Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.
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Supporting information

Multi-element (C, H, Cl, Br) stable isotope fractionation as a tool to investigate transformation processes for halogenated hydrocarbons

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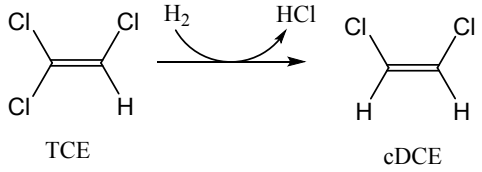
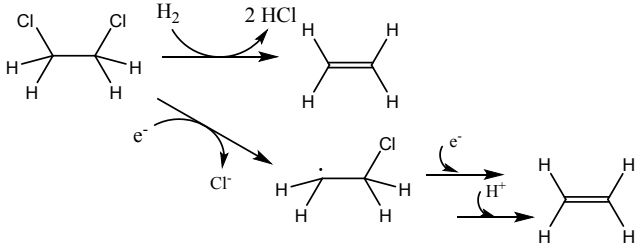
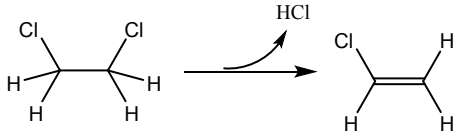
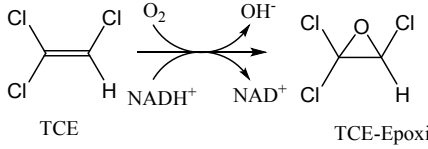
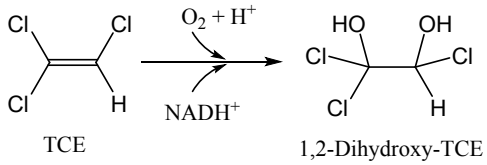
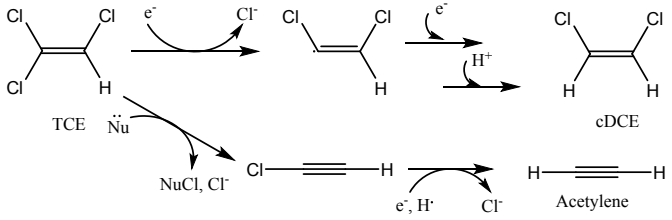
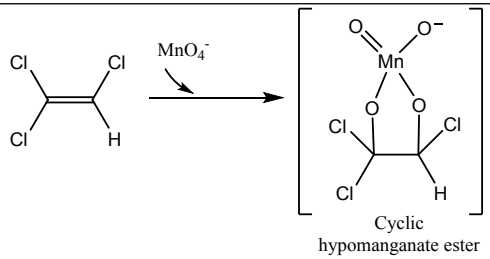
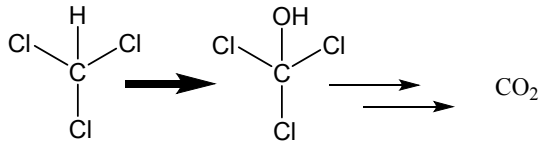
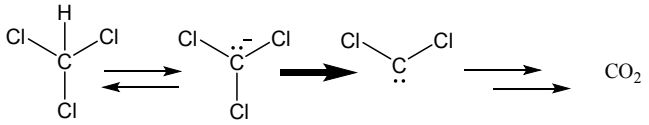
Table S1. Conditions, transformation pathways, and reaction mechanisms for halogenated hydrocarbons

Conditions		**Scheme**	Pathway	Possible Reaction Mechanisms	Ref	Expected isotope effects (1° = primary; 2° = secondary)
Anaerobic OHRB respiration	Reductive dechlorination		Hydrogenolysis (RDase enzymes)	Addition-protonation Addition elimination S_N1 SET	[1,2]	1°: C, Cl 2°: H (?)
			Dihaloelimination – concerted	Addition elimination	[3]	1°: C 2°: Cl, H
			Dihaloelimination – stepwise	SET	[3]	1°: C 2°: Cl, H
Anaerobic OHRB (not respiratory)			Dehydro-dehalogenation		[3]	1°: C, Cl 2°: H
Aerobic	Oxidation			Epoxidation (sMMO, pMMO, T2MO, T4MO	[4–7]	1°: C 2°: Cl, H

				enzymes)		
				Dioxygenation (TDO enzyme)	6,8	1°: C 2°: Cl, H
Engineered remediation strategies	Mineral Reductive dechlorination		Hydrogenolysis (ZVI, Fenton)	Addition elimination SET	9,10	1°: C, Cl 2°: H
			Dihaloelimination (ZVI)	Addition elimination		1°: C, Cl 2°: H
	Permanganate Oxidation		Permanganate Oxidation	Concerted addition	11,12	1°: C 2°: Cl, H
	Persulfate Oxidation		Persulfate Oxidation	$E1_{CB}$ elimination (stepwise elimination)	13	1°: C, Cl 2°: H
	Alkaline hydrolysis		Alkaline hydrolysis			1°: C, Cl 2°: H

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