Supplementary Information

Theoretical Studies on Gas-Phase Kinetics and Mechanism of H-abstraction Reaction from Methanol by ClO and BrO Radicals

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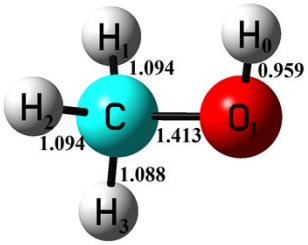
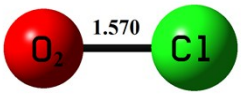
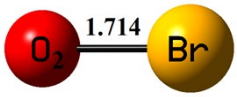
Figure S1: Structural parameters of the optimized geometries of Reactants, Transition States, Molecular Complexes and Products of CH_3OH+XO (X=Cl, Br) reaction at M06-2X/cc-pVTZ level of theory.



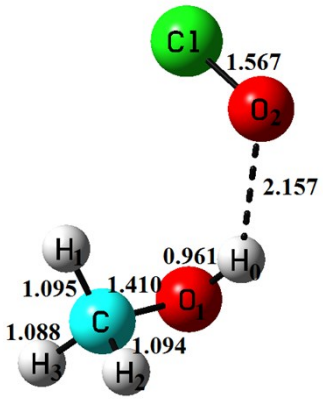
CH_3OH



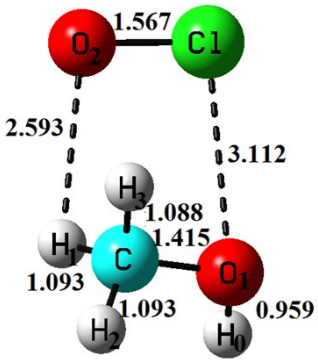
OCl



OBr



PreM11



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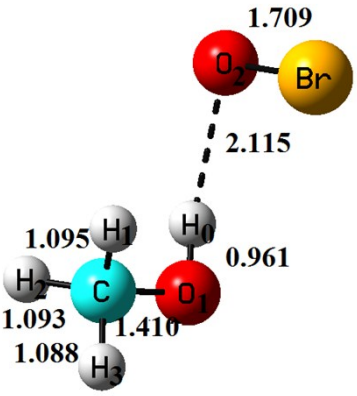
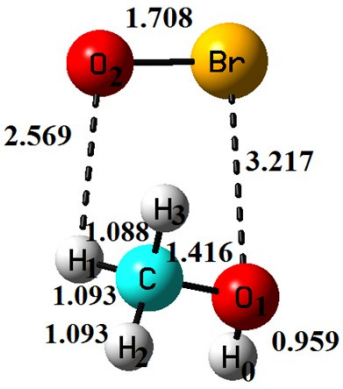
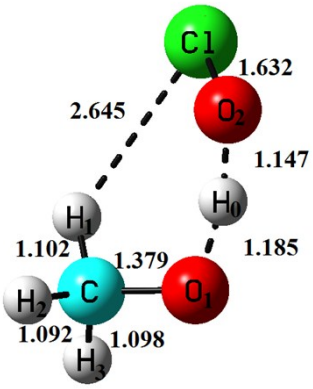


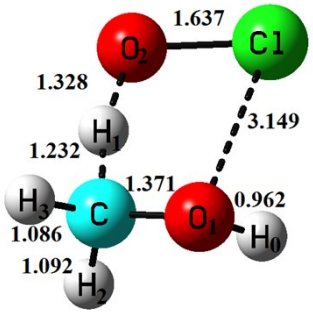
PreM21



PreM22



TS11



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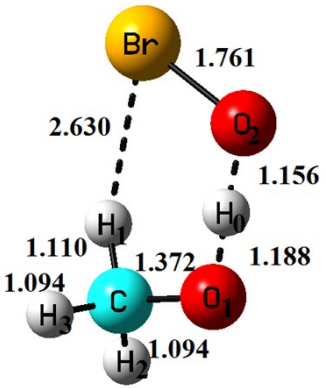

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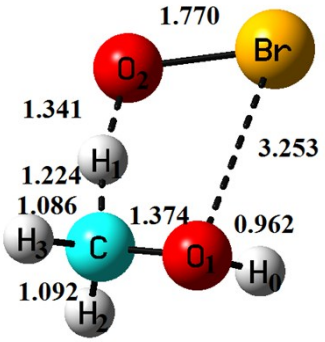

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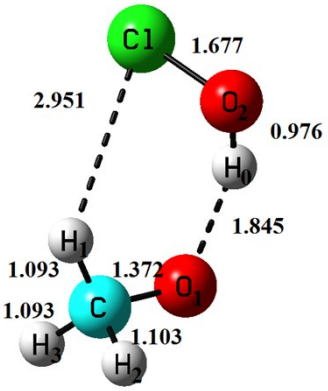
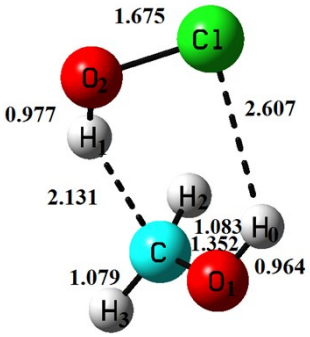


PostM11



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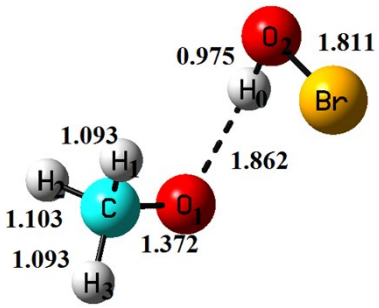

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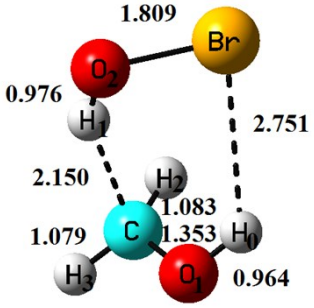

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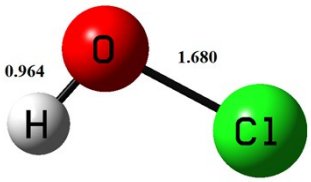
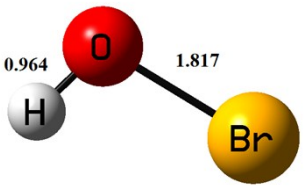
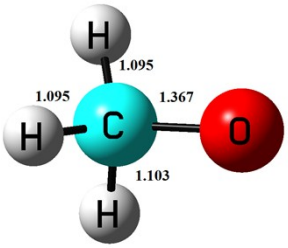


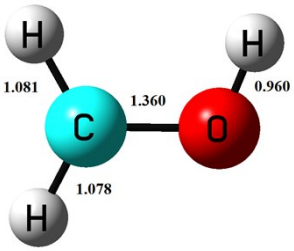
HOCl



HOBr



CH_3O



CH_2OH

Table S1: Cartesian Coordinates for Optimized Geometries of Reactants, Transition States, Molecular Complexes and Products of CH_3OH+XO (X=Cl, Br) reaction at M06-2X/cc-pVTZ level of theory.

Species	Centre number	Symbol	Cartesian Coordinates (Å)		
			X	Y	Z
CH_3OH	1	C	0.0463880	0.6597110	0.0000000
	2	H	1.0865980	0.9780330	0.0000000
	3	H	-0.4373220	1.0733510	0.8891920
	4	H	-0.4373220	1.0733510	-0.8891920
	5	O	0.0463880	-0.7528140	0.0000000
	6	H	-0.8613870	-1.0604880	0.0000000
OCl	1	O	0.0000000	0.0000000	-1.0679150
	2	Cl	0.0000000	0.0000000	0.5025480
OBr	1	O	0.0000000	0.0000000	-1.3949130
	2	Br	0.0000000	0.0000000	0.3188370
PreM11	1	C	-0.1485570	-0.1063410	0.2205410
	2	H	-0.6203780	0.0680940	1.1854640
	3	H	0.9157530	-0.2993670	0.3915170
	4	H	-0.5956900	-0.9999330	-0.2238790
	5	O	-0.3598190	1.0444680	-0.5671330
	6	H	0.0904200	0.9123620	-1.4054730
	7	O	2.0705410	0.6549340	-2.2213310
	8	Cl	2.8424690	1.5388080	-1.1833120
PreM12	1	C	0.0124350	0.0029720	0.0100440
	2	H	0.0302250	0.0196010	1.0977110
	3	H	1.0426290	0.0157540	-0.3544300
	4	H	-0.4676960	-0.9271240	-0.3059540
	5	O	-0.7102440	1.1447520	-0.4106400
	6	H	-0.7645790	1.1374490	-1.3679640
	7	O	-2.5164260	-1.3290490	1.2310360
	8	Cl	-3.2000710	0.0766310	1.1198830
PreM21	1	C	0.0066080	-0.1546740	-0.1462890

	2	H	0.2686780	-0.2281530	0.9072480
	3	H	0.9125950	-0.3290120	-0.7362040
	4	H	-0.3435320	0.8623440	-0.3432590
	5	O	-0.9880790	-1.1207040	-0.4031330
	6	H	-1.1803820	-1.0993470	-1.3448520
	7	O	-0.3711300	-1.4780930	-3.2615090
	8	Br	0.6999080	-2.7464890	-2.8558170
PreM22	1	C	-0.1473210	-0.0187920	0.1036750
	2	H	-0.6032690	0.4105330	0.9931900
	3	H	0.7898190	-0.4957060	0.4021680
	4	H	0.0681500	0.7880610	-0.6012430
	5	O	-1.0718250	-0.9497210	-0.4289530
	6	H	-0.6764270	-1.3692590	-1.1952330
	7	O	0.3790090	-1.7196300	2.6228220
	8	Br	-0.9978410	-2.6731490	2.2859740
TS11	1	C	0.0383190	-0.0063610	-0.0656440
	2	H	-0.0608070	0.0279840	1.0269430
	3	H	1.1021320	0.2016210	-0.2637720
	4	H	-0.2265430	-1.0000820	-0.4318000
	5	O	-0.7586830	0.9930020	-0.5818280
	6	H	-0.3616720	1.3952300	-1.6232640
	7	O	0.2202050	1.5785020	-2.5942080
	8	Cl	1.7704960	1.8867270	-2.1897620
TS12	1	C	-0.0083290	0.1055660	0.1680390
	2	H	0.6791530	0.2589450	0.9949850
	3	H	0.4072920	-0.5078260	-0.6338720
	4	H	-0.9185430	-0.5921370	0.6187210
	5	O	-0.5287020	1.3089580	-0.2344930
	6	H	-1.0711080	1.1843230	-1.0194530
	7	O	-2.0656120	-1.2111200	0.8737530
	8	Cl	-3.1909410	-0.3477630	0.0558580

TS21	1	C	0.0780600	0.1016320	-0.1681330
	2	H	0.2728640	-0.3842650	0.7921130
	3	H	1.0311910	0.1023020	-0.7376300
	4	H	-0.1828480	1.1557310	-0.0345970
	5	O	-0.8956820	-0.5257600	-0.9039660
	6	H	-0.4719520	-1.4766720	-1.4762970
	7	O	0.0701200	-2.1866500	-2.2103340
	8	Br	1.8124820	-2.0796820	-1.9812650
TS22	1	C	-0.0806540	-0.0530220	0.1529580
	2	H	-0.5287680	0.4858740	0.9830550
	3	H	0.9625010	-0.5188910	0.5919300
	4	H	0.2457150	0.6003520	-0.6583880
	5	O	-0.9088350	-1.0796340	-0.2318460
	6	H	-0.5654150	-1.4964770	-1.0280550
	7	O	2.0611570	-1.2283260	0.8902290
	8	Br	1.8072760	-2.8240520	0.1671090
PostM11	1	C	0.0368590	0.0331510	-0.0355900
	2	H	0.0937440	0.1372270	1.0513380
	3	H	1.0242060	-0.0295170	-0.5003240
	4	H	-0.4924150	-0.9150090	-0.2319310
	5	O	-0.7552510	1.0045470	-0.5930750
	6	H	0.0242680	1.3339770	-2.2330530
	7	O	0.7398910	1.3911320	-2.8941990
	8	Cl	1.9037680	2.2943880	-2.0921390
PostM12	1	C	-0.0162040	0.0332020	0.0044850
	2	H	-0.1564140	0.0758810	1.0730340
	3	H	2.0110290	-0.0826050	-0.6427190
	4	H	-0.1559880	0.9206890	-0.6006320
	5	O	-0.3186650	-1.1697590	-0.5343950
	6	H	-0.2127030	-1.1324790	-1.4916580
	7	O	2.6898000	-0.2061420	-1.3350480

	8	Cl	1.8161560	-0.0978190	-2.7602250
PostM21	1	C	0.0226270	-0.0733780	-0.1000340
	2	H	0.1953430	-0.1749860	0.9748560
	3	H	0.9504980	-0.1178840	-0.6765680
	4	H	-0.4247880	0.9236280	-0.2527670
	5	O	-0.9251620	-0.9601450	-0.5439970
	6	H	-0.3638630	-1.3797150	-2.2691360
	7	O	0.2736630	-1.5239670	-2.9922480
	8	Br	1.4192700	-2.7314780	-2.2790000
PostM22	1	C	-0.0179520	0.0455040	0.0004030
	2	H	-0.1759830	0.1026810	1.0657720
	3	H	2.0548510	-0.0964150	-0.5536090
	4	H	-0.1451340	0.9248670	-0.6188270
	5	O	-0.3126120	-1.1645690	-0.5271680
	6	H	-0.1954130	-1.1396530	-1.4836030
	7	O	2.7817100	-0.2369100	-1.1897990
	8	Br	1.9768700	-0.0872830	-2.8028640
CH_3O	1	C	-0.0419720	-0.0664870	0.0099260
	2	H	0.0326360	-0.0376070	1.1020080
	3	H	0.9283660	0.1181730	-0.4627570
	4	H	-0.3396710	-1.0925850	-0.2633030
	5	O	-1.0323320	0.7396580	-0.4772330
CH_2OH	1	C	0.6815210	0.0278930	-0.0669220
	2	H	1.1126860	0.9896560	0.1737740
	3	H	1.2321630	-0.8814410	0.1091210
	4	O	-0.6671610	-0.1255370	0.0221020
	5	H	-1.0966880	0.7287240	-0.0581780
HOCl	1	H	-0.9005760	1.3193070	0.0000000
	2	O	0.0360230	1.0897670	0.0000000
	3	Cl	0.0360230	-0.5904380	0.0000000
HOBr	1	H	-0.9138380	1.6740790	0.0000000

2	O	0.0212520	1.4396430	0.0000000
3	Br	0.0212520	-0.3768920	0.0000000