crystals

Supplementary Materials: A Solid-Solid Phase Transformation of Triclabendazole at High Pressures

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Table S1. The calculated and experimental [1] crystal structures of triclabendazole forms I and II at different pressures.

TCBZ Form I							
P (GPa)	**a/Å**	**b/Å**	**c/Å**	**α°**	**β°**	**γ°**	**V/Å^3**
atm (Exp. [1])	9.658	10.183	17.775	81.75	75.63	62.34	1499.087
atm (Cal.)	9.632	10.184	17.694	81.75	75.63	62.34	1488.381
1	9.383	10.009	17.467	81.75	75.63	62.34	1406.773
5	8.898	9.647	16.692	81.75	75.63	62.34	1228.731
5.5	8.866	9.606	16.646	81.75	75.63	62.34	1215.607
6	8.833	9.569	16.604	81.75	75.63	62.34	1203.488
7	8.770	9.499	16.527	81.75	75.63	62.34	1180.769
11	8.577	9.281	16.271	81.75	75.63	62.34	1110.72
TCBZ Form II							
atm (Exp. [1])	21.277	8.8962	16.447	90	112.69	90	1436.111
atm (Cal.)	21.282	8.891	16.725	90	112.69	90	1459.874
1	20.966	8.606	16.389	90	112.69	90	1364.130
5	20.335	8.102	15.705	90	112.69	90	1193.605
5.5	20.285	8.051	15.682	90	112.69	90	1181.443
6	20.235	8.006	15.648	90	112.69	90	1169.402
7	20.145	7.920	15.606	90	112.69	90	1148.604
11	19.880	7.657	15.369	90	112.69	90	1079.213

Table S1 shows the experimental [1] and calculated crystal structure parameters of TCBZ forms I and II at different pressures. We found phase transition at pressure of 5.5 GPa which is highlighted in Table S1. The comparison of experimental and calculated crystal structures for both forms of TCBZ are given in Figures S1 and S2. Where Figure S1 provides crystal structures for TCBZ form I at atmospheric pressure and high pressures. Figure S2 provides crystal structures for TCBZ form II at atmospheric pressure and high pressures.

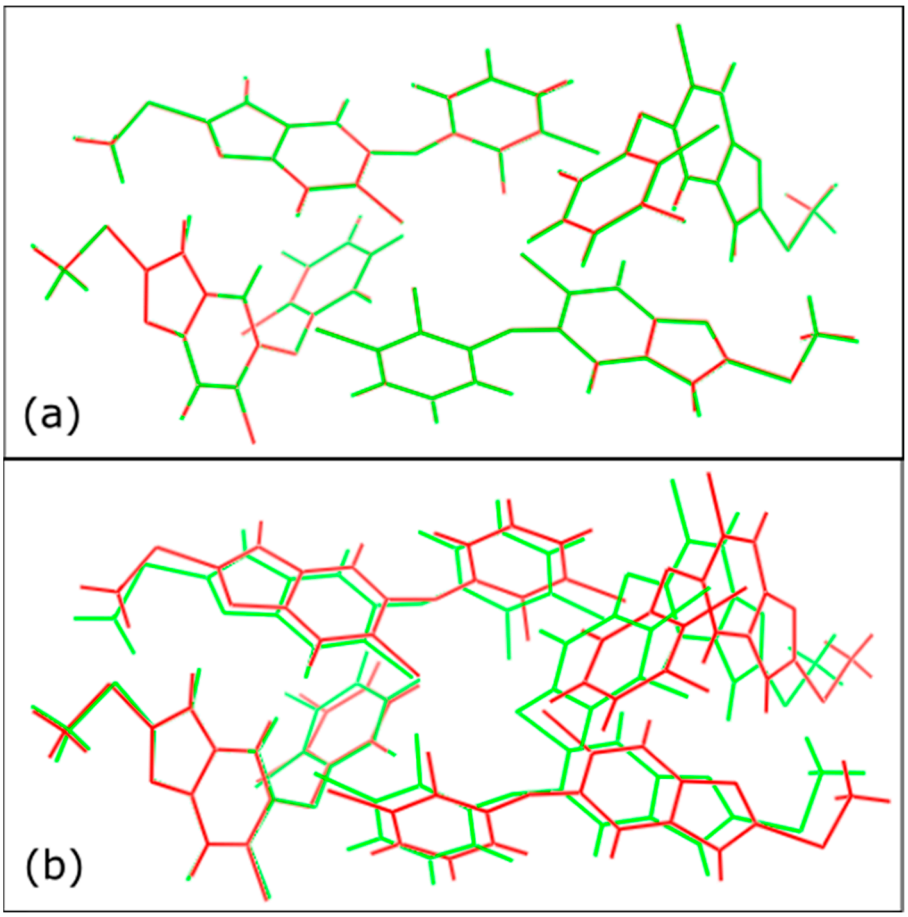

Figure S1. Experimental [1] (red) and calculated (green) crystal structures of TCBZ form I. (**a**) shows overlay of experimental [1] and predicted crystal structures at atmospheric pressure. (**b**) shows over-lay of experimental [1] at atmospheric pressure and computed structure at 5.5 GPa.

The comparison between experimental [1] (Red) and calculated (Green) crystal struc-ture of TCBZ form I is given in Figure S1a, where both structures were found at room tem-perature and atmospheric pressure. The root mean squire deviation (RMSD) was found to be 0.081 (Å), which is evidence of both structures matches well. However, RMSD for overlay of experimental form I at atmospheric pressure to calculated form I at high pres-sure (5.5 GPa) was found to be 0.436 (Å), which is evidence of change in crystal structure, can be seen in Figure S1 b.

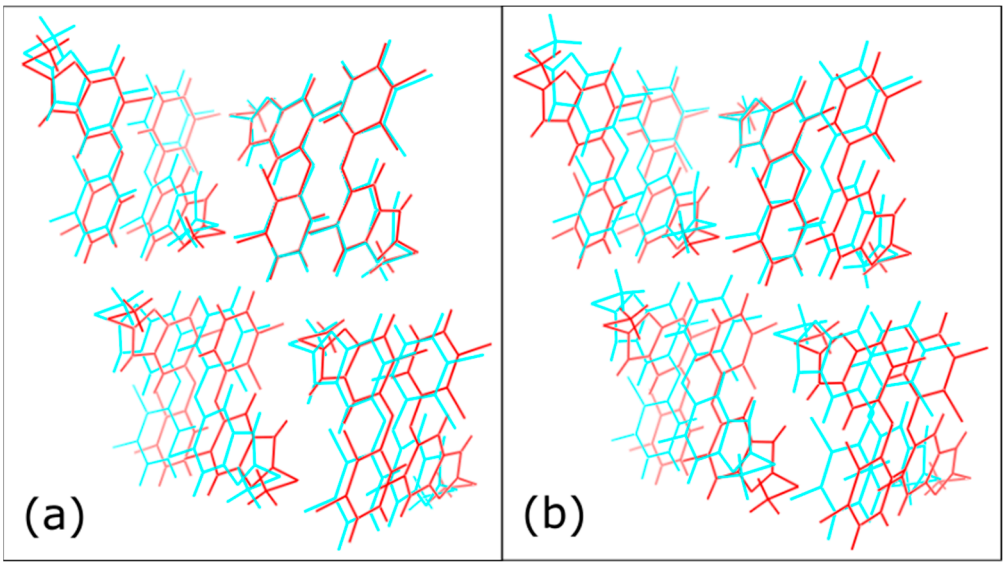

Figure S2. Experimental [1] (red) and calculated (cyan) crystal structures of TCBZ form II. (**a**) shows overlay of experimental [1] and predicted crystal structures at atmospheric pressure. (**b**) shows over-lay of experimental [1] at atmospheric pressure and computed structure at 5.5 GPa.

The comparison between experimental [1] (Red) and calculated (Green) crystal struc-ture of TCBZ form II is given in Figure S2a, where both structures were found at room temperature and atmospheric pressure. The root mean squire deviation (RMSD) was found to be 0.262 (Å), which shows less accuracy in prediction of crystal structure of form II. Moreover, RMSD for overlay of experimental form II at atmospheric pressure to calcu-lated form II at high pressure (5.5 GPa) was found to be 0.626 (Å), which is an evidence of change in crystal structure, can be seen in Figure S2 b.

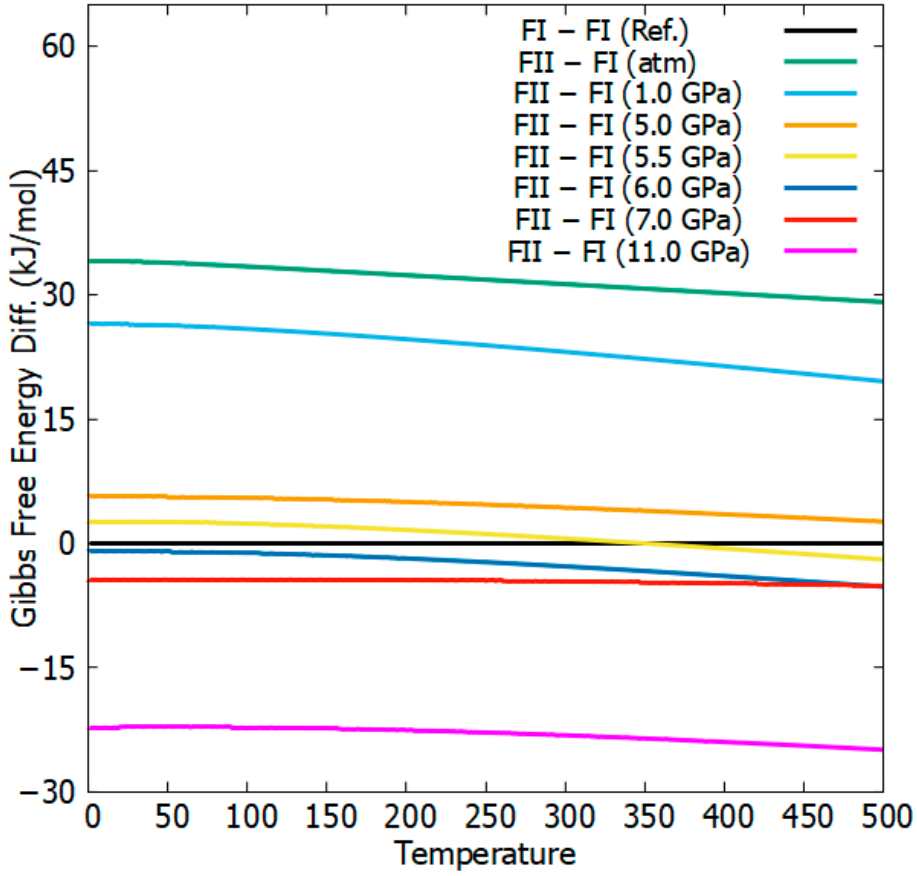

Figure S3. Calculated Gibbs free energy differences between TCBZ forms I and II at different pressures with respect to temperatures from 0 K to 500 K.

Reference

1. Tothadi, S.; Bhogala, B.R.; Gorantla, A.R.; Thakur, T.S.; Jetti, R.K.R.; Desiraju, G.R. Triclabendazole: An Intriguing Case of Co-Existence of Conformational and Tautomeric Polymorphism. *Chem. Asian J.* **2012**, *7* (2), 330–342, https://doi.org/10.1002/asia.201100638.