603	0.40580
	0.28723	0.28596	0.28960	0.28178	0.28297	0.32969	0.31927	0.35842	0.38429	0.40689	0.39962	0.39779

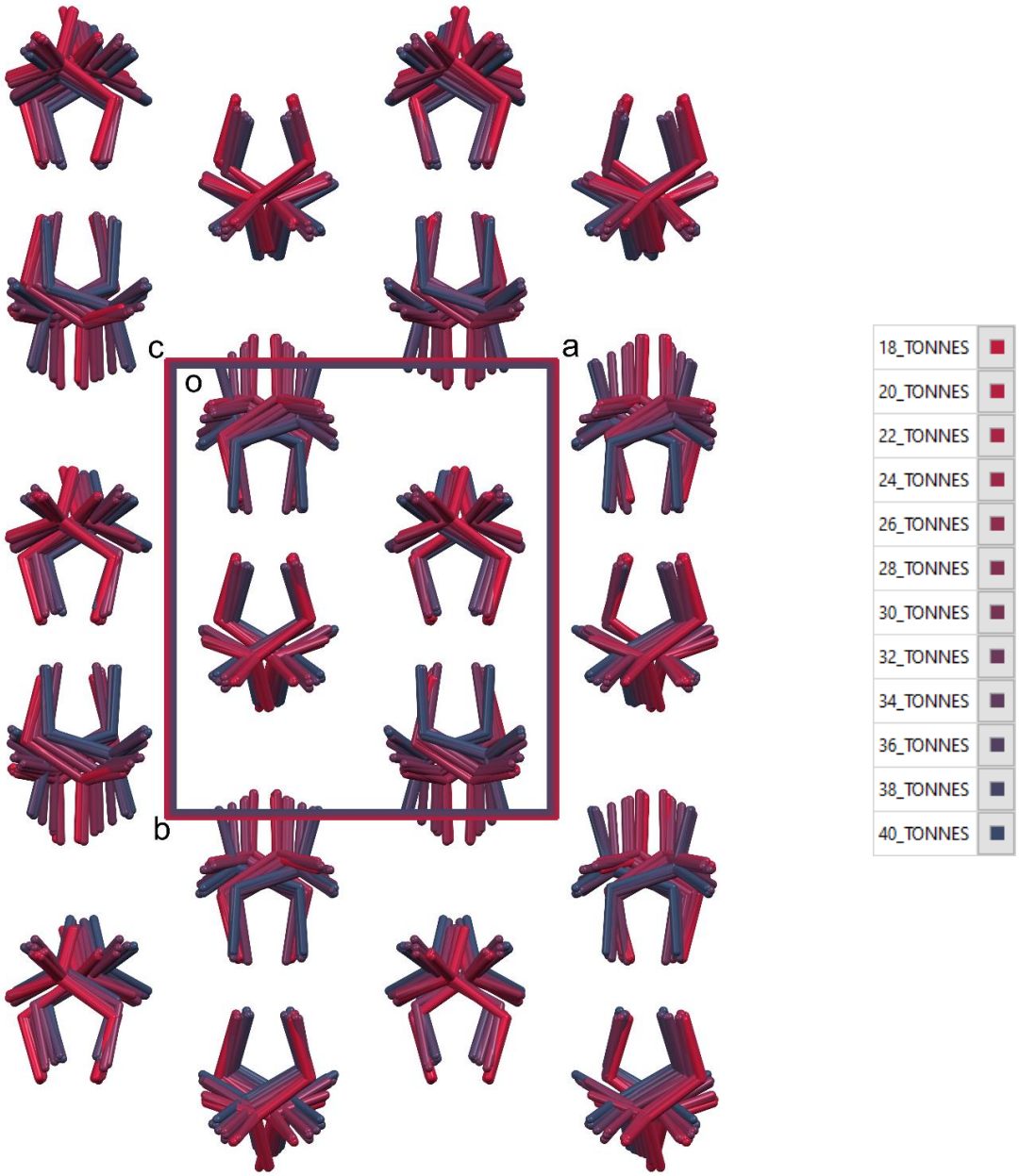


Figure S2.9: Packing of the TFE structures refined from the neutron powder-diffraction data from PEARL at 200 K showing an overlay of packing of Form 1 at pressures from 0.10(3) GPa to 1.59(3) GPa. Progression from 0.10 GPa (18T, red) to 1.59 GPa (40T, blue) is show by successively bluer shading.

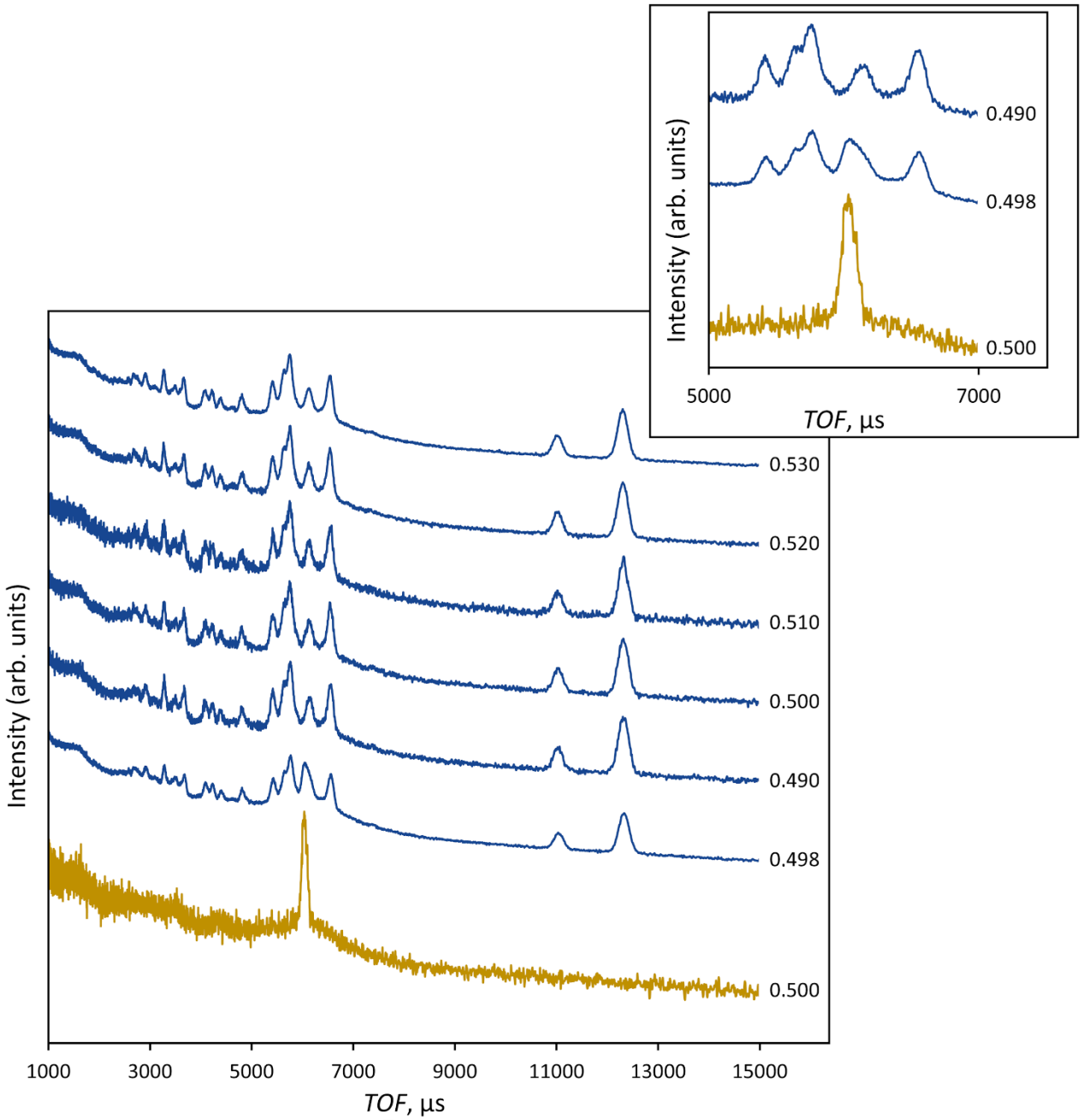


Figure 2.10: Neutron powder-diffraction patterns of TFE obtained from GEM, collected at 290 K, shown in the order the data was collected and labelled by starting pressure, in GPa (Form 5 – gold; Form 2 – blue). Insert shows the peak at ~6000 µs at 0.498 GPa looks to be composed of both Form 5 and Form 2.

Table S2.7: Crystallographic data for the high-pressure neutron powder studies of TFE at 290 K on GEM

Pressure (GPa)	wR	Form	Space Group	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	V (Å^3)	Density (g/cm^3)	Z / Z'
0.50	0.06247	5	*Im*-3*m*	5.708(2)	5.708(2)	5.708(2)	90	90	90	185.9(2)	1.8412	2 / 1
0.53	0.03729	2	*P*-1	4.911(4)	8.849(17)	9.12(2)	111.49(5)	102.92(2)	90.628(16)	357.62(11)	1.9141	4 / 2

Table S2.8: Atomic positions for the Form 2 structure refined from the high-pressure neutron powder-diffraction study on GEM at 0.53 GPa.

	C1	D1A	D1B	O1	D1	C2	F1	F2	F3	C3	D3A	D3B	O2	D2	C4	F4	F5	F6
x	0.96432	1.13494	0.89341	1.03042	0.91907	0.75459	0.85440	0.53017	0.61988	0.62321	0.77431	0.45429	0.57878	0.44834	0.70847	0.76932	0.51179	0.93715
y	0.22168	0.23335	0.32514	0.16285	0.16710	0.10668	-0.03156	0.06961	0.14535	0.28434	0.25835	0.28988	0.16066	0.16165	0.44304	0.55939	0.49118	0.47150
z	0.36163	0.32700	0.40140	0.48647	0.54254	0.22071	0.14827	0.26320	0.10283	0.78259	0.85661	0.81877	0.62879	0.55518	0.77903	0.92598	0.68621	0.74178

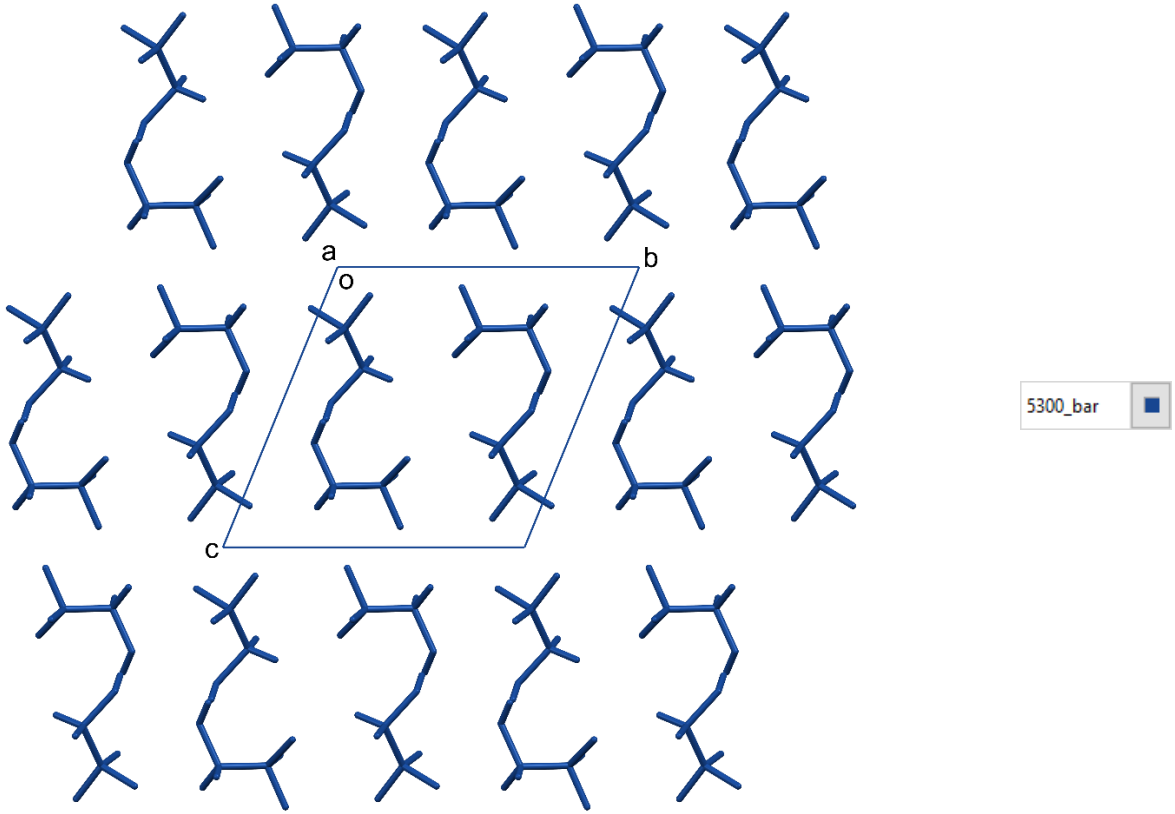


Figure S2.11: Packing of the TFE structure refined from the neutron powder-diffraction data from GEM at 290 K showing Form 2 at 0.53 GPa.

References

1 A. D. Fortes, *RAL Technical Reports*, 2019, **RAL-TR-2019-002**, 2019.