

Supplementary information

Table S1. Calculated B-B, Os-B, and Os-Os bond length (Å) for the lowest energy structures of Os-B system.

bond length			
	B-B	Os-B	Os-Os
Os ₇ B ₃		2.136	2.731
		2.155	2.747
		2.219	2.767
		2.230	2.776
			2.872
			2.890
			2.890
			2.891
			2.901
			2.901
OsB		2.204	
Os ₂ B ₃	1.872	2.205	
		2.215	
59-OsB ₂	1.817	2.174	
	1.908	2.230	
11-OsB ₃	1.999	2.177	2.933
	1.660	2.223	
	1.909	2.231	
	1.933		
	2.185		
	1.891		
59-OsB ₄	1.653	2.188	
	1.889	2.243	
	1.991	2.246	
	2.187		
	2.219		

Table S2. Calculated B-B, Ru-B, and Ru-Ru bond length (Å) for the lowest energy structures of Ru-B system.

bond length			
	B-B	Ru-B	Ru-Ru
Ru ₇ B ₃		2.138	2.628
		2.154	2.714
		2.177	2.719
		2.206	2.782
			2.851
			2.858
			2.864
			2.864
			2.874
			2.872
RuB		2.185	
Ru ₂ B ₃	1.857	2.190	
		2.197	
		2.181	
59-RuB ₂	1.816	2.162	2.995
	1.889	2.218	
62-RuB ₃	1.675	2.195	2.942
	1.812	2.322	
	1.818	2.112	
	1.823	2.183	
	1.864	2.287	
		2.322	
		2.846	
194-RuB ₄	1.685	2.192	
	1.895	2.224	
	1.898		