

Supplementary Materials:

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Table S1. Optimized geometries of the reactants, pre-reactive complex, transition state, product complex, and products at the MP2/aug-cc-pV(T+d)Z level of theory for the reaction of O₃ with the Cl atom.

Cartesian Coordinates (Angstroms) - Optimized parameters of O ₃ .					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	8	0	0	0	0.420134
2	8	0	0	1.056220	-0.210067
3	8	0	0	-1.056220	-0.210067
Cartesian Coordinates (Angstroms) - Optimized parameters of Cl.					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	17	0	0	0	0
Cartesian Coordinates (Angstroms) - Optimized parameters of pre-reactive complex of Cl+O ₃ reaction.					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	8	0	-1.702988	-0.789394	0
2	8	0	-2.557785	0.035187	0
3	8	0	0.577797	0.989754	0
4	17	0	1.684610	-0.107741	0
Cartesian Coordinates (Angstroms) - Optimized parameters of transition state of Cl+O ₃ reaction.					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	8	0	-1.086783	-0.468820	0
2	8	0	-2.157925	0.068714	0
3	8	0	0.070418	0.674397	0
4	17	0	1.493055	-0.129962	0
Cartesian Coordinates (Angstroms) - Optimized parameters of product complex of Cl+O ₃ reaction.					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	8	0	-1.702988	-0.789394	0
2	8	0	-2.557785	0.035187	0
3	8	0	0.577797	0.989754	0

4	17	0	1.684610	-0.107741	0
Cartesian Coordinates (Angstroms) - Optimized parameters of ClO.					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	17	0	0	0	0.498790
2	8	0	0	0	-1.059928
Cartesian Coordinates (Angstroms) - Optimized parameters of O₂.					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	8	0	0	0	0.593322
2	8	0	0	0	-0.593322

Table S2: Optimized geometries of the reactants, pre-reactive complex, transition state, product complex, and products at the MP2/aug-cc-pV(T+d)Z level of theory for the reaction of O₃ with the Br atom.

Cartesian Coordinates (Angstroms) - Optimized parameters of Br.					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	35	0	0	0	0
Cartesian Coordinates (Angstroms) - Optimized parameters of pre-reactive complex of Br+O₃ reaction.					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	8	0	-1.953072	-0.286930	0
2	8	0	-3.177209	2.863394	0
3	8	0	-1.356469	1.305684	0
4	35	0	1.482686	-0.053635	0
Cartesian Coordinates (Angstroms) - Optimized parameters of transition state of Br+O₃ reaction.					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	8	0	1.621000	-0.468379	0
2	8	0	2.708111	0.029014	0
3	8	0	0.490844	0.732646	0
4	35	0	-1.099067	-0.069345	0
Cartesian Coordinates (Angstroms) - Optimized parameters of product complex of Br+O₃ reaction.					

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	8	0	-2.238208	-0.688766	0.048749
2	8	0	-2.906150	0.288864	-0.048257
3	8	0	0.202535	1.244663	0.032983
4	35	0	1.129559	-0.193088	-0.007651
Cartesian Coordinates (Angstroms) - Optimized parameters of BrO.					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	35	0	0	0	0.318397
2	8	0	0	0	-1.392986

Table S3: Optimized geometries of the reactants, pre-reactive complex, transition state, product complex, and products at the MP2/aug-cc-pV(T+d)Z level of theory for the reaction of O₃ with the I atom.

Cartesian Coordinates (Angstroms) - Optimized parameters of I.					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	53	0	0	0	0
Cartesian Coordinates (Angstroms) - Optimized parameters of pre-reactive complex of I+O₃ reaction.					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	8	0	2.509754	-0.315419	0.030231
2	8	0	3.728511	-0.200810	-0.026223
3	8	0	1.826451	0.712525	0.005593
4	53	0	-1.217316	-0.029630	-0.001449
Cartesian Coordinates (Angstroms) - Optimized parameters of transition state of I+O₃ reaction.					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	8	0	-1.996993	-0.467396	0.064798
2	8	0	-3.089017	-0.001598	-0.057426
3	8	0	-0.870796	0.769881	0.026762
4	53	0	0.895046	-0.049235	-0.034063
Cartesian Coordinates (Angstroms) - Optimized parameters of product complex.					
Center Number	Atomic Number	Atomic Type	X	Y	Z

1	8	0	2.667901	-0.731269	0.058650
2	8	0	3.331149	0.246668	-0.062196
3	8	0	0.313502	1.256386	0.042716
4	53	0	-0.952838	-0.116496	-0.005912

Cartesian Coordinates (Angstroms) - Optimized parameters of IO.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	53	0	0	0	0.245218
2	8	0	0	0	-1.624568