Supporting information

Full citation for reference 22: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Gaussian, Inc.: Wallingford CT, 2004.

Table S1: Free energy of reaction using SDD/ECP (g03) and all electron TZ (p6) basis sets.

Reactions	Basis set	
	SDD/ECP	All electron TZ
$CH_3HgOH + HSR \rightarrow CH_3HgSR + H2O$	-12.65	-11.56
$CH_3HgOH + HSeR \rightarrow CH_3HgSeR + H2O$	-18.17	-17.67

Table S2: The K values for different steps in the degradation of CH_3Hg (seleno)amino acid complexes at 298.15 K.

	Reactions	Complexes		
		S	Se	Mixed
1	$CH_3HgOH + REH \rightarrow CH_3HgER + H_2O$	1.88×10^{9}	2.09×10^{13}	
2	$CH_3HgOH + 2REH \rightarrow CH_3Hg(ER)_2^- + H^+ + H_2O$	5.11×10^{-9}	2.29	
2a	$CH_3HgOH + RSH + RSeH \rightarrow CH_3Hg(SR)(SeR)^- + H^+ + H_2O$			8.31×10^{-6}
3	$CH_3HgER + REH \rightarrow CH_3Hg(ER)_2^- + H^+$	2.77×10^{-18}	1.09×10^{-13}	
3a	$CH_3HgSR + RSeH \rightarrow CH_3Hg(SR)(SeR)^- + H^+$			1.26×10^{-14}
3b	$CH_3HgSeR + ReH \rightarrow CH_3Hg(SR)(SeR)^- + H^+$			4.55×10^{-14}
4	$CH_3HgOH + CH_3HgER \rightarrow (CH_3Hg)_2E + R\text{-}OH$	2.19×10^{16}	1.29×10^{19}	
5	$CH_3HgER + CH_3HgER \rightarrow (CH_3Hg)_2E + R\text{-}E\text{-}R$	1.75×10^{9}	3.51×10^{9}	
5a	$CH_3HgSR + CH_3HgSeR \rightarrow (CH_3Hg)_2S + R\text{-}Se\text{-}R$			5.84×10^{6}
5b	$CH_3HgSeR + CH_3HgSR \rightarrow (CH_3Hg)_2Se + R\text{-}S\text{-}R$			3.60×10^{10}
6	$CH_3HgER + HER + CH_3HgER \rightarrow (CH_3Hg)_2E + R\text{-}E\text{-}E\text{-}R + R\text{-}H$	5.15×10^{12}	1.36×10^{21}	
6a	$CH_3HgSR + HSeR + CH_3HgSR \rightarrow (CH_3Hg)_2S + R\text{-}S\text{-}Se\text{-}R + R\text{-}H$			2.09×10^{18}
6b	$CH_3HgSR + HSeR + CH_3HgSR \rightarrow (CH_3Hg)_2Se + R\text{-}S\text{-}S\text{-}R + R\text{-}H$			3.44×10^{19}
6c	$CH_3HgSeR + HSR + CH_3HgSeR \rightarrow (CH_3Hg)_2S + R\text{-}Se\text{-}Se\text{-}R + R\text{-}H$			2.04×10^{14}
6d	$CH_3HgSeR + HSR + CH_3HgSeR \rightarrow (CH_3Hg)_2Se + R\text{-}S\text{-}Se\text{-}R + R\text{-}H$			1.11×10^{17}
6e	$CH_3HgSR + HSR + CH_3HgSeR \rightarrow (CH_3Hg)_2S + R\text{-}S\text{-}Se\text{-}R + R\text{-}H$			1.88×10^{14}
6f	$CH_3HgSR + HSR + CH_3HgSeR \rightarrow (CH_3Hg)_2Se + R\text{-}S\text{-}S\text{-}R + R\text{-}H$			3.66×10^{15}
6g	$CH_3HgSR + HSeR + CH_3HgSeR \rightarrow (CH_3Hg)_2S + R\text{-}Se\text{-}Se\text{-}R + R\text{-}H$			2.27×10^{18}
6h	$CH_3HgSR + HSeR + CH_3HgSeR \rightarrow (CH_3Hg)_2Se + R\text{-}S\text{-}Se\text{-}R + R\text{-}H$			1.23×10^{21}
7	$(CH_3Hg)_2E \rightarrow (CH_3)_2Hg + HgE$	1.43×10^{17}	1.59×10^{18}	
8	$HgE(g) \rightarrow HgE(s)$		1.49×10^{47}	
9	$(CH_3)_2Hg + H_2O \rightarrow CH_3HgOH + CH_4(g)$	8.99×10^{7}		

Table S3: Free energy of reactions in Kcal/mol.

	Reactions	Complexes containing	
		S	Se
1s1	$CH_3HgCl + HER \rightarrow CH_3HgER + HCl$	19.46	13.04
1s2	$CH_3HgCl + 2HER \rightarrow CH_3Hg(ER)_2^- + H^+ + HCl$	43.41	31.63
1s3	$CH_3HgCl + CH_3HgER \rightarrow (CH_3Hg)_2E + R\text{-}Cl$	9.91	6.12
1s4	$(CH3)_2Hg + HCl \rightarrow CH_3HgCl + CH_4$	-42.97	-42.97

Table S4: Enthalpy of reaction (Kcal/mol) in the gas phase

	Reactions	Complexes containing	
		S	Se
2s1	$CH_3HgOH + HER \rightarrow CH_3HgER + H_2O$	-19.14	-22.46
2s2	$CH_3HgOH + CH_3HgER \rightarrow (CH_3Hg)_2E + R\text{-}OH$	-21.78	-25.53
2s3	$CH_3HgER + CH_3HgER \rightarrow (CH_3Hg)_2E + R\text{-}E\text{-}R$	-3.46	-4.05
2s4	$CH_3HgER + HER + CH_3HgER \rightarrow (CH_3Hg)_2E + R\text{-}E\text{-}E\text{-}R + R\text{-}H$	-14.93	-24.70