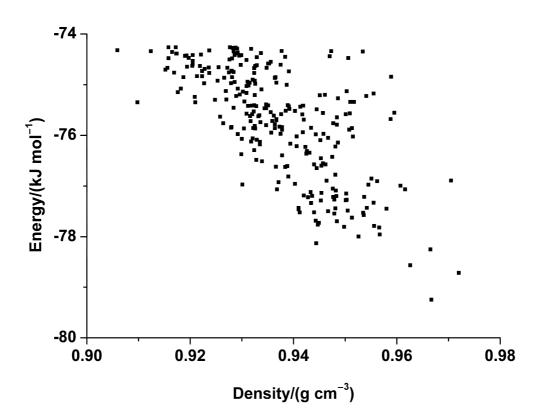
Supplementary material for "Predicted and experimental crystal structures of ethyl-*tert*-butyl ether" Sonja M. Hammer, Edith Alig, Lothar Fink and Martin U. Schmidt

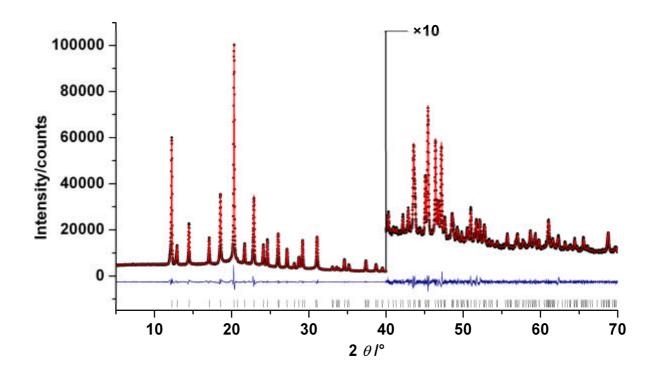
Figure S1

Distribution of energies and densities for the predicted structures with low energies. Note that all structures are within only 5 kJ mol⁻¹ above the energetically-lowest packing.



Supplementary material for "Predicted and experimental crystal structures of ethyl-*tert*-butyl ether" Sonja M. Hammer, Edith Alig, Lothar Fink and Martin U. Schmidt

Figure S2Pawley-fit of ETBE



Supplementary material for "Predicted and experimental crystal structures of ethyl-*tert*-butyl ether" Sonja M. Hammer, Edith Alig, Lothar Fink and Martin U. Schmidt

Formula S1

$$E(\boldsymbol{t}) = \sum_{n=0}^{7} A_n \cdot \cos(n \cdot \boldsymbol{t})$$

with:

n	$A_{\rm n}(t_1)$	$A_{\rm n}(t_2)$
0	16.3396	9.3073
1	18.9941	3.6367
2	5.34595	1.6991
3	3.1909	8.0333
4	1.1482	0.2171
5	0.6831	0.0000
6	0.0000	0.3916
7	0.0000	- 0.0548

All values in kJ mol⁻¹