Electronic Supplementary Information for PCCP

Table S1: Calculated CP-corrections (kJ mol^{-1}) at post-HF levels

	Hg			X	
	MP2	**CCSD**	**CCSD(T)**	**CCSD**	**CCSD(T)**
HgF_4	26.0	23.0	24.8	3.8	-[a]
$HgCl_4$	20.5	18.0	19.4	3.2	-[a]
HgH_4	29.9	26.5	28.6	0.0	0.0
HgF_2	12.9	11.3	12.2	1.5	1.5
$HgCl_2$	10.4	9.1	9.8	1.1	1.2
HgH_2	15.0	13.3	14.3	0.0	0.0
F_2				1.2	1.3
Cl_2				0.9	1.0
H_2				0.0	0.0

[a] CP correction was not possible, due to system size.

Table. S2: Structure of the transition state for H_2 elimination from HgH_4 calculated at different levels[a]

	Geometry	**SVWN5**	**BP86**	**B1LYP**	**B3LYP**	**MPW1PW91**	**BHandHLYP**
this work, basis B	rHg-H1	1.699	1.709	1.693	1.696	1.683	1.672
	rHg-H2	1.674	1.687	1.684	1.684	1.675	1.674
	rH1-H1	1.324	1.353	1.394	1.386	1.382	1.422
	∠ H2-Hg-H2	104.1	102.8	101.7	101.9	101.7	101.2
	∠ H2-Hg-H1	105.0	105.3	104.8	105.0	104.9	104.3
ref. 8	Hg-H1				1.692		
	Hg-H2				1.668		
	H1-H1				1.329		
	∠ H2-Hg-H2				103.6		
	∠ H2-Hg-H1				105.1		

[a]Bond lengths in Å, bond angles in deg. See Figure S1 for atom labels.