

Supplementary Material

Kinetics Tables

Supplementary Material Table 1 Compilation of known gas-phase kinetics of mercury

Gas Phase Reaction	Reaction Type ^a	Gas Type, Press	Temp (K)	Rate ($\text{cm}^3 \text{molec}^{-1} \text{s}^{-1}$) ^b [R] = J K ¹ mol ⁻¹ [T] = Kelvin	Reference
Hg(⁶ P ₁) + N ₂ → Hg(⁶ P ₀) + N ₂	Absolute	N ₂ , 1 atm	298	$3.9\text{--}7.1 \times 10^{-12}$	Hall <i>et al.</i> ¹
Hg(⁶ P ₀) + N ₂ → Hg(⁶ S ₀)	Absolute			6.1×10^{-15}	
Hg ⁰ + I ₂ → HgI ₂	Absolute	N ₂ , 1 atm	296 ± 1	$< (1.27 \pm 0.58) \times 10^{-19}$	Raofie <i>et al.</i> ²
	M06-2X/aug-cc-pVTZ-PP	High pressure limit		$3.94 \times 10^{-14} \text{T}^{1.06} \text{e}^{-159080/\text{RT}}$	Auzmendi-Murua <i>et al.</i> ³
Hg ⁰ + I → HgI	RRKM/B3LYP	N ₂ , 1 atm	180-400	$4.0 \times 10^{-13} (\text{T}/298)^{-2.38}$	Goodsite <i>et al.</i> ⁴
Hg ⁰ + Br ₂ → HgBr ₂	Absolute	Air, N ₂ , 1 atm	298 ± 1	$< (9 \pm 2) \times 10^{-17}$	Ariya <i>et al.</i> ⁵
	Absolute	Air, 1 atm	~298	No reaction detected	Sumner <i>et al.</i> ⁶
	Absolute	Air, 1 atm	296	$(6.0 \pm 0.5) \times 10^{-17}$	Liu <i>et al.</i> ⁷
	CCSD(T)/AVTZ	1 atm	298-2000	$1.62^{-9} \text{e}^{-110800/\text{RT}}$	Wilcox and Okano ⁸
	M06-2X/aug-cc-pVTZ-PP	High pressure limit		$4.70 \times 10^{-14} \text{T}^{1.06} \text{e}^{-169190/\text{RT}}$	Auzmendi-Murua <i>et al.</i> ³
Hg ⁰ + BrO → HgBrO	Relative	N ₂ , 1 atm	298	$10^{-15} < k < 10^{-13}$	Raofie and Ariya ⁹
Hg ⁰ + Br → HgBr	Ab initio	N/A, 1 atm		$1.01 \times 10^{-12} \text{e}^{1738/\text{RT}}$	Khalizov <i>et al.</i> ¹⁰
	RRKM/B3LYP	N ₂ , 1 atm	200-300	$3.7 \times 10^{-13} (\text{T}/298)^{-2.76}$	Goodsite <i>et al.</i> ⁴ ; Goodsite <i>et al.</i> ¹¹
	Absolute	N ₂ , 0.26-0.79 atm	243-293	$(1.46 \pm 0.36) \times 10^{-32} [\text{cm}^6 \text{molec}^{-2} \text{s}^{-1}]$	Donohoue <i>et al.</i> ¹²

				$(T/298)^{(-1.86 \pm 1.49)}$	
	CCSD(T)	Ar, 1 atm	260	1.2×10^{-12}	Shepler <i>et al.</i> ¹³
	Relative	Air, N ₂ , 1 atm	298 ± 1	$(3.2 \pm 0.9) \times 10^{-12}$	Ariya <i>et al.</i> ⁵
	Absolute	CF ₃ Br, 0.26 atm	397	$\sim 3 \times 10^{-16} \text{ molec}^{-1} \text{ s}^{-1}$	Greig, G. <i>et al.</i> ¹⁴
	CCSD(T)/AVTZ	1 atm	298-2000	$6.64 \times 10^{-14} (T/298)^{-0.859}$	Wilcox and Okano ⁸
HgBr + Br → HgBr ₂	Absolute	CF ₃ Br, 0.26 atm	397	$\sim 7 \times 10^{-14}$	Greig, G. <i>et al.</i> ¹⁴
	RRKM/B3LYP	N ₂ , 1 atm	180-400	$2.5 \times 10^{-10} (T/298)^{-0.57}$	Goodsite <i>et al.</i> ⁴
	CCSD(T)/AVTZ	1 atm	298-2000	$3.32 \times 10^{-12} (T/298)^{-9.18}$	Wilcox and Okano ⁸
	CCSD(T)/aVTZ	1 atm	298	6.33×10^{-11}	Dibble <i>et al.</i> ¹⁵ ; Wang <i>et al.</i> ¹⁶
HgBr → Hg + Br	CCSD(T)/aVTZ		200 - 320	$(1.6 \pm 0.4) \times 10^{-9} (T/298)^{-(1.86 \pm 1.49)} e^{(-64860 \pm 1670)/RT}$	Dibble <i>et al.</i> ¹⁵
HgBr + Br ₂ → HgBr ₂ + Br	CCSD(T)/AVTZ	1 atm	298-2000	$6.68 \times 10^{-13} e^{-3600/RT}$	Wilcox and Okano ⁸
HgBr + HBr → HgBr ₂ + H	B3LYP/ECP60MDF	1 atm	298-2000	$1.56 \times 10^{-11} e^{-78160/RT}$	Wilcox and Okano ⁸
HgBr + HgBr → (HgBr ₂ + Hg) or Hg ₂ Br ₂	Absolute	CF ₃ Br, 0.26 atm	397	$(2.1 \pm 1.3) \times 10^{-14} \text{ molec}^{-1} \text{ s}^{-1}$	Greig, G. <i>et al.</i> ¹⁴
HgBr + HO ₂ → BrHgHO ₂	CCSD(T)/aVTZ	1 atm	298	8.2×10^{-11}	Dibble <i>et al.</i> ¹⁵ ; Wang <i>et al.</i> ¹⁶
HgBr + NO ₂ → BrHgNO ₂	CCSD(T)/aVTZ	1 atm	298	2.81×10^{-11}	
HgBr + NO ₂ → BrHgONO	CCSD(T)/aVTZ	1 atm	298	5.82×10^{-11}	
HgBr + BrO → BrHgOH	CCSD(T)/aVTZ	1 atm	298	1.09×10^{-10}	
Hg ⁰ + BrCl → Hg ²⁺	Absolute	Air, 1 atm	373	$(2.3 \pm 0.2) \times 10^{-17}$	Qu <i>et al.</i> ¹⁷
Hg ⁰ + ICl → Hg ²⁺	Absolute	Air, 1 atm	373	$(5.7 \pm 0.3) \times 10^{-17}$	

$\text{Hg}^0 + \text{Cl}_2 \rightarrow \text{HgCl}_2$	Absolute	Air, N ₂ , 1 atm	298 ± 1	$(2.6 \pm 0.2) \times 10^{-18}$	Ariya <i>et al.</i> ⁵
	Absolute	Humid air	298	$< 0.4 (13\% \text{ RH}) - 2.5(80\% \text{ RH}) \times 10^{-15}$	Menke and Wallis ¹⁸ ; Schroeder <i>et al.</i> ¹⁹
	Absolute	Air	293-973	5.6×10^{-15}	Sliger <i>et al.</i> ²⁰
	Absolute	N ₂ , 1 atm	297 ± 1	$(1.82 \pm 0.05) \times 10^{-19}$	Yan <i>et al.</i> ²¹
	Absolute	Air, 1 atm	~298	$(2.5 \pm 0.9) \times 10^{-18}$	Sumner <i>et al.</i> ⁶
	Absolute		470-870	0.386 (units?) e ^{-607/RT}	Agarwal <i>et al.</i> ²²
	M06-2X/aug-cc-pVTZ-PP	High pressure limit		$2.76 \times 10^{-14} \text{ T}^{1.20} \text{ e}^{-190430/\text{RT}}$	Auzmendi-Murua <i>et al.</i> ³
$\text{Hg} + \text{Cl}_2 \rightarrow \text{HgCl} + \text{Cl}$	B3LYP/RCEP60 VDZ	1 atm	298 - 2000	$1.02 \times 10^{-10} \text{ e}^{-181000/\text{RT}}$	Wilcox ²³
	QCISD/ CEP-121G	N/A	298 - 2000	$7.51 \times 10^{-11} \text{ e}^{-150590/\text{RT}}$	Krishnakumar and Helble ²⁴
$\text{Hg} + \text{HOCl} \rightarrow \text{HgCl} + \text{OH}$	QCISD/ CEP-121G	N/A	298 - 2000	$4.47 \times 10^{-10} \text{ e}^{-133020/\text{RT}}$	Krishnakumar and Helble ²⁴
	QCISD/RCEP28 DVZ	1 atm	298 - 1500	$1.89 \times 10^{-10} \text{ e}^{-62270/\text{RT}}$	Liu <i>et al.</i> ²⁵
	B3LYP/RCEP60 VDZ	1 atm	298 - 2000	$5.08 \times 10^{-11} \text{ e}^{-153000/\text{RT}}$	Wilcox ²³
$\text{Hg}^0 + \text{HCl} \rightarrow \dots \rightarrow \text{HgCl}_2 (\text{g})$	Absolute	N ₂ , 1 atm	673-1173	$3.65 \times 10^{-14} \text{ e}^{-45400/\text{RT}}$	Widmer <i>et al.</i> ²⁶
$\text{Hg} + \text{HCl} \rightarrow \text{HgCl} + \text{H}$	QCISD(T)/SDD	N/A	298 - 2000	$4.58 \times 10^{-9} \text{ e}^{-333790/\text{RT}}$	Krishnakumar and Helble ²⁴
	QCISD/RCEP28 DVZ	1 atm	298 -	$2.81 \times 10^{-10} \text{ e}^{-372640/\text{RT}}$	Liu <i>et al.</i> ²⁵

			1500		
	B3LYP/RCEP60 VDZ	1 atm	298 -	$3.21 \times 10^{-11} e^{-390000/RT}$	Wilcox ²³
			2000		
HgCl + HCl → HgCl ₂ + H	QCISD/1997	1 atm	298 -	$3.2 \times 10^{-15} e^{-104640/RT}$	Wilcox <i>et al.</i> ²⁷
			2000		
	B3LYP/MHF60	N/A	298 -	$4.13 \times 10^{-11} e^{-104460/RT}$	Krishnakumar and Helble ²⁴
			2000		
HgCl + M → Hg + Cl + M	QCISD/1997	1 atm	298 -	$9.0 \times 10^{-11} e^{-89800/RT}$	Wilcox <i>et al.</i> ²⁷
			2000		
	MP2/CEP-121G	N/A	298 -	$1.92 \times 10^{13} e^{-8912/RT} \text{ cm}^6 \text{ mol}^{-2} \text{ s}^{-1}$	Krishnakumar and Helble ²⁴
			2000		
HgCl + Cl + M → HgCl ₂ + M	MP4/SDD	N/A	298 -	$1.66 \times 10^{12} e^{5030/RT} \text{ cm}^6 \text{ mol}^{-2} \text{ s}^{-1}$	
			2000		
Hg ⁰ + Cl → HgCl	Ab initio	N/A, 1 atm		$1.38 \times 10^{-12} e^{1729/RT}$	Khalizov <i>et al.</i> ¹⁰
	Absolute	N ₂	243-293	$(2.2 \pm 0.5) \times 10^{-32} e^{[(680 \pm 400)(1/T-1/298)]} \text{ cm}^6$ $\text{molec}^{-2} \text{ s}^{-1}$	Donohoue <i>et al.</i> ²⁸
	Absolute, fitted equation	Ar, 0.93 atm	383-443	1.5×10^{-11}	Horne <i>et al.</i> ²⁹
	Relative	Air, N ₂ , 1 atm	298 ± 1	$(1.0 \pm 0.2) \times 10^{-11}$	Ariya <i>et al.</i> ⁵
	Absolute, extrapolated	?	> 873	2.5×10^{-11}	Senior <i>et al.</i> ³⁰
HgCl + HgCl → Hg ₂ Cl ₂	Absolute	Ar, 0.93 atm	383-443	$(3 \pm 2) \times 10^{-10}$	Horne <i>et al.</i> ²⁹
Hg ⁰ + F ₂ → Prod	Absolute	Air, 1 atm	<298	$(1.8 \pm 0.4) \times 10^{-15}$	Sumner <i>et al.</i> ⁶
Hg ⁰ + F → HgF	ab initio	N/A, 1 atm		$9.2 \times 10^{-13} e^{1720/RT}$	Khalizov <i>et al.</i> ¹⁰
Me ₂ Hg + OH → MeHgOH + Me	Relative	Air, 0.92 atm	303	$(1.9 \pm 0.2) \times 10^{-11}$	Niki <i>et al.</i> ³¹

	Estimation			2.72×10^{-13}	Lin and Pehkonen ³²
$\text{Me}_2\text{Hg} + \text{O}_3 \rightarrow ?$	Model estimation			$< 10^{-21}$	Lin and Pehkonen ³² ; Niki <i>et al.</i> ³¹
$\text{Me}_2\text{Hg} + \text{Cl} \rightarrow \text{CH}_3\text{HgCl}$	Relative	N_2 , 0.93 atm	300	$(2.75 \pm 0.30) \times 10^{-10}$	Niki <i>et al.</i> ³¹
$\text{Me}_2\text{Hg} + \text{NO}_3 \rightarrow \text{Hg}^0, \text{HgO(s)}$	Absolute	He, 2.7 - 5.0 hPa	258-358	$3.2 \times 10^{-11} \text{ e}^{(14600 \pm 3300)/\text{RT}}$	Sommar <i>et al.</i> ³³
$\text{Me}_2\text{Hg} + \text{O}(^3\text{P}) \rightarrow \text{HgO}$	Absolute	He, 1 Torr	~294	$(2.5 \pm 0.20) \times 10^{-11}$	Thomsen and Egsgaard ³⁴
$\text{Me}_2\text{Hg} + \text{F} \rightarrow ?$	Relative	H_2 , 4 atm	287	$< (4.7 \pm 0.5) \times 10^{-10}$	Mckeown <i>et al.</i> ³⁵
$\text{Hg}^0 + \text{OH} \rightarrow \text{HgOH}$	Relative	N_2 , 1 atm	283-353	$3.55 \times 10^{-14} \text{ e}^{(2440 \pm 130)/\text{RT}}$	Pal and Ariya ³⁶
	Absolute	Air, 1 atm	298	$< 1.2 \times 10^{-13}$	Bauer <i>et al.</i> ³⁷
	RRKM/B3LYP	N_2 , 1 atm	180-400	$3.2 \times 10^{-13} \times (\text{T}/298)^{-3.06}$	Goodsite <i>et al.</i> ⁴
	Relative	Air, 1 atm	298	$(8.7 \pm 2.8) \times 10^{-14}$	Sommar <i>et al.</i> ³⁸
$\text{Hg}^0(\text{g}) + \text{h}\nu + \frac{1}{2}\text{O}_2 \rightarrow \text{HgO}_{(\text{g/s})}$	Absolute	Air, 1 atm	293	1×10^{-23}	Hall <i>et al.</i> ³⁹
			973	4×10^{-23}	
$\text{Hg}^0 + \text{O}_3 \rightarrow \text{HgO(s)} + \text{O}_2$	Absolute, extrapolated	N_2 , 1 atm	283-323	$8.43 \times 10^{-17} \text{ e}^{-(11700 \pm 270)/\text{RT}}$	Pal and Ariya ³⁶
	Absolute, S/V extrapolated	N_2/O_2 , 1 atm	293	$(3 \pm 2) \times 10^{-20}$	Hall ⁴⁰
	Absolute	Air, 1 atm	~298	$(6.4 \pm 2.3) \times 10^{-19}$	Sumner <i>et al.</i> ⁶
	Absolute, re-plotted data	1 atm	293	4.9×10^{-18}	Schroeder <i>et al.</i> ¹⁹ ; P'yankov ⁴¹
			303	8.4×10^{-18}	
			293	$4.2 \times 10^{-19} (?)$	Slemr ⁴² ; P'yankov ⁴¹
	Absolute	Air, 1 atm, 71% RH	293	1.7×10^{-18}	Schroeder <i>et al.</i> ¹⁹ ;
					Iverfeldt and Lindqvist ⁴³
	QCISD(T)/MP2; TST theory	1 atm	~298	$1.2 \times 10^{-9} \text{ e}^{-176500/\text{RT}}$	Xu <i>et al.</i> ⁴⁴

	Absolute	~ 1 atm	298 ± 2	$(6.2 \pm 1.1) \times 10^{-19}$	Snider <i>et al.</i> ⁴⁵
Hg + O ₃ → HgO + O ₂	QCISD/RCEP28 DVZ	1 atm	298 - 1500	$2.39 \times 10^{-10} e^{-135170/RT}$	Liu <i>et al.</i> ²⁵
Hg + NO → HgO + N	QCISD/RCEP28 DVZ	1 atm	298 - 1500	$2.19 \times 10^{-11} e^{-675140/RT}$	
Hg ⁰ + NO ₂ → ?	Absolute	N ₂ , 1 atm	293	$(2.8 \pm 0.5) \times 10^{-35} \text{ cm}^6 \text{ molec}^{-2} \text{ s}^{-1}$, 2 nd order in [NO ₂]	Hall <i>et al.</i> ⁴⁰
	Absolute	Air, 1 atm	295 ± 1	$(3.5 \pm 0.5) \times 10^{-35} \text{ cm}^6 \text{ molec}^{-2} \text{ s}^{-1}$, 2 nd order in [NO ₂]	Snider and Ariya ⁴⁶
Hg ⁰ + NO ₃ → HgO + NO ₂	S/V extrapolation	N ₂ , 5.4 - 9.5 hPa	294 ± 2	$< 4 \times 10^{-15}$	Sommar <i>et al.</i> ³³
	Relative	Air, 1 atm	~298	$< 7 \times 10^{-15}$, $< 1.3 \times 10^{-14}$, 3×10^{-14}	Sumner <i>et al.</i> ⁶
Hg ⁰ + H ₂ O ₂ → ?	Absolute	N ₂	293	$< 8.5 \times 10^{-19}$	Tokos <i>et al.</i> ⁴⁷

^a ab initio, semi-empirical, relative, absolute, extrapolated

^b unless otherwise stated

Supplementary Material Table 2 Aqueous phase kinetics of mercury

Aqueous Phase Reaction	Type of study	Environment <i>pH</i>	Temp (<i>K</i>)	Rate ($M^{-1} s^{-1}$) ^a	Reference
$Hg^0(aq) + O_3 + H_2O \rightarrow Hg^{2+} + OH^- + O_2$	Lab, relative	Water, pH=4.5-9.5	~293 (T-ind)	$(4.7 \pm 2.2) \times 10^7$	Munthe, 1992 ⁴⁸
$Hg(OH)_2(aq) + h\nu \rightarrow Hg^0 + H_2O$	Lab, absolute	pH = 7	293 ± 0.5	$1.2 \times 10^{-4} s^{-1}$	Xiao <i>et al.</i> , 1995 ⁴⁹
$Hg^{2+}(aq)/humic\ acid + h\nu \rightarrow Hg(g)$	Lab, absolute	Water/air	Ambient	$2 \times 10^{-2} s^{-1}$	
$HgCl_2 + e^- \rightarrow Cl^- + HgCl$	Avg'd Lit. Cit.	pH = 5	Ambient	4.0×10^{10}	Buxton <i>et al.</i> , 1988 ⁵⁰
$HgBr_2 + e^- \rightarrow Br^- + HgBr$	Avg'd Lit. Cit.		Ambient	3.7×10^{10}	
$HgI_2 + e^- \rightarrow I^- + HgI$	Avg'd Lit. Cit.		Ambient	3.0×10^{10}	
$Hg(CN)_2 + e^- \rightarrow CN^- + HgCN$	Avg'd Lit. Cit.		Ambient	1.4×10^{10}	
$Hg(SCN)_2 + e^- \rightarrow SCN^- + HgSCN$	Lit. Cit.		Ambient	4.5×10^{10}	
$Hg(EDTA)^{2-} + e^- \rightarrow Products$	Avg'd Lit. Cit.	pH = ~ 11.5	Ambient	$2.1, 5.1 \times 10^9$	
$Hg^{2+} + e^- \rightarrow Hg^{(I)}$	Avg'd Lit. Cit.		Ambient	7.1×10^9	Zhang, 2006 ⁵¹ ; Buxton <i>et al.</i> , 1988 ⁵⁰
$H + Hg_2^{2+} \rightarrow H^+ + Hg_2^+$	Lit. Cit.	pH = 1.0	Ambient	4.7×10^9	
$H + Hg^{2+} \rightarrow H^+ + Hg^+$	Avg'd Lit. Cit.	pH = 1.5	Ambient	2.0×10^9	
$H + Hg(OH)_2 \rightarrow H_2O + HgOH$	Avg'd Lit. Cit.	pH = 7	Ambient	2.4×10^9	
$H + HgCl_2 \rightarrow HCl(aq) + HgCl$	Lit. Cit.	pH = 1	Ambient	1.0×10^{10}	
$H + HgI_2 \rightarrow HgI_2(H)$	Lit. Cit.		Ambient	1.5×10^{10}	
$OH + HgCl \rightarrow OH^- + HgCl^+$	Lit. Cit.	pH = 5	Ambient	$\sim 1 \times 10^{10}$	
$OH + HgBr_2 \rightarrow Br + HgBrOH$	Lit. Cit.	pH = 5	Ambient	$> 9 \times 10^8$	
$OH + HgCN \rightarrow products$	Lit. Cit.		Ambient	3.1×10^9	
$Hg^0(aq) + OH \rightarrow Hg^+ + OH^-$	Relative	Water, pH = 7.9	295 ± 1	$(2.4 \pm 0.3) \times 10^9$	Gardfeldt <i>et al.</i> , 2001 ⁵²
	Lab, absolute	Water, pH = 5.6 - 5.9	298 ± 2	2.0×10^9	Lin and Pehkonen, 1997 ⁵³

	Field	Mid latitudes, June (noon)	Ambient	1.0×10^9	Hines and Brezonik, 2004 ⁵⁴
$\text{Hg}^+(\text{aq}) + \text{OH}^- \rightarrow \text{Hg}^{2+} + \text{OH}^-$	Lit. Cit.		Ambient	1×10^{10}	Zhang, 2006 ⁵¹
$\text{HgOH} + \text{OH}^- \rightarrow \text{Hg}(\text{OH})_2$	Lit. Cit.		Ambient	1×10^{10}	
$\text{HgOH} + \text{H}_2\text{O} + \text{O}_2 \rightarrow \text{Hg}(\text{OH})_2 + \text{H}^+ + \text{O}_2^-$	Lit. Cit.		Ambient	1×10^9	
$\text{HO}_2 + \text{Hg}^{2+} \rightarrow \text{Hg}^+ + \text{O}_2 + \text{H}^+$	Lab	pH = 3.9	298 ± 2	1.7×10^4	Pehkonen and Lin, 1998 ⁵⁵
	Lab	pH = 3.9	298 ± 2	1.1×10^4 (chloride present)	
$\text{Hg}(\text{HSO}_3)^-(\text{aq}) \rightarrow \text{Hg}^0(\text{aq}) + \text{S}^{(\text{VI})}$	Lit. Cit.			$4 \times 10^{-6} \text{ s}^{-1}$	Lin and Pehkonen, 1997 ⁵³ ; Munthe <i>et al.</i> , 1991 ⁵⁶
$\text{HgSO}_3(\text{aq}) \rightarrow \text{Hg}^0(\text{aq}) + \text{S}^{(\text{VI})}$	Lab	pH = 3.0 and pH = 4.8, excess SO_3^{2-}	299 ± 2	0.6 s^{-1}	Munthe <i>et al.</i> , 1991 ⁵⁶
	Lab, absolute	pH = 3.0, excess Hg^{2+}	279 - 308	$T \times 2.083 \times 10^{10} \exp[(8.2 \pm 0.7) - (1.26 \pm 0.02) \times 10^4/T]$ s^{-1}	Van Loon <i>et al.</i> , 2000 ⁵⁷
	Lab, absolute	pH = 1.0, excess Hg^{2+}	279 - 308	$T \times 2.083 \times 10^{10} \exp[(9.7 \pm 0.6) - (1.29 \pm 0.01) \times 10^4/T]$ s^{-1}	
$\text{Hg}(\text{SO}_3)_2^{2-}(\text{aq}) \rightarrow \text{Hg}^0(\text{aq}) + \text{S}^{(\text{VI})}$	Lit. Cit.	pH = 3.0 and pH = 4.8, excess SO_3^{2-}		$< 10^{-4} \text{ s}^{-1}$	Lin and Pehkonen, 1997 ⁵³ ; Munthe <i>et al.</i> , 1991 ⁵⁶
$\text{Hg}(\text{OH})_2(\text{aq}) \rightarrow \text{Hg}^0(\text{aq}) + \text{prod.}$	Lit. Cit.	Midday, at 60°N latitude		$3 \times 10^{-7} \text{ s}^{-1}$	Lin and Pehkonen, 1999 ³²
$\text{MeHg} + \text{OH}^- \rightarrow \text{products}$	Lab	pH = 6.2-8.2	293	1.2×10^9	Zepp <i>et al.</i> , 1987 ⁵⁸
$\text{Hg}^{2+}(\text{aq}) \rightarrow \text{MeHg}(\text{aq})$	Field	Estuarine sediment	Ambient	$1.4 - 144 \times 10^8 \text{ s}^{-1}$	Jonssen <i>et al.</i> , 2012 ⁵⁹
	Lab	pH $\approx$ 7.5, methylating	304	Init. methylation rate:	Graham <i>et al.</i> , 2012 ⁶⁰

		bacteria		0.60 - 21.8 pM min ⁻¹	
$\text{Hg}^{2+}(\text{aq}) + \text{DOM} \rightarrow \text{MeHg}(\text{aq})$	Lab	pH = 6.8, bacteria	311	Hg^{2+} was most bioavailable < 24 h after addition to DOM	Chiasson-Gould <i>et al.</i> , 2014 ⁶¹
$\text{Hg}^{2+} + h\nu \rightarrow \text{Hg}^0(\text{aq})$	Field	Lake water, daylight radiation	Ambient	2.4 - 9 times $\text{Hg}^0(\text{aq})$ production than dark: 1.6%/h	Amyot <i>et al.</i> , 1994 ⁶²
	Field	Lake water	Ambient	UV-A: $7.76 \times 10^{-5} \text{ s}^{-1}$ UV-B: $8.91 \times 10^{-5} \text{ s}^{-1}$	O'Driscoll <i>et al.</i> , 2006 ⁶³
		River water		UV-A: $1.78 \times 10^{-4} \text{ s}^{-1}$ UV-B: $1.81 \times 10^{-4} \text{ s}^{-1}$	
	Field	Coastal water, midday	Ambient	$4.4 - 11 \times 10^{-4} \text{ s}^{-1}$	Whalin and Mason, 2006 ⁶⁴
	Field	Fresh water, midday	Ambient	$2.9 - 11 \times 10^{-4} \text{ s}^{-1}$	
$\text{Hg}(\text{NO}_3)_2(\text{aq}) + h\nu \rightarrow \text{Hg}^0(\text{aq})$	Lab	Milli-Q water, pH = 4	303	$1 \times 10^{-5} \text{ s}^{-1}$	Zhang <i>et al.</i> , 2012 ⁶⁵
$\text{Hg}^{2+} + \text{Fe(III)} + h\nu \rightarrow \text{Hg}^0(\text{g})$	Field	Freshwater, UV exposed		$0.3 - 0.6 \times 10^{-4} \text{ s}^{-1}$	Zhang and Lindberg, 2001 ⁶⁶
$\text{Hg}^{2+} + \text{MerA bacteria} \rightarrow \text{Hg}^0(\text{aq})$	pH = 7.0	MerA, intact cells, pH = 7.0	Ambient	$8.2 - 20.6 \text{ nmol Hg}^{2+} \text{ min}^{-1} \text{ mg protein}^{-1}$	Philippidis <i>et al.</i> , 1991 ⁶⁷
$\text{Hg}^0(\text{aq}) + h\nu \rightarrow \text{Hg}^{2+}$	Field	Coastal water, midday	Ambient	$2.6 - 5.3 \times 10^{-4} \text{ s}^{-1}$	Whalin and Mason, 2006 ⁶⁴
	Field	Fresh water, midday	Ambient	$8 - 15 \times 10^{-4} \text{ s}^{-1}$	
	Field	Brackish water, Vis light	288	$0.25 \times 10^{-4} \text{ s}^{-1}$	Lalonde <i>et al.</i> , 2004 ⁶⁸
	Field	Brackish water, UV light	288	$1.7 - 1.9 \times 10^{-4} \text{ s}^{-1}$	
	Field	Saline water, UV	Ambient	$(1.9 \pm 0.3) \times 10^{-4} \text{ s}^{-1}$	Lalonde <i>et al.</i> , 2001 ⁶⁹
$\text{Hg}^0(\text{aq}) \rightarrow \text{Hg}^{2+}(\text{aq})$	Field	Saline water, dark	Ambient	$0.17 \times 10^{-4} \text{ s}^{-1}$	
	Lab	HPLC water, dark	Ambient	$6 \times 10^{-7} \text{ s}^{-1}$	Hines and Brezonik, 2004 ⁵⁴
	Field	Lake water, dark	Ambient	$6 \times 10^{-6} \text{ s}^{-1}$	

	Field	Brackish water, dark	288	not statistically significant	Lalonde <i>et al.</i> , 2004 ⁶⁸
$\text{Hg}^0(\text{aq}) + h\nu \rightarrow \text{Hg}^{2+}(\text{HgO?})$	Field	Lake water, Hg lamp	Ambient	$1.1 - 2.1 \times 10^{-4} \text{ s}^{-1}$	Hines and Brezonik, 2004 ⁵⁴
$\text{Hg}^0(\text{aq}) + \text{Cl}^- + h\nu \rightarrow \text{Hg}^{2+}(\text{aq})$	Lab	Seawater, River water + 0.5 M Cl^-	Ambient	$0.28 - 1.1 \times 10^{-4} \text{ s}^{-1}$	Amyot <i>et al.</i> , 1997 ⁷⁰
	Field	Lake water	Ambient	$1.53 \times 10^{-3} \text{ s}^{-1}$	Hines and Brezonik, 2004 ⁵⁴
	Field	Fresh water	Ambient	$1.6 \times 10^{-4} \text{ s}^{-1}$	Lalonde <i>et al.</i> , 2001 ⁷¹
$\text{Hg}^0(\text{aq}) + \text{Cl}^- + h\nu(\text{UV}) + \text{benzoquinone} \rightarrow \text{Hg}^{2+}$	Field	Natural water spiked	298	$1.7 \times 10^{-4} \text{ s}^{-1}$	
$\text{Hg}^0(\text{aq}) + \text{bacteria exudates} + \text{Cl}^- \rightarrow \text{Hg}^{2+}$	Lab	Spiked water	277 ± 2	Dark reaction; 40% decrease in $\text{Hg}^0(\text{aq})$ after 3.5 h	Poulain <i>et al.</i> , 2007 ⁷²
$\text{Hg}^0(\text{aq}) + \text{semiquinones} + \text{Cl}^- \rightarrow \text{Hg}^{2+}$	Lab	Artificial water, 0.5 M HCl	Ambient	$10 - 20 \times 10^{-4} \text{ s}^{-1}$	Whalin and Mason, 2006 ⁶⁴ ; Lalonde <i>et al.</i> , 2001 ⁷¹
$\text{Hg}^0(\text{aq}) + \text{fulvic acid} \rightarrow \text{Hg}^{2+}$	Lab	Artificial water	Ambient	$0.28 \times 10^{-4} \text{ s}^{-1}$	
$\text{Hg}^0(\text{aq}) + \text{DOM} \rightarrow \text{Hg}^{2+}(\text{aq})$	Lab	pH = 7, dark, anoxic	~295	$1.6 - 15.3 \times 10^{-4} \text{ s}^{-1}$	Zheng <i>et al.</i> , 2011 ⁷³
$\text{Hg}^0(\text{aq}) + \text{UV} + \text{DOC} \rightarrow \text{Hg}^{2+}$	Field	Lake water	Ambient	$0.7 \times 10^{-4} \text{ s}^{-1}$	Lalonde <i>et al.</i> , 2001 ⁷¹
$\text{Hg}^0(\text{aq}) + \text{Fe}^{3+} \rightarrow \text{Hg}^{2+}$	Field	Freshwater, dark (prev. UV expos.)		$0.6 - 0.8 \times 10^{-4} \text{ s}^{-1}$	Zhang and Lindberg, 2001 ⁷⁴
$\text{Hg}^0(\text{aq}) + \text{NO}_3^- + \text{octanol} + h\nu \rightarrow \text{Hg}^{2+}$	Lab	Milli-Q water	Ambient	$1.4 \times 10^{-4} \text{ s}^{-1}$	Hines and Brezonik, 2004 ⁵⁴
$\text{Hg}^0(\text{aq}) + \text{Br}_2 \rightarrow \text{prod.}$	Lab	pH = 2	295 ± 1	0.20 ± 0.03	Wang and Pehkonen, 2004 ⁷⁵
$\text{Hg}^0(\text{aq}) + \text{HOBr} \rightarrow \text{prod.}$	Lab	pH = 6.8		0.28 ± 0.02	
$\text{Hg}^0(\text{aq}) + \text{OBr}^- \rightarrow \text{prod.}$	Lab	pH = 11.7		0.27 ± 0.04	
$\text{Hg}^0(\text{aq}) + \text{HOCl} + \text{H}^+ \rightarrow \text{Hg}^{2+} + \text{Cl}^- + \text{H}_2\text{O}$	Lab	pH = 6.5 - 8.5	297 ± 1	$(2.09 \pm 0.06) \times 10^6$	Lin and Pehkonen, 1998 ⁷⁶

$\text{Hg}^0(\text{aq}) + \text{OCl}^- + \text{H}_2\text{O} \rightarrow \text{Hg}^{2+} + \text{Cl}^- + 2\text{OH}^-$	Lab	pH = 6.5 - 8.5	297 ± 1	$(1.99 \pm 0.05) \times 10^6$	
$\text{Hg}^0(\text{aq}) + \text{H}_2\text{O}_2 \rightarrow \text{HgO}(\text{s}) + \text{Hg}^{2+} + \text{H}_2\text{O}$	Lab	pH = 1.3, pH = 3.3		< 150	Munthe and McElroy, 1992 ⁷⁷
$\text{Hg}^0(\text{aq}) + 2\text{-mercaptopropionic acid} \rightarrow \text{Hg}^{2+}(\text{aq})$	Lab	pH = 7, dark anoxic conditions	Ambient	$(3.6 \pm 0.3) \times 10^{-5} \text{ s}^{-1}$	Zheng <i>et al.</i> , 2013 ⁷⁸
$\text{Hg}^0(\text{aq}) + \text{cysteine} \rightarrow \text{Hg}^{2+}(\text{aq})$	Lab	pH = 7, dark anoxic conditions	Ambient	$(1.7 \pm 0.3) \times 10^{-5} \text{ s}^{-1}$	
$\text{Hg}^0(\text{aq}) + \text{glutathione} \rightarrow \text{Hg}^{2+}(\text{aq})$	Lab	pH = 7, dark anoxic conditions	Ambient	$(2.2 \pm 0.3) \times 10^{-5} \text{ s}^{-1}$	
$\text{HgS}_2^{2-}(\text{aq}) + h\nu \rightarrow \text{HgS}(\text{s}) + \text{S}^{2-}(\text{aq}) \rightarrow \text{Hg}^0(\text{g})$	Lab		Ambient	Not significant	Xiao <i>et al.</i> , 1994 ⁷⁹ ; Zhang, 2006 ⁵¹
$\text{Hg}^{2+}(\text{aq}) + \text{cysteine}(\text{aq}) + h\nu \rightarrow \text{Hg}^0(\text{g})$	Lab	pH = 3.6	294 ± 1	$1.3 \times 10^{-5} \text{ s}^{-1}$	Zheng and Hintelmann, 2010 ⁸⁰
$\text{Hg}^{2+}(\text{aq}) + \text{serine}(\text{aq}) + h\nu \rightarrow \text{Hg}^0(\text{g})$	Lab	pH = 3.8	294 ± 1	$1.78 \times 10^{-4} \text{ s}^{-1}$	
$\text{Hg}^{2+}(\text{aq}) + 2\text{RS}^-(\text{aq}) \rightleftharpoons \text{Hg}(\text{SR})_2(\text{aq}) + h\nu \rightarrow \text{Hg}^0(\text{g}) + \text{RS-SR}(\text{aq})$	Lab, absolute	pH = 7	296 ± 2	$(2.0 \pm 0.2) \times 10^{-7} \text{ s}^{-1}$ (1-propanethiol) $(1.4 \pm 0.1) \times 10^{-7} \text{ s}^{-1}$ (1-butanethiol) $(8.3 \pm 0.5) \times 10^{-8} \text{ s}^{-1}$ (1-pentanethiol)	Si and Ariya, 2011 ⁸¹

$\text{Hg}^{2+}_{(\text{aq})} + \text{DCA}_{(\text{aq})} + h\nu \rightarrow \text{Hg}^0(\text{g})$	Lab, absolute	pH = 3, absence of Cl^- and O_2	296 ± 2	$(2.0 \pm 0.3) \times 10^{-17}$ (oxalic acid) $(8 \pm 1) \times 10^{-18}$ (malonic acid) $(4.7 \pm 0.8) \times 10^{-18}$ (succinic acid)	Si and Ariya, 2008 ⁸²
$\text{Hg}^{2+}_{(\text{aq})} + \text{DOM} \rightarrow \text{Hg}^0_{(\text{aq})}$	Lab	pH = 7, dark, anoxic	~295	$6.13 - 15.1 \times 10^{-4} \text{ s}^{-1}$	Zheng <i>et al.</i> , 2011 ⁷³
$\text{FeOH}^+_{(\text{aq})} + \text{Hg}(\text{OH})_2(\text{aq}) \rightarrow \text{Fe}(\text{OH})_2^+ + \text{OH}^- + \text{Hg}^+(\text{g})$	Lab, model	Water, pH = 6.3 - 8.1	293 - 296	1.20×10^2	Amirbahman <i>et al.</i> , 2013 ⁸³

^a unless otherwise stated

Supplementary Material Table 3 Inter-phase (heterogeneous/surface) kinetics and emission rates of mercury

Surfaces	Type of expt.	Interface	Temp (K)	Rates/rate constants/results;	Reference
Hg ⁰ (g) → Hg (ads)	Absolute	N ₂ , 1 atm, N ₂ /Teflon wall (s/v=0.58 cm ⁻¹)	293	4.5 × 10 ⁻⁶ s ⁻¹	Hall 1995 ⁴⁰
			323	1.7 × 10 ⁻⁵ s ⁻¹	
			348	3.0 × 10 ⁻⁵ s ⁻¹	
	Absolute	Air, 1 atm, air/carbon	293	90 - 120 × 10 ⁻⁴ s ⁻¹	Hall <i>et al.</i> , 1995 ³⁹
			373 - 523	1.3 - 5.0 × 10 ⁻⁴ s ⁻¹	
			573	~ 0 s ⁻¹	
	Absolute	Air, 1 atm, air/fly ash	293	8.1 × 10 ⁻³ s ⁻¹	
			373 - 523	1.12 - 2.72 × 10 ⁻³ s ⁻¹	
			573	6.8 - 7.7 × 10 ⁻⁴ s ⁻¹	
	Lab	Air/unburned carbon from fly ash	293, 313	More mercury adsorption at 20 °C than 40 °C	Li <i>et al.</i> , 2002 ⁸⁴
	Model/Field data	Air/Forest canopy (summer)	Ambient	0.12 cm s ⁻¹	Lindberg <i>et al.</i> , 1992 ⁸⁵
		Air/Forest canopy (winter)		0.006 cm s ⁻¹	
	Field study	Air/ground dry deposition (Arctic)	Ambient	0.1 cm s ⁻¹ (particulate; Hg(p)) 0.5 cm s ⁻¹ (Hg ²⁺ (g))	Schroeder <i>et al.</i> , 1998 ⁸⁶
	Field study	Air/snow/barren ground (Arctic)	Ambient	12.5 ± 2.5 pmol m ⁻² h ⁻¹	
	Lab	N ₂ /Gold	411	25 nm thick Au sheet absorbs for 33 min vs. 5 min for 2.5 nm sheet. Hg diffuses into Au film.	Turchi, 2000 ⁸⁷

	Lab	Simulated flue gas/ sulfur impregnated activated carbon	423	Order of enhancing adsorption: NO > HCl > O ₂ > SO ₂ ; SO ₂ + O ₂ inhibited ads.	Hsi and Chen, 2012 ⁸⁸
	Lab	N ₂ + O ₂ /activated carbon + 20% H ₂ SO ₄	473	Ads. capacity exceeded 500 mg (g Hg) ⁻¹	Morris <i>et al.</i> , 2012 ⁸⁹
	Lab	N ₂ + O ₂ /activated carbon	363-424	O ₂ enhanced the adsorption capacity of activated carbon	Karatza <i>et al.</i> , 2013 ⁹⁰
	Lab	Simulated flue gas/ KI-impregnated bamboo charcoal	413, 453	> 99% capture, NO and SO ₂ inhibit capture	Tan <i>et al.</i> , 2012 ⁹¹
Hg ⁰ /HgF ₂ /HgNO ₃ (aq) + hv → Hg (l)	Lab, Hg lamp	Water/TiO ₂ surface	298	90% conversion after 40 min irradiation. Lower pH, less reduction	Habibi <i>et al.</i> , 2003 ⁹² ; Zhang, 2006 ⁵¹
Hg (l) + Δ → Hg ⁰ (g)		TiO ₂ surface/N ₂ flow	423	Removes Hg ^(l) in 1 hour	
Hg ⁰ (g) + H ₂ O (g) + O ₂ (g) + hv → HgO (s)	Lab	Air/TiO ₂ surface, differential bed reactor	297 - 408	k=Ae ^{-(Es-λ)/RT} d[Hg]/dt = k[Hg] ^(1.4±0.1) [J _{UV}] ^(0.35±0.05)	Lee <i>et al.</i> , 2004 ⁹³
	Lab	Humid air/TiO ₂ surface	298	Surface mechanism developed, removal rate incr. with humidity, Hg removal < 80%, > 30%	Rodriguez <i>et al.</i> , 2004 ⁹⁴
	Lab	Humid air/SiO ₂ -TiO ₂ surface	316	L-H mech., removal rate decreases with humidity, up to 95% removal when dry.	Li and Wu, 2007 ⁹⁵
HgCl ₂ (aq) + dodecyl sulfate (DS) + hv → Hg ⁺	Lab	Water/TiO ₂ surface, pH = 6	295	97% reduction in 6 min	Hegyi and Horvath, 2004 ⁹⁶ ; Zhang, 2006 ⁵¹

HgCl ₂ (aq) + hv + cetyltrimethylammonium (CTA ⁺) → Hg ⁺	Lab	Water/TiO ₂ surface, pH = 6	295	99% reduction in 25 min	
HgCl ₂ (aq) + hv + arginine → Hg ⁺	Lab	Water/TiO ₂ surface	Ambient	arginine binds Hg ²⁺ to TiO ₂ , facilitates charge transfer. 99.9% removal in 128 min	Skubal and Meshkov, 2002 ⁹⁷
HgCl ₂ (aq) + hv (UV) → Hg ⁰ (aq) + 2Cl ⁻	Lab	Water/TiO ₂ semiconductor	293 ± 5	E=0.41 V, poss. Catalytic TiO ₂ action, initial rate oxidation=0.051[Hg] ^{1/2}	Prairie <i>et al.</i> , 1993 ⁹⁸
Hg ⁰ (g) + H ₂ O ₂ (ads) + hv → Hg ²⁺	Field study	Air/snow pack	267	5-fold increase in Hg ⁰ (g) deposition with H ₂ O ₂ -spiked snow	Lahoutifard <i>et al.</i> , 2006 ⁹⁹
Hg (I/II) _g → Hg (I/II)(ads)	Field study	Air/snow; dry dep.	Ambient	1 cm s ⁻¹	Lindberg <i>et al.</i> , 2002 ¹⁰⁰
Hg ²⁺ (ads) → Hg ²⁺ (snowpack)	Field study	Snow air/Snow vertical diffusion	238-260	5.8 - 7.0 pg m ⁻² h ⁻¹	Ferrari <i>et al.</i> , 2004 ¹⁰¹
Hg (ads, II) + hv → Hg ⁰ (g)	Field study	Snow/air	Ambient	20% reduction loss in 3 h	Ariya <i>et al.</i> , 2004 ¹⁰²
	Field study	Snow/air	< 260	> 40% reduction loss in 24 h	Lalonde <i>et al.</i> , 2003 ¹⁰³
	Field study	Snow/air	< 273	6.7 × 10 ⁻⁵ s ⁻¹ , 1.9 pmol m ⁻² h ⁻¹ . Reduction enhanced by H ₂ O (l)	Fain <i>et al.</i> , 2007 ¹⁰⁴
	Field study	Air/melted snow	277	2.2 - 29 × 10 ⁻⁵ s ⁻¹	Mann <i>et al.</i> , 2014 ¹⁰⁵
	Lit. Cit. Field study	Temperate, boreal soil volatilization	Ambient	55 pmol m ⁻² h ⁻¹	Grigal, 2002 ¹⁰⁶ ; Zhang and Lindberg
	Lit. Cit. Field study	Contaminated soil volatilization	Ambient	~6500 pmol m ⁻² h ⁻¹	1999 ¹⁰⁷

	Lab	Air/Coal fly ash, solar radiation (400 W m ⁻²)	Ambient	12.2 - 18.8 % h ⁻¹ (similar rates for reaerosolized soluble components of ash)	Tong <i>et al.</i> , 2014 ¹⁰⁸
	Lab	Air/synthetic aerosols, solar radiation (400 W m ⁻²)	Ambient	9.2 ± 1.5 % h ⁻¹ (carbon black) ± 5.7 % h ⁻¹ (adipic acid) 2.4 % h ⁻¹ (levoglucosan)	64.8 17.5 ±
	Lab	Air/synthetic aerosols, solar radiation (400 W m ⁻²)	Ambient	19.8 ± 2.2 % h ⁻¹ (NaCl) 1.5 % h ⁻¹ (NaCl and FeCl ₃) 2.6 % h ⁻¹ (NaCl and FeCl ₂)	2.6 ± 12.2 ± Tong <i>et al.</i> , 2013 ¹⁰⁹
Hg ⁰ (g) + hν → Hg (ads, II)	Lab study, Xe-lamp	Air/snow	261 - 269	5.0 - 6.9 × 10 ⁻⁵ s ⁻¹	Dommergue <i>et al.</i> , 2007 ¹¹⁰
	Field study	Air/melted snow	277	2.5 - 4.7 × 10 ⁻⁵ s ⁻¹	Mann <i>et al.</i> , 2014 ¹¹¹
Hg (g) → Hg (ads, II)	Lit. Cit. Field study	Throughfall + litterfall	Ambient	22 pmol m ⁻² h ⁻¹	Grigal, 2002 ¹⁰⁶ ;
		Precipitation	Ambient	5.8 pmol m ⁻² h ⁻¹	Zhang and Lindberg 1999 ¹⁰⁷
Hg ⁰ /Hg(CH ₃) ₂ → Hg ⁰ (g)/Hg(CH ₃) ₂ (g)	Avg. Lit. Cit. Field studies	Soil/air	Ambient	< 1 nmol m ⁻² h ⁻¹	Schlüter, 2000 ¹¹²
Hg(ads, 0, II) → Hg (ads, 0, II)	Lit. Cit. Field study	Soil sequestration	Ambient	2.9 pmol m ⁻² h ⁻¹	Grigal, 2002 ¹⁰⁶ ; Zhang and Lindberg 1999 ¹⁰⁷
Hg ⁰ (soil) → Hg ⁰ (g)	Model/Field data	Forest soil/air	Ambient	250 pmol m ⁻² h ⁻¹	Lindberg <i>et al.</i> , 1992 ⁸⁵
Hg ²⁺ [Cl ⁻ /NO ₃ ⁻] + surface sediment → Hg ⁰ (aq)	Field	Lake water/sediment, pH = 6	~298	(1.6 - 10) × 10 ⁻⁷ s ⁻¹	Peretyazhko <i>et al.</i> , 2006 ¹¹³

$\text{Hg}^0(\text{aq}) \rightarrow \text{Hg}^0(\text{g})$	Model fit, empirical data	Water/air	293	5.7 $\text{pmol m}^{-2} \text{h}^{-1}$ loss	Hines and Brezonik, 2004 ⁵⁴
	Field	Water/air (East Atlantic: 0-50 °N)	Ambient	9.5 $\text{pmol m}^{-2} \text{h}^{-1}$ loss (Nov.) 0.5 $\text{pmol m}^{-2} \text{h}^{-1}$ loss (May)	Kuss <i>et al.</i> , 2011 ¹¹⁴
	Field	Water/air (East Atlantic: 60-63 °N)	Ambient	2.1 $\pm$ 1.8 $\text{pmol m}^{-2} \text{h}^{-1}$ loss (July)	Andersson <i>et al.</i> , 2011 ¹¹⁵
	Field	Water/air (West Atlantic: 0-45 °N)	Ambient	10 - 34 $\text{pmol m}^{-2} \text{h}^{-1}$ loss (June-Oct)	Soerensen <i>et al.</i> , 2013 ¹¹⁶
$\text{Hg}^0(\text{aq}) + \text{h}\nu \rightarrow \text{Hg}^0(\text{g})$	Lab study	River water + 0.5 M Cl^- /air	Ambient	0.2 $\times 10^{-4} \text{s}^{-1}$	Amyot <i>et al.</i> , 1997 ⁷⁰
		Seawater/air		0.3 $\times 10^{-4} \text{s}^{-1}$	
$\text{Hg}^0(\text{ads}) + \text{Br} \rightarrow \text{HgBr}$	Field study	In snow (20 - 60 cm deep)	261-265	8 $\times 10^{-13} \text{cm}^3 \text{molec}^{-1} \text{s}^{-1}$	Fain <i>et al.</i> , 2006 ¹¹⁷
$\text{Hg}^0(\text{g}) + \text{Cl}_2(\text{g}) \rightarrow (\text{HgCl})_n(\text{aq/s})$	Lab	Air/surface, p = 0.95 atm	525	50 second reaction	Medhekar <i>et al.</i> , 1979 ¹¹⁸
	Lab	Air/water	~298	No homogeneous reaction. Heterogeneous interactions occur.	Skare and Johansson, 1992 ¹¹⁹
	Lab	Air/water + sulfite, pH = 4.7, pH = 5.7	298	(6.1 $\pm$ 0.8) $\times 10^9 \text{M}^{-1} \text{s}^{-1}$	Roy and Rochelle, 2004 ¹²⁰
$\text{Hg}^0(\text{g}) + \text{Cl}_2(\text{g}) \rightarrow \text{HgCl}_2(\text{g})$	Lab	Air/Au surface	448 - 498	40 - 60% oxidation, k $\sim 10^{-8} \text{cm}^3 \text{molec}^{-1} \text{s}^{-1}$ (473 K), Langmuir-Hinshelwood mechanism proposed	Zhao <i>et al.</i> , 2006 ¹²¹
$\text{Hg}^0(\text{g}) + \text{Cl}_2(\text{aq}) \rightarrow \text{Hg}^{2+} + 2\text{Cl}^-$	Absolute	Water + NaOCl, pH = 9.0 - 11.1	298	1.7 $\times 10^{15} \text{M}^{-1} \text{s}^{-1}$	Zhao and Rochelle, 1999 ¹²²
	Absolute	Water + NaOCl, pH = 9.3 -	328	1.4 $\times 10^{17} \text{M}^{-1} \text{s}^{-1}$	

10.1

$\text{Hg}^0(\text{g}) + \text{ICl}(\text{g}) \rightarrow \text{Hg}^{2+}(\text{g})$	Absolute	Air/Fly ash (20 g m ⁻³)	393	~94% oxidation, HgCl ₂ is the major product	Qu <i>et al.</i> , 2010 ¹²³
$\text{Hg}^0(\text{g}) + \text{BrCl}(\text{g}) \rightarrow \text{Hg}^{2+}(\text{g})$	Absolute	Air/Fly ash (20 g m ⁻³)	373	Up to 90% oxidation, HgCl ₂ is the major product	Qu <i>et al.</i> , 2009 ¹⁷
$\text{Hg}^0(\text{g}) + \text{Br}_2(\text{g}) \rightarrow \text{Hg}^{2+}(\text{g})$	Absolute	Simulated flue gas/fly ash	298 ± 1	~0.2 s ⁻¹ , enhanced over homogeneous case	Liu <i>et al.</i> , 2007 ⁷
$\text{Hg}^0_{(\text{g, ads})} + \text{O}_{2(\text{g, ads})} \rightarrow \text{prod.}$	Langmuir-	Air/Fly ash surface	423 - 573	$1.5 - 6.5 \times 10^{-12} (\text{cm}^3 \text{ molec}^{-1})^{0.5} \text{ s}^{-1}$	Hall <i>et al.</i> , 1995 ³⁹
	Hinshelwood mech.	Air/Carbon surface	423 - 523	$0.1 - 4.4 \times 10^{-12} (\text{cm}^3 \text{ molec}^{-1})^{0.5} \text{ s}^{-1}$	
$\text{Hg}^0(\text{g}) + \text{SO}_2 + \text{O}_2 \rightarrow \text{HgSO}_4(\text{s})$	Lab	Air/Pt	348-673	3.5 mg Hg hr ⁻¹ (348 - 600 K)	Schofield, 2004 ¹²⁴
$\text{Hg}^0(\text{g}) \rightarrow \text{Hg}^{2+}$	Avg. Lit. Cite.	Air/Pd	~420	> 90% oxidation	Presto and Granite,
	Lit. Cite. Field test	Air/SCR catalyst		~70% oxidation, declines over time to < 30%	2006 ¹²⁵
	Lab	Simulated flue gas/ MnO _x - CeO ₂ /TiO ₂ catalyst	473	> 90% oxidation; NH ₃ inhibited oxidation, however oxid. activity recovered after NH ₃ removed	Li <i>et al.</i> , 2012 ¹²⁶
	Lab	Simulated flue gas/ CeO ₂ /TiO ₂	473	(107 ± 24) s ⁻¹	Li <i>et al.</i> , 2013 ¹²⁷
$\text{Hg}^0(\text{g}) \rightarrow \text{prod.}$	Field Test	Air/TMT-15 catalyst ^a		Inconclusive; intended to prevent re-emission of Hg	Blythe, 2006 ¹²⁸
$\text{Hg}^0(\text{g}) + \text{SO}_2 + \text{NO}_2 + \text{HCl} \rightarrow \text{Hg}^{2+}(\text{g})$	Lab	Air/Fly ash	453	~30% Hg (g) oxidation	Norton <i>et al.</i> , 2003 ¹²⁹
$\text{Hg}^0(\text{g}) + \text{h}\nu \rightarrow \text{prod.}$	Lab study, Xe-lamp	Air/quartz surface	293	$1.2 \times 10^{-5} \text{ s}^{-1}$	Sheu and Mason, 2004 ¹³⁰
$\text{Hg}^0(\text{g}) + \text{h}\nu + \text{H}_2\text{O}(\text{l}) \rightarrow \text{prod.}$	Lab study, Xe-lamp	Air/quartz surface	293	$4.0 \times 10^{-5} \text{ s}^{-1}$	
$\text{Hg}^0(\text{g}) + \text{h}\nu + \text{NaCl} \rightarrow \text{prod.}$	Lab study, Xe-lamp	Air/quartz surface	293	$1.6 \times 10^{-3} \text{ s}^{-1}$	

$\text{Hg}^0(\text{g}) + \text{hv} + \text{NaCl} + \text{H}_2\text{O}(\text{l}) \rightarrow$ prod.	Lab study, Xe-lamp	Air/quartz surface	293	$1.7 \times 10^{-3} \text{ s}^{-1}$	
$\text{HgCl}_2(\text{g}) + \text{H}_2 \rightarrow \text{Hg}_2\text{Cl}_2(\text{s}) +$ 2HCl	Lab, laser	N_2 /Stainless steel surface	473	Unknown mech for reaction	Wang <i>et al.</i> , 1983 ¹³¹
$\text{Hg}^0(\text{g}) + \text{HCl} \rightarrow \text{Hg}(\text{ads})$	Lab	N_2 /Stainless steel surface or PTFE teflon	423	HCl enhances Hg^0 removal, retention on PTFE: (0 $\rightarrow$ 44 ng), SS: (66 $\rightarrow$ 128 ng)	Turchi, 2000 ⁸⁷
$\text{HgCl}_2(\text{g}) \rightarrow \text{HgCl}_2(\text{ads})$	Simulated flue gas	N_2 and trace gas/Gold	422	Acid gases (HCl or NO_2) + SO_2 reduce ads. capacity. HgCl_2 adsorbs; no rxn. Similar to carbon surface ads.	
	Lab	Air/Cysteine over silica	298 - 408	Cature eff. CE: 12 mg Hg g^{-1} < CE < 33 mg Hg g^{-1}	Abu-Daabes and Pinto, 2005 ¹³²
	Lab	N_2 / sulfur impregnated activated carbon	423	Ads. increased with sulfur cotent. Max CE = 5.236 mg (g C) $^{-1}$	Ie <i>et al.</i> , 2012 ¹³³
$\text{HgCl}_2(\text{aq}) + \text{N719-TiO}_2 \rightarrow \text{Hg}^{2+}$ (ads)	Lab	Water/N719-TiO ₂ , pH= 6.6	~298	Hg^{2+} binding constant = $3 \times 10^5 \text{ M}^{-1}$; 65% scavenging eff.	Li <i>et al.</i> , 2007 ¹³⁴
$\text{Hg}^{2+}(\text{aq}) \rightarrow \text{Hg}(\text{ads})$	Lab	Water/ZnO nanoparticles, pH=5.5	303	Ads. capacity: 714 mg Hg g^{-1}	Sheela <i>et al.</i> , 2012 ¹³⁵
$\text{Hg}(\text{NO}_3)_2(\text{aq}) \rightarrow \text{Hg}(\text{ads})$	Lab	Water/Fly ash	303 $\pm$ 1	Freundlich parameters: k = 1.230, 1/n = 0.361 @ pH = 4.2, > 90% adsorption	Sen and De, 1987 ¹³⁶
	Lab	Water/Modified sulfur- impregnated activated carbon	Ambient	Up to 99% adsorption	Wade <i>et al.</i> , 2012 ¹³⁷

	Lab	Water/Activated carbon, pH = 2.0	300	Freundlich parameters: k = 0.1427, 1/n = 0.71	Mohan <i>et al.</i> , 2000 ¹³⁸
			318	k = 0.0663, 1/n = 0.75	
			338	k = 0.01073, 1/n = 1.38	
	Lab	Water/polyaniline/ hexagonal mesoporous silica		Ads. Capacity at pH 10: 843 mg Hg g ⁻¹ ; 88% recovery using H ₂ SO ₄	Javadian <i>et al.</i> , 2014 ¹³⁹
Hg(NO ₃) ₂ (aq) + 2e ⁻ → Au-Hg (s)	Simulated flue gas	Au-coated microparticle	298	0.35 V causes AuHg amalgam formation	Barrosse-Antle <i>et al.</i> , 2007 ¹⁴⁰
Hg ⁰ (g) + H ₂ S (g) + O(ads) → HgS(ads) + H ₂ O	Lab, simulated flue comb.	Flue gas/Fe ₂ O ₃ (N)	353	H ₂ S (g) initiates Hg removal rxn up to 65% Hg loss in stream - no effect from H ₂ or CO. H ₂ O reduces Hg adsorbance	Wu <i>et al.</i> , 2006 ¹⁴¹
	Lab, simulated flue comb.	Fe ₂ O ₃ , Fe ₂ O ₃ -Ca(OH) ₂ , FeS ₂ , Fe ₂ O ₃ (1% wt)/ TiO ₂ surfaces	353	Fe ₂ O ₃ : 50% removal, Fe ₂ O ₃ /TiO ₂ : 80%, Fe ₂ O ₃ - Ca(OH) ₂ : 70%, FeS ₂ : 60%; HCl (g) suppressed Fe ₂ O ₃ activity only	Wu <i>et al.</i> , 2008 ¹⁴²
Hg ⁰ (g) + hν → HgO (s)	Lab, simulated flue comb.	SiO ₂ -TiO ₂ surface	408	99% removal in dry conditions. Humidity and NO inhibited oxid., HCl and SO ₂ promoted oxid.	Li <i>et al.</i> , 2008 ¹⁴³
Hg ⁰ (g) + Δ → HgO _(ad)	Lab, simulated flue comb.	Extensive list of metal oxide surface mixtures, Mars- Maessen mech.	410	Cr ₂ O ₃ /Al ₂ O ₃ , MnO ₂ /Al ₂ O ₃ , and MoS ₂ show high Hg adsorption capacities.	Granite <i>et al.</i> , 2000 ¹⁴⁴
Hg ⁰ (g) + Δ → Hg _(II, ads)	Lab, glass tube diffusion	Various metal surface catalysts. Het. rate constants measured.	411	Rank: Ir > Ir/HCl > Darco > Thief/HCl (in terms of oxidation efficiency	Presto <i>et al.</i> , 2006 ¹²⁵

$\text{HgBr}_2(\text{s}) + \text{Ag}_2\text{WO}_4(\text{s}) \rightarrow \text{HgWO}_4(\text{s}) + 2\text{AgBr}(\text{s})$		Solid-state reaction	393 - 443	$K = 1.10 \times 10^{-4} \text{ cm h}^{-1} @ 120^\circ\text{C}$ (thickness) ² = Kt	Jain and Beg, 1995 ¹⁴⁵
$\text{HgCl}_2(\text{s}) + \text{Ag}_2\text{WO}_4(\text{s}) \rightarrow \text{HgWO}_4(\text{s}) + 2\text{AgCl}(\text{s})$	Lab		418 - 461	$K = 2.29 \times 10^{-4} \text{ cm h}^{-1} @ 145^\circ\text{C}$	
$\text{Hg}^0(\text{g}) \rightarrow \text{Hg}(\text{ads})$	Lab, model	Activated carbon- Ptolemais lignite, impregnated with sulfur (S)	323	Ads. capacity: without S = 175 - 458 ng Hg/mg C, with S = 359 - 915 ng Hg/mgRT C	Skodras <i>et al.</i> , 2007 ¹⁴⁶
$\text{Hg}^0(\text{g}) + \text{O}_3 \rightarrow \text{HgO}_{(\text{s})} + \text{O}_2$	Lab	Air/Secondary organic aerosol (SOA)	295 ± 1	$(7.5 \pm 0.5) \times 10^{-19} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$, rate not affected by SOA	Rutter <i>et al.</i> , 2012 ¹⁴⁷
$\text{Hg}^{2+}(\text{aq}) \rightarrow \text{Hg}^0(\text{g})$	Lab, model	Water/Magnetite, pH = 4.77 - 6.73	Ambient	$3 - 16 \times 10^{-3} \text{ s}^{-1}$; rate increases for increasing magnetite SA and pH, decreases for increasing [Cl ⁻]	Wiatrowski <i>et al.</i> , 2009 ¹⁴⁸
$\text{Hg}(\text{OH})_2(\text{aq}) + (\text{s})\text{-OH} \rightarrow (\text{s})\text{-OHg}^+ + \text{H}_2\text{O} + \text{OH}^-$	Lab, model	Water/Goethite or Hematite or γ -alumina, pH = 6.3 -8.1	296	$150 \text{ M}^{-1} \text{ s}^{-1}$ (Goethite); $188 \text{ M}^{-1} \text{ s}^{-1}$ (Hematite); $0.190 \text{ M}^{-1} \text{ s}^{-1}$ (γ -alumina)	Amirbahman <i>et al.</i> , 2013 ⁸³
$\text{Hg}(\text{OH})_2(\text{aq}) + (\text{s})\text{-OH} \rightarrow (\text{s})\text{-OHg}^+ + \text{H}_2\text{O} + \text{OH}^-$	Lab, model	Water/Goethite or Hematite or γ -alumina, pH = 6.3 - 8.1	296	$3.15 \times 10^{-4} \text{ s}^{-1}$ (Goethite); $2.50 \times 10^{-4} \text{ s}^{-1}$ (Hematite); $6.10 \times 10^{-5} \text{ s}^{-1}$ (γ -alumina)	
$\text{Hg}(\text{OH})_2(\text{aq}) + \text{FeOH}^+(\text{aq}) \rightarrow \text{Hg}^0(\text{g})$	Lab	Water/Goethite or Hematite or γ -alumina, pH = 6.3 - 8.1	296	$78.2 \text{ M}^{-1} \text{ s}^{-1}$ (Goethite); $52.0 \text{ M}^{-1} \text{ s}^{-1}$ (Hematite); $1.80 \text{ M}^{-1} \text{ s}^{-1}$ (γ -alumina)	
$\text{Hg}(\text{OOCCH}_2\text{S})(\text{aq}) \rightarrow \text{Hg}^0 + \text{HgS}(\text{s}) + \text{prod.}$	Lab	Water/HgS nanoparticles, pH = 4.0	296 ± 2	$(2.3 \pm 0.4) \times 10^{-5} \text{ s}^{-1}$ (without K ⁺) $(6.2 \pm 0.6) \times 10^{-5} \text{ s}^{-1}$ ([K ⁺] = 0.02 M)	Si and Ariya, 2015 ¹⁴⁹
$\text{Hg-DOM}(\text{aq}) + \text{HS}^- \rightarrow \text{HgS}(\text{s}) + \text{DOM} + \text{H}^+$	Lab	Water/HgS nanoparticles, pH = 7.5	298	Increasing DOM concentrations inhibited HgS(s) growth rates	Deonaraine and Hsu-Kim, 2009 ¹⁵⁰

$\text{Hg-DOM (aq)} + \text{HS}^- \rightarrow \text{HgS(s)} + \text{DOM} + \text{H}^+$	Lab	Water/HgS nanoparticles, pH = 7.0 ± 0.2	295 ± 2	3 subgroups of Hg^{2+} : 60% react readily with sulfide, 20% react slowly (inhibited by DOM), and 20% do not react at all	Slowey, 2010 ¹⁵¹
	Lab	Water/HgS nanoparticles, pH = 6.5 ± 0.1 , low [Hg]:[DOM]	Ambient	More hydrophobic compounds at lower [Hg]:[DOM]. Structure of HgS(s) is nanoscale or disordered metacinnabar	Gerbig <i>et al.</i> , 2011 ¹⁵²
$\text{HgS (s)} + \text{Cl}^- + h\nu \rightarrow \text{Hg}_{(\text{ad})}^0$	Lab	Water/ α -HgS Pt electrode, 1 M NaCl		HgS(s) reduction to $\text{Hg}_{(\text{ad})}^0$ requires NaCl, visible radiation	Anaf <i>et al.</i> , 2013 ¹⁵³
$\text{HgCl}_{2(\text{ad})} \rightarrow \text{Hg}^0 + \text{Cl}_2$	Lab	Activated carbon/Air	448 - 548	$[(3.0 \pm 0.3) \times 10^4] \exp[-(9.75 \pm 0.56) \times 10^4/\text{RT}]$	Bentley <i>et al.</i> , 2013 ¹⁵⁴
		FeCl ₃ /Air	448 - 548	$[(1.7 \pm 0.1) \times 10^8] \exp[-(1.157 \pm 0.053) \times 10^5/\text{RT}]$	

^a TMT-15 is a 15 % aqueous solution of Trimercapto-s-triazine, a trisodium salt ($\text{C}_3\text{N}_3\text{S}_3\text{Na}_3$)

Additional information ¹⁵⁵:

- In the reactions listed, (s)- is used to denote surface bound groups.
- For comparative discussion of Hg^0 (g) oxidation surface mechanisms (Langmuir-Hinshelwood, Eley-Rideal, Mars-Maessen), see Presto and Granite ¹²⁵
- For large-scale fluxes to/from ocean, land, and anthropogenic sources, see Lindberg *et al* ¹⁵⁶
- For detailed photochemical information of mercury reactions in solid, liquid, and gas phases, see Zhang ⁵¹
- Concentrations of $[\text{Hg}^0 (\text{aq})]$ in various northern lakes: Peretyazhko *et al.* ¹¹³
- Large compilation of Henry's Law values for atmospherically relevant species: Sander, 1999. ¹⁵⁷

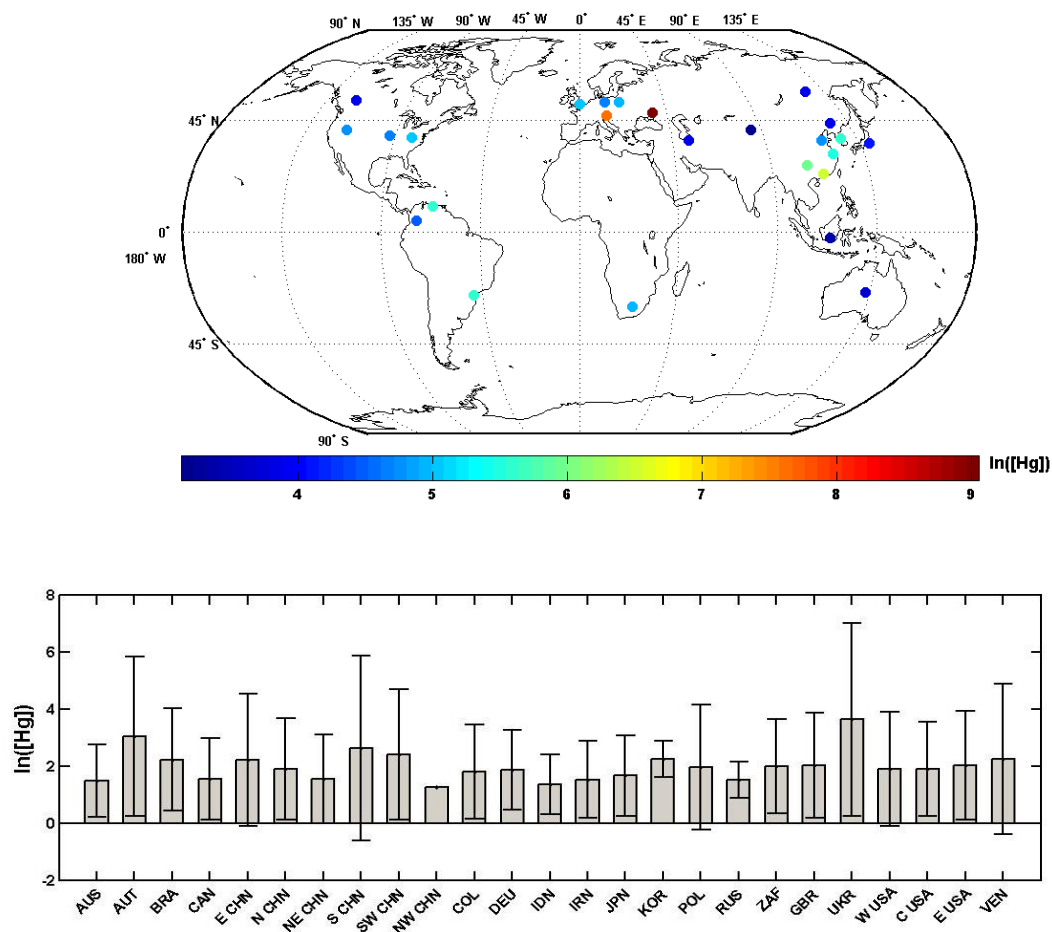
- Other possible catalysis surfaces: Au, Ag, Cu, Ir, Pd, C (fly ash, thief carbon) (Presto and Granite ¹²⁵), Fe₂O₃, iron oxide—Ca(OH), FeS₂ (Wu *et al.* ¹⁴²), TiO₂-SiO₂ (Li *et al.* ¹⁴³), CuCl₂ (Li *et al.* ¹²⁷), RuO₂ (Yan *et al.* ¹⁵⁸), CuO-TiO₂ (Xu *et al.* ¹⁵⁹). Expensive catalysts can often be deposited over a bed of Al₂O₃, TiO₂, or other comparatively cheaper metal oxides.
- Other sorbents for aqueous Hg²⁺ include: thiol-functionalized Zn-doped biomagnetite particles (He *et al.* ¹⁶⁰), attapulgite clay, granular Cu + S, Fe + S (Gibson *et al.* ¹⁶¹), magnetic powdered activated carbon (Faulconer *et al.* ¹⁶²), nanozeolites (Alijani *et al.* ¹⁶³)
- Hg²⁺ (aq) complexes with: CH₃⁻, Cl⁻, H₂O, HCO₃⁻, CO₃⁻, SO₄⁻, OH⁻, fulvic acid, humic acid, oxalate, citrate,...
- Detailed discussion of Hg emissions and deposition to/from soil, see Schlüter ¹¹², Grigal ¹⁰⁶, and Gabriel and Williamson ¹⁶⁴ (includes some details of aquatic Hg distribution).
- Estimated cost of removing mercury from coal fire plant (using SCR catalyst): 29,000 USD lb⁻¹ (Turchi ⁸⁷). Aerosol pH = 2–5; Surface water (lake, river, ocean) pH = 6–8.
- For a detailed review of Hg reactions and fluxes in the cryosphere, see Durnford and Dastoor ¹⁶⁵ and Mann *et al.* ¹⁰⁵.
- For recent density functional theory studies (DFT) on reactions and sorption of mercury, see Castro *et al.* ¹⁶⁶, Lim *et al.* ¹⁶⁷, Sun *et al.* ¹⁶⁸, Lim and Wilcox ¹⁶⁹, Suarez Negreira and Wilcox ¹⁷⁰.

Case Study: Mercury content and occurrence in coal

If the mercury content of coal is known together with the specifications of control technology, then reported coal consumption and/or sales data can be used to develop a bottom-up emissions inventory to better constrain the regional and global impact of mercury emissions related to coal-fired power production. Over the past decades the scientific community has made a large effort to measure the mercury content of coal from the major coal-producing regions, world-wide ¹⁷¹. Although measured mercury contents in coal range from 1 ppb to 330 ppm, the majority of coals sampled contain less than 1 ppm Hg. The average Hg contents for regions studied typically range between 70 and 240 ppb Hg (Supplementary Material Figure 1). Regional Hg coal contents are step-averages of available data starting with the highest resolution possible (*i.e.*, seam averages→ basin averages→ regional or country average) weighted by the number of measurements in each dataset. Despite considerable inter-basin variability in coal Hg content, it is relatively constant worldwide, with notable exceptions in Eastern Europe and Southern China. Results from Austria and Ukraine tend to be early in the compiled dataset ^{171a,b} and it is possible that they are elevated due to unaccounted-for analytical blanks. High inter-laboratory variability in measured Hg in coal suggests that the naturally observed variability in coal Hg may be due to either heterogeneity in coal seams or to the comparison of differing analytical techniques ^{171u}. The estimated worldwide average Hg content of coal, from the compiled data is $(3\pm1)\times10^2$ ppb, consistent with previous estimates ¹⁷². Statistical differences were not found between varying coal ranks (*i.e.* anthracite $[(2.2\pm0.9)\times10^2$ ppb] vs. bituminous $[(1.3\pm0.9)\times10^2$ ppb] vs. lignite $[(1.3\pm0.8)\times10^2$ ppb] vs. sub-bituminous $[(0.7\pm0.4)\times10^2$ ppb]), with the exception of anthracite vs. sub-bituminous coals. Supplementary Material Figure 1 summarizes the average mercury content in coal (in ppb, by mass) binned by country and/or region.

The mercury content of coal typically correlates well with the quantity of pyritic sulfur present ^{171ar,173}, suggesting that Hg is associated with epigenetic pyrites. Leaching experiments on coals also

found that Hg is mainly associated with sulfides and to a lesser extent with organic compounds, and infrequently with silicates and carbonates^{171y,171au,174}. However, high silicate-associated Hg contents have been found in the presence of igneous intrusions into coal seams^{171au,174}. Additionally, SEM-EDX analyses of southwestern Chinese coal suggest the association of Hg with low-temperature hydrothermal minerals related to gold mineralization¹⁷⁵. In most cases, Hg is associated with denser fractions of the bulk coal^{171f,171y}, allowing for significant Hg reductions via the physical cleaning of coal prior to combustion. Coal cleaning has been shown to reduce the Hg coal content by 12-78% (average of 37%)^{171z}.



Supplementary Material Figure 1 The average mercury content in coal (in ppb, by mass) binned by country and/or region. Error bars are equal to one standard deviation from the mean. Despite

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considerable inter- and intra-regional variability, the mercury content in coal worldwide is typically on the order of 10^2 ppb. (AUS=Australia, AUT=Austria, BRA=Brazil, CAN=Canada, CHN = China, COL=Colombia, DEU=Germany, IDN=Indonesia, IRN=Iran, JPN=Japan, KOR=Korea, POL=Poland, RUS=Russia (Siberia), ZAF=South Africa, GBR=Great Britain and Scotland, UKR=Ukraine, USA=United States of America, VEN=Venezuela)

Mercury Isotopes in Coal

One emerging field of study in coal Hg is the fingerprinting of coal via mercury isotopes^{171bi,176}. Mercury has isotopes that are influenced by either mass dependent fractionation (MDF) or mass independent fractionation (MIF), and the combination of MDF and MIF can be used to trace Hg from coal through the environment. The isotopes Hg-199 and Hg-201 undergo MIF and are not expected to be influenced by combustion, and may be traced back to their source coal and the associated Hg emitter^{171bi,176}. Hg-202 abundance (expressed in per-mil as $\delta^{202}\text{Hg}$) ranges from -3 to 0.77 ‰, Hg-199 abundance ($\Delta^{199}\text{Hg}$) ranges from -2.3 to 0.38 ‰ and Hg-201 ($\Delta^{201}\text{Hg}$) abundance from -1.2 to 0.25 ‰^{171bi,176}. Data plotted in $\Delta^{201}\text{Hg}$ - $\Delta^{199}\text{Hg}$ space have a slope of 1 – 1.1, consistent with the photoreduction of Hg^{2+} prior to coal formation. The $\delta^{202}\text{Hg}$ - $\Delta^{199}\text{Hg}$ signatures of different coal-producing regions and different seams within a given region have been shown to be distinct^{171bi,176}. The mercury isotope signature of pyrites in coal is unfractionated with respect to Hg standards^{176b} suggesting that Hg may be hydrothermal in origin, and that Hg isotopes may also be used to distinguish between epigenetic and syngeneic Hg in a given coal sample.

Mercury Mass Balance For Coal-Fired Power Plants

The local and regional impact of coal combustion processes depends not only on the mercury content of coal but also on the flow of mercury throughout the flue of the power plant. Numerous studies have

established mercury mass balances for individual coal fire power plants (CFPPs) in order to track the fate of mercury released during combustion. The rate and chemical makeup of mercury emissions from CFPPs has been found to depend on a wide range of parameters, such as boiler type, coal rank, flue gas temperature, carbon, sulfur and the chlorine content of coal, and the presence of pollutant controls such as electrostatic precipitators (ESPs) and/or fabric filters (FFs) for particulates, flue gas desulphurization (FGD) units and selective catalytic reduction (SCR) units for NO_x. Despite the wide variety of variables that exist, some general conclusions can be made. For example, the quantity of residual mercury in bottom ash or slag collected in the boiler after combustion is very low, 0.04 - 7% (average of 1±2%)^{171h,171k,l,171q,171v,171av,171az,177}, suggesting that the overwhelming majority of Hg trapped in coal is released to the flue during combustion. At combustion temperatures this Hg will be predominately Hg⁰ but is expected to repartition to Hg²⁺ and Hg(p) as temperatures decrease^{171ab,178}.

If an SCR is installed, the flue gas will likely pass from the boiler through the SCR; mercury speciation measurements indicate that Hg⁰ is converted efficiently to Hg²⁺ within the SCR^{171az,177e,179}. The flue gas then typically passes through an ESP and/or FF baghouse, wherein the overwhelming majority of Hg(p) is removed^{171ah,171az,179b,180}, resulting in the average reductions in total mercury of 30(±30)%. The proportion of total Hg captured onto fly ash in the ESP/FF has been shown to correlate well with the carbon content and surface area of the fly ash^{171ao,181}. Pulverized coal boilers produced fly ash with higher surface area than cyclone or stoke ash boilers^{181d}, promoting higher Hg capture in the ESP/FF. Some oxidation of elemental mercury to Hg²⁺ occurs across the ESP/FF, with rates appearing to depend on the Cl content of the coal being burnt^{171ab,171aq,180b,182}. Fabric filter bag houses have been shown to capture higher quantities of particulates than ESPs due to a higher surface area, and may also promote greater conversion of Hg⁰ to Hg²⁺^{177g}. Hg capture by fly ash in the ESP is temperature sensitive, with a greater Hg uptake as the temperature decreases^{181c}.

When installed, flue gas desulphurization units downstream of particulate pollutant controls efficiently remove Hg^{2+} from the gas stream^{171q,171ab,171ah,171az,ba,178a,179b,180} with average total mercury reductions of 30($\pm$ 20)%. The rate of Hg^{2+} capture depends on the liquid-to-gas ratio in the FGD¹⁸³. Hg^0 may also be reemitted from captured Hg^{2+} in the FGS, possibly via reaction with sulfite (HSO_3^-) in the FGD slurry¹⁸⁴. The stack mercury speciation of gases emitted from a CFPP equipped with both ESP and FGD would be anticipated to consist predominately of Hg^0 ^{171ba,171bf,177f,g,178b}.

In 1999, the U.S. EPA issued an Information Collection Request (ICR) with regards to mercury emissions from U.S. power plants, including mercury speciation of emissions. The speciation of mercury in the plume of a power plant will control whether CFPP emissions are a source of local pollution ($\text{Hg}(\text{p})$ and Hg^{2+}) or regional/global pollution (Hg^0). An analysis of the EPA ICR data confirmed that Hg speciation varies widely depending on the pollution controls installed, with Hg^0 ranging from 23 to 96% of emissions, Hg^{2+} 2.7 to 76.4% of emissions and $\text{Hg}(\text{p})$ from 0.4 to 2% of emissions¹⁸⁵. For comparison, the global average speciation of emissions is thought to be 50:40:10 Hg^0 : Hg^{2+} : $\text{Hg}(\text{p})$ from CFPP¹⁸⁶.

In-plume measurements of mercury after emission are rare in the literature.^{171j} studied the plume of a CFPP by helicopter and found that the Hg speciation shifts from 90:10 $\text{Hg}(\text{p})$: $\text{Hg}(\text{g})$ (i.e. $\text{Hg}^0 + \text{Hg}^{2+}$) near the stacks to essentially 100% $\text{Hg}(\text{g})$ at a distance (22 km), possibly due solely to dilution with ambient air containing minor quantities of $\text{Hg}(\text{p})$. A multi-year ground-level monitoring campaign of Hg speciation from CFPP in the southern US found discrepancies in lesser quantities of Hg^{2+} and greater quantities of Hg^0 in-plume than expected based on estimated emissions from nearby plants¹⁸⁷. The authors attributed the discrepancy to in-plume reduction of Hg^{2+} although the in-stack vs. in-plume comparison relied on national average Hg emissions ratios that may not have been appropriate for the CFPPs studied.¹⁸⁸ also observed lower Hg^{2+} in the plume of a CFPP than expected based on recent in-stack Hg speciation measurements, although in-plume Hg^0 concentrations were

consistent with in-stack emissions. The authors attributed the discrepancy to Hg^{2+} chiefly due to biases in Hg measurement techniques although corrections for said biases were insufficient to completely account for differences in Hg^{2+} . Recent work by ¹⁸⁹ found that root mean square errors and biases in modeled local mercury deposition near coal-fired power plants decreased significantly when the emitted mercury speciation was shifted from the average speciation of 50:40:10 to 90:8:2 Hg^0 : Hg^{2+} : Hg(p)

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