Electronic Supplementary Material (ESI) for CrystEngComm

Supporting information

New Insights into the BiB_3O_6 Melt Structure

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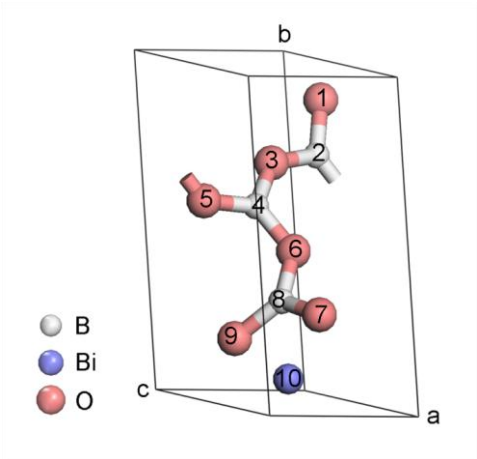

Fig. 1S The optimized structure of the fundamental unit in BiB_3O_6 melt.

Table 1S Geometrical parameters of the optimized structural unit.

Bond length (Å)		Bond angle (degree)	
B(2)-O(1)	1.358	O(1)-B(2)-O(3)	115.17
B(2)-O(3)	1.393	B(4)-O(3)-B(2)	135.50
B(4)-O(3)	1.372	O(3)-B(4)-O(5)	119.40
B(4)-O(5)	1.378	O(3)-B(4)-O(6)	122.01
B(4)-O(6)	1.358	O(5)-B(4)-O(6)	118.24
B(8)-O(6)	1.385	B(4)-O(6)-B(8)	127.85
B(8)-O(7)	1.366	O(6)-B(8)-O(7)	118.48
B(8)-O(9)	1.373	O(6)-B(8)-O(9)	123.29
Bi(10)-O(7)	2.024	O(7)-B(8)-O(9)	118.18
Bi(10)-O(9)	2.916		

Unit cell parameters: a = 4.71 Å; b = 9.04 Å; c = 4.40 Å; α = 107.33°; β = 83.25°; γ = 125.14°.