The molecular transformations of arsenic species in the flue gas of typical power plants: a DFT study

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Structures not shown in the paper are given in the following tables. All the structures have been fully optimized at the level of B3LYP/6-311G*.

Table s1, the structures related to figure 2 in the paper.

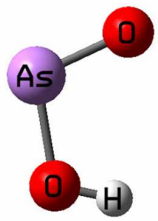
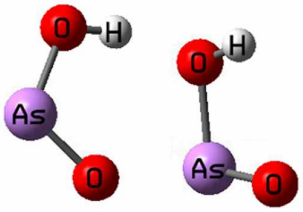
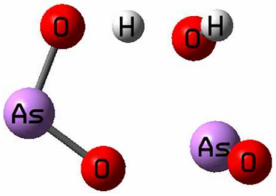
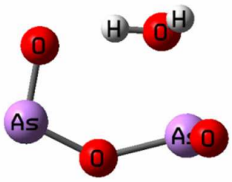
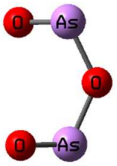
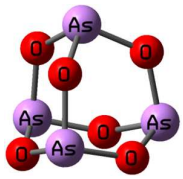
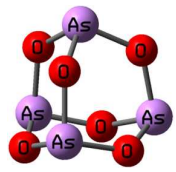
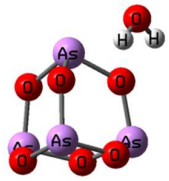
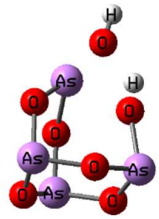
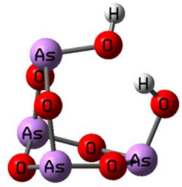
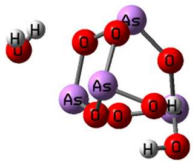
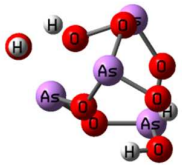
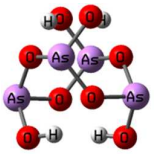
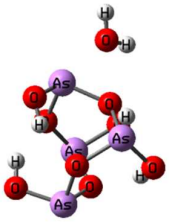
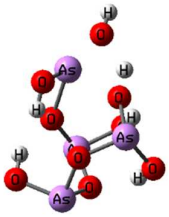
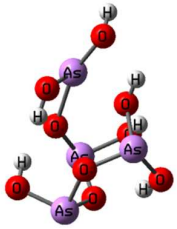
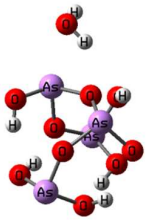
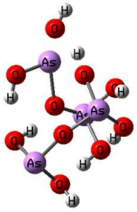
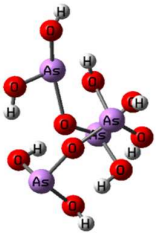
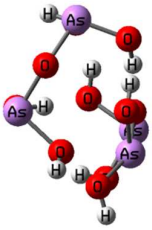
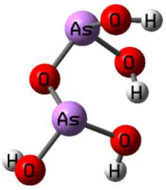
AsOOH	AsOOH-AsOOH	TS
		
As_2O_3-H_2O	As_2O_3	As_4O_6
		

Table s2, the structures related to figure 5 in the paper.

S1 (As_4O_6+6H_2O)	S2 As_4O_6-H_2O+5 H_2O	TS1 As_4O_6-H_2O(TS) +5H_2O	S3 $As_4O_6H_2O$+5 H_2O	S4 $As_4O_6H_2O$-H_2O+ 4H_2O
				
TS2 $As_4O_6H_2O$-H_2O(TS)+4H_2O	S5 $As_4O_6H_2OH_2O$+4H_2O	S6 $As_4O_6H_2OH_2O$-H_2O+3H_2O	TS3 $As_4O_6H_2OH_2O$-H_2O(TS)+3 H_2O	S7 $As_4O_6H_2OH_2OH_2O$+3H_2O
				
S8 $As_4O_6H_2OH_2OH_2O$-H_2O+2 H_2O	TS4 $As_4O_6H_2OH_2OH_2O$-H_2O(TS)+2H_2O	S9 $As_4O_6H_2OH_2OH_2OH_2O$+2H_2O	TS5 TS(Decompose) + 2H_2O	S10 2$As(OH)_2OAs(OH)_2$+2H_2O
				
S11 2$As(OH)_2OAs(OH)_2$-H_2O	TS6 2$As(OH)_2OAs(OH)_2$-H_2O(TS)	S12 2$As(OH)_2OAs(OH)_2H_2O$	S13 4$As(OH)_3$	

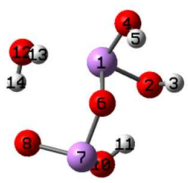
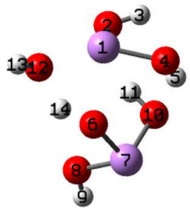
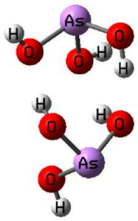
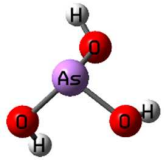
				

Table s3, the structures related to figure 6 in the paper.

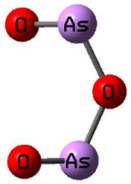
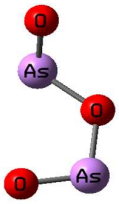
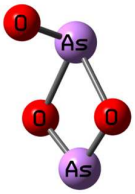
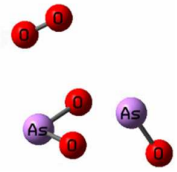
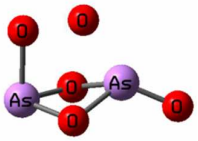
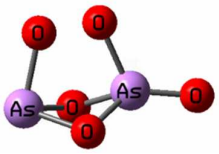
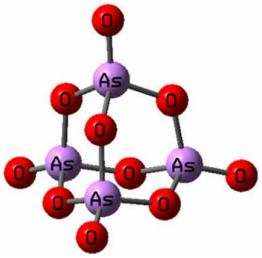
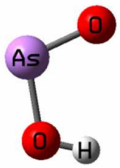
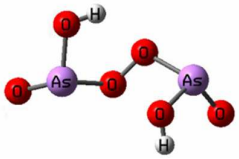
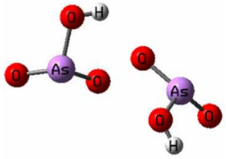
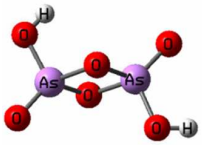
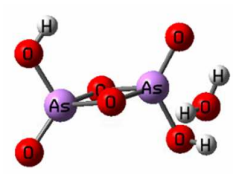
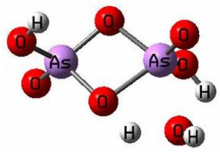
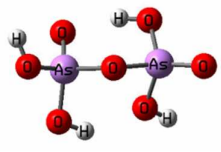
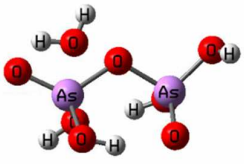
As_2O_3	TS1	AsO_2AsO	$AsO_2AsO\text{-}O_2$
			
IS2	V2O5	V4O10	
			

Table s4, the structures related to figure 7 in the paper.

AsOOH	IS1	TS1	IS2
			
IS2-H2O	TS2	IS3	IS3-H2O

			
TS3	IS4	H3AsO4