

Supporting Information

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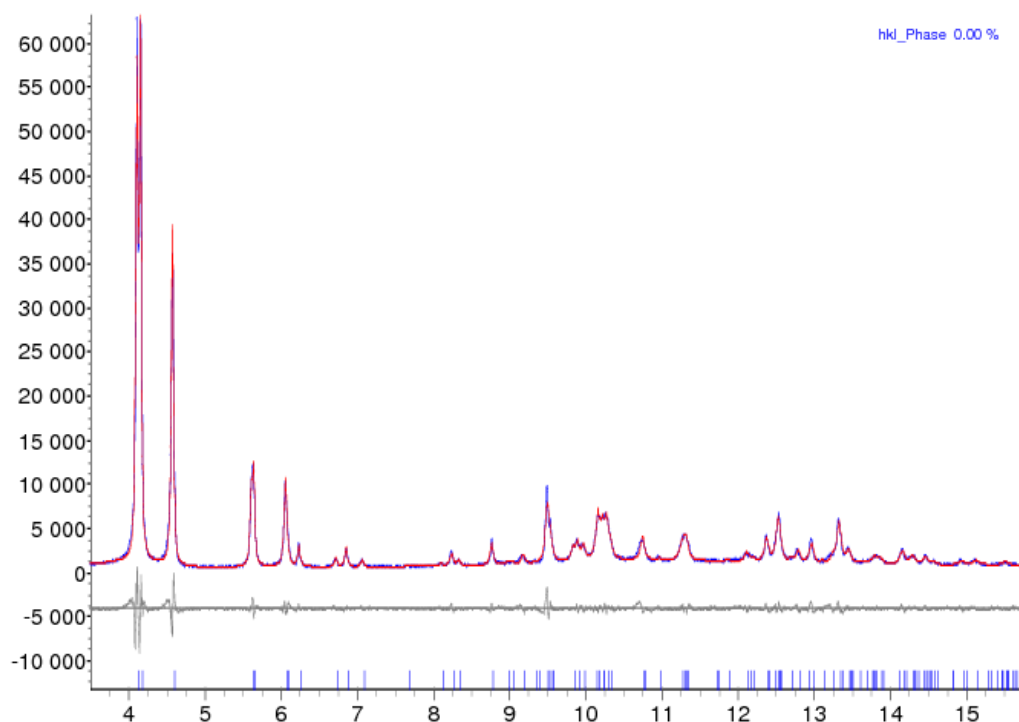


Figure SM1. XRPD pattern of IBUPOSS at RT refined employing the Pawley method [space group P-1; cell parameters: $a=10.17$, $b=11.16$, $c=11.22$ $\alpha=93.8$, $\beta=100.1$, $\gamma=90.8$].

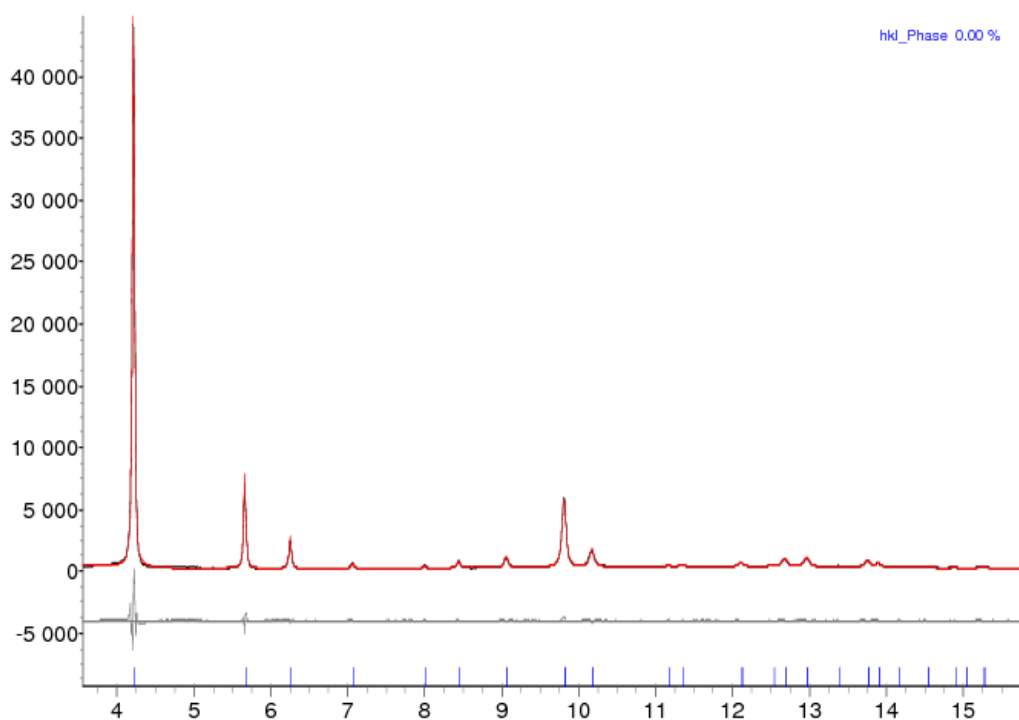


Figure SM2. XRPD pattern of IBUPOSS at HT refined employing the Pawley method space group R-3m; cell parameters: $a=b=16.15$, $c=17.16$].

h	k	l	2-Theta [degree]	Dspacing [Å]	h	k	l	2-Theta [degree]	Dspacing [Å]
0	1	0	4,11444	11,13823	1	-2	2	12,65697	3,62733
0	0	1	4,15621	11,02634	0	-3	1	12,76816	3,59587
1	0	0	4,57864	10,00951	0	-1	3	12,87674	3,56568
1	0	-1	5,61377	8,16493	1	1	-3	12,94573	3,54676
0	-1	1	5,64017	8,12675	1	-3	0	13,07571	3,51165
0	1	1	6,05177	7,57449	2	-2	1	13,19745	3,47940
1	-1	0	6,07494	7,54562	1	3	0	13,30602	3,45113
1	1	0	6,23829	7,34823	0	3	1	13,32529	3,44616
1	0	1	6,70825	6,83395	1	-1	-3	13,42038	3,42186
1	1	-1	6,86064	6,68233	0	1	3	13,42945	3,41956
1	-1	-1	7,06201	6,49203	1	3	-1	13,43171	3,41898
1	-1	1	7,65192	5,99219	2	0	2	13,43964	3,41698
1	1	1	8,08609	5,67095	1	2	2	13,55116	3,38898
0	2	0	8,23419	5,56912	3	0	-1	13,65770	3,36267
0	0	2	8,31790	5,51317	1	-3	1	13,70834	3,35031
1	0	-2	8,75830	5,23644	1	-3	-1	13,74336	3,34181
0	-2	1	8,96166	5,11785	2	2	-2	13,74603	3,34117
0	-1	2	9,01949	5,08511	3	0	0	13,76533	3,33650
2	0	0	9,16460	5,00476	2	-1	2	13,81411	3,32478
1	-2	0	9,31782	4,92264	2	2	1	13,85552	3,31489
2	0	-1	9,37086	4,89484	1	0	3	14,05453	3,26818
1	1	-2	9,48075	4,83823	2	0	-3	14,13651	3,24933
0	2	1	9,48478	4,83618	2	-2	-2	14,15102	3,24601
1	2	0	9,53178	4,81239	3	-1	-1	14,24806	3,22402
0	1	2	9,53946	4,80852	3	-1	0	14,26655	3,21986
1	2	-1	9,82927	4,66707	3	1	-1	14,29119	3,21434
1	-1	-2	9,87530	4,64538	2	1	2	14,30351	3,21158
2	-1	0	9,94853	4,61127	1	-1	3	14,36424	3,19808
1	-2	-1	10,11119	4,53727	0	-3	2	14,42367	3,18497
2	1	0	10,14933	4,52027	1	3	1	14,44162	3,18103
1	0	2	10,18586	4,50410	3	1	0	14,47827	3,17302
2	1	-1	10,21864	4,48969	0	-2	3	14,48401	3,17177
2	-1	-1	10,25739	4,47277	2	1	-3	14,54947	3,15758
1	-2	1	10,30090	4,45393	1	2	-3	14,58034	3,15093
2	0	1	10,71784	4,28114	3	0	-2	14,78071	3,10844
1	-1	2	10,72041	4,28012	1	3	-2	14,78718	3,10709
1	2	1	10,94578	4,19225	2	-1	-3	14,90636	3,08239
2	0	-2	11,24107	4,08247	1	1	3	14,93088	3,07735
1	1	2	11,25230	4,07840	3	0	1	15,07781	3,04754
2	-1	1	11,28988	4,06487	2	-3	0	15,21306	3,02060
0	-2	2	11,29405	4,06337	3	1	-2	15,28963	3,00556
2	1	1	11,67645	3,93074	2	-2	2	15,33822	2,99610
1	2	-2	11,70982	3,91958	0	3	2	15,40113	2,98393
2	1	-2	11,85675	3,87118	3	-1	-2	15,40785	2,98264
2	-1	-2	12,09201	3,79613	1	-2	-3	15,41693	2,98089
0	2	2	12,12050	3,78724	0	2	3	15,45774	2,97307
2	-2	0	12,16704	3,77281	3	-1	1	15,45917	2,97280
1	-2	-2	12,34640	3,71821	1	-3	2	15,48560	2,96776
0	3	0	12,36464	3,71274	2	3	-1	15,49795	2,96541
2	2	-1	12,45485	3,68596	1	-3	-2	15,54771	2,95597
0	0	3	12,49061	3,67545	2	-3	-1	15,57509	2,95081
2	2	0	12,49516	3,67411	2	3	0	15,60859	2,94451
2	-2	-1	12,51856	3,66727	1	-2	3	15,79183	2,91056
1	0	-3	12,52135	3,66646	3	1	1	15,80973	2,90728

Table SM1. hkl values and relative peak positions of the IBUPOSS pattern at RT after Palwey refinement in space group P-1.

h	k	l	2-Theta [degree]	Dspacing [Å]
1	0	1	4,22652	10,84299
1	1	0	5,67575	8,07584
0	1	2	6,26680	7,31483
0	2	1	7,07862	6,47681
0	0	3	8,01496	5,72119
2	0	2	8,45880	5,42150
2	1	1	9,07762	5,05261
1	1	3	9,82645	4,66841
0	3	0	9,83875	4,66259
1	2	2	10,19229	4,50126
1	0	4	11,18677	4,10222
2	2	0	11,36548	4,03792
1	3	1	12,13076	3,78405
0	2	4	12,55244	3,65741
3	0	3	12,70268	3,61433
0	3	3	12,70268	3,61433
3	1	2	12,98869	3,53507
4	0	1	13,40193	3,42655
0	1	5	13,77658	3,33379
2	1	4	13,78540	3,33167
2	2	3	13,92257	3,29901
0	4	2	14,18443	3,23841
3	2	1	14,56440	3,15436
2	0	5	14,91044	3,08155
4	1	0	15,05374	3,05238
2	3	2	15,28869	3,00575
1	2	5	15,96566	2,87907
1	3	4	15,97329	2,87771
0	0	6	16,06946	2,86060

Table SM2. hkl values and relative peak positions of the IBUPOSS pattern at HT after Palwey refinement in space group R-3m.

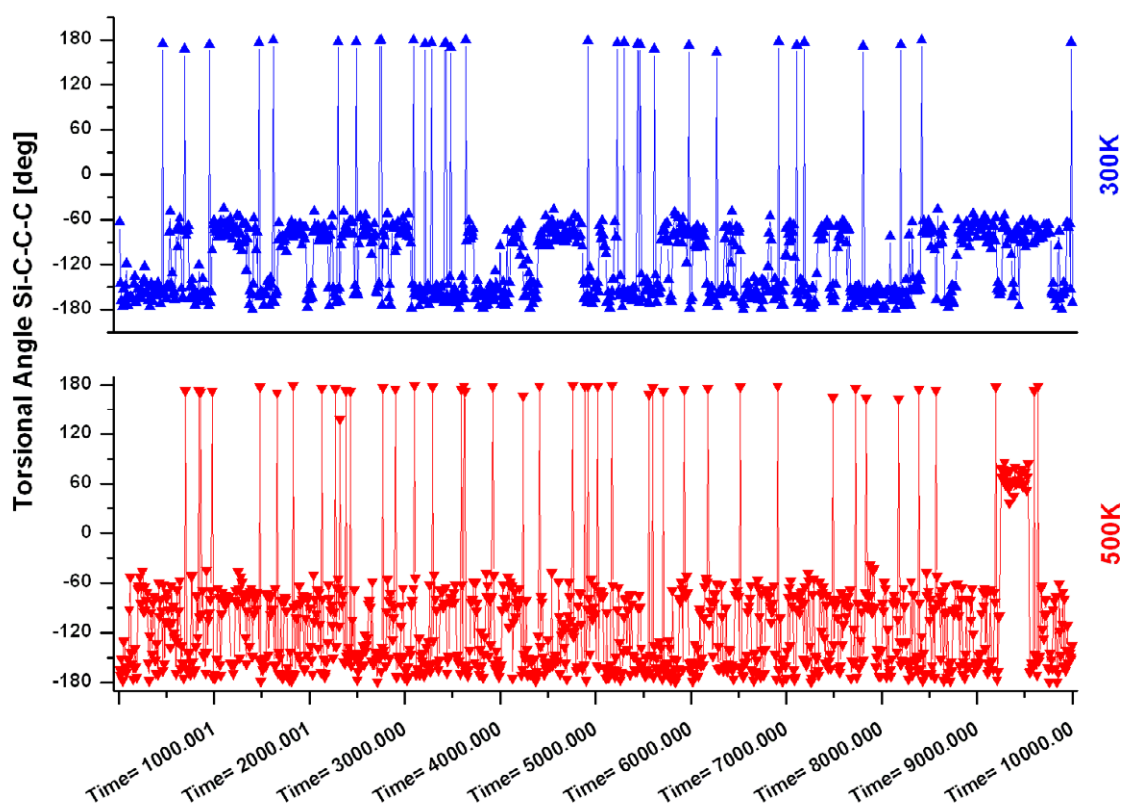


Figure SM3. Conformational motion of Si-C-C-C at 300 K and 500 K.

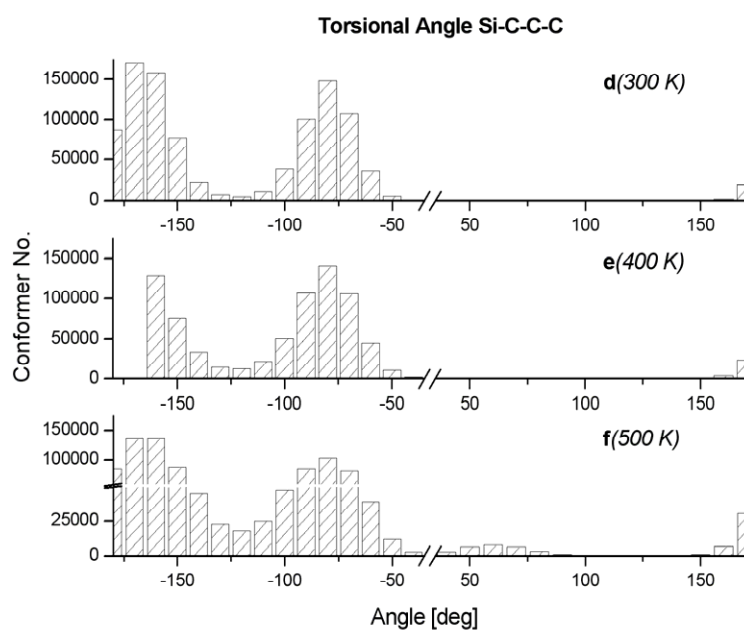


Figure SM4. Population distribution of one of the Si-C-C-C torsion angles at different temperatures.