Table S-I. NMR shielding constants for CO.

C						
	cc-pCV5Z		aug-cc-pCVQZ		CTOCD-1[a]	
	σ	Δσ	σ	Δσ	σ	Δσ
RPA	-27.55	444.66	-28.46	442.82	-25.86	444.89
CCS	-27.93	406.95	-29.03	405.31	-26.26	407.21
CC2	5.75	397.01	5.02	394.65	8.14	395.42
CCSD	-2.45	322.54	-3.19	405.00	0.03	405.76
CC3	2.83	401.90	2.06	399.68	5.16	400.48
O						
	cc-pCV5Z		aug-cc-pCVQZ		CTOCD-1[a]	
	σ	Δσ	σ	Δσ	σ	Δσ
RPA	-90.05	746.23	-90.48	742.51	-87.16	745.74
CCS	-46.91	629.44	-47.88	626.35	-44.19	629.10
CC2	-62.76	703.51	-63.24	699.48	-60.50	702.57
CCSD	-56.23	691.85	-57.01	688.35	-54.78	692.28
CC3	-55.12	693.34	-55.69	689.54	-53.28	693.05

(a) aug-cc-pCVTZ-CTOCD-uc basis from Reference [20].

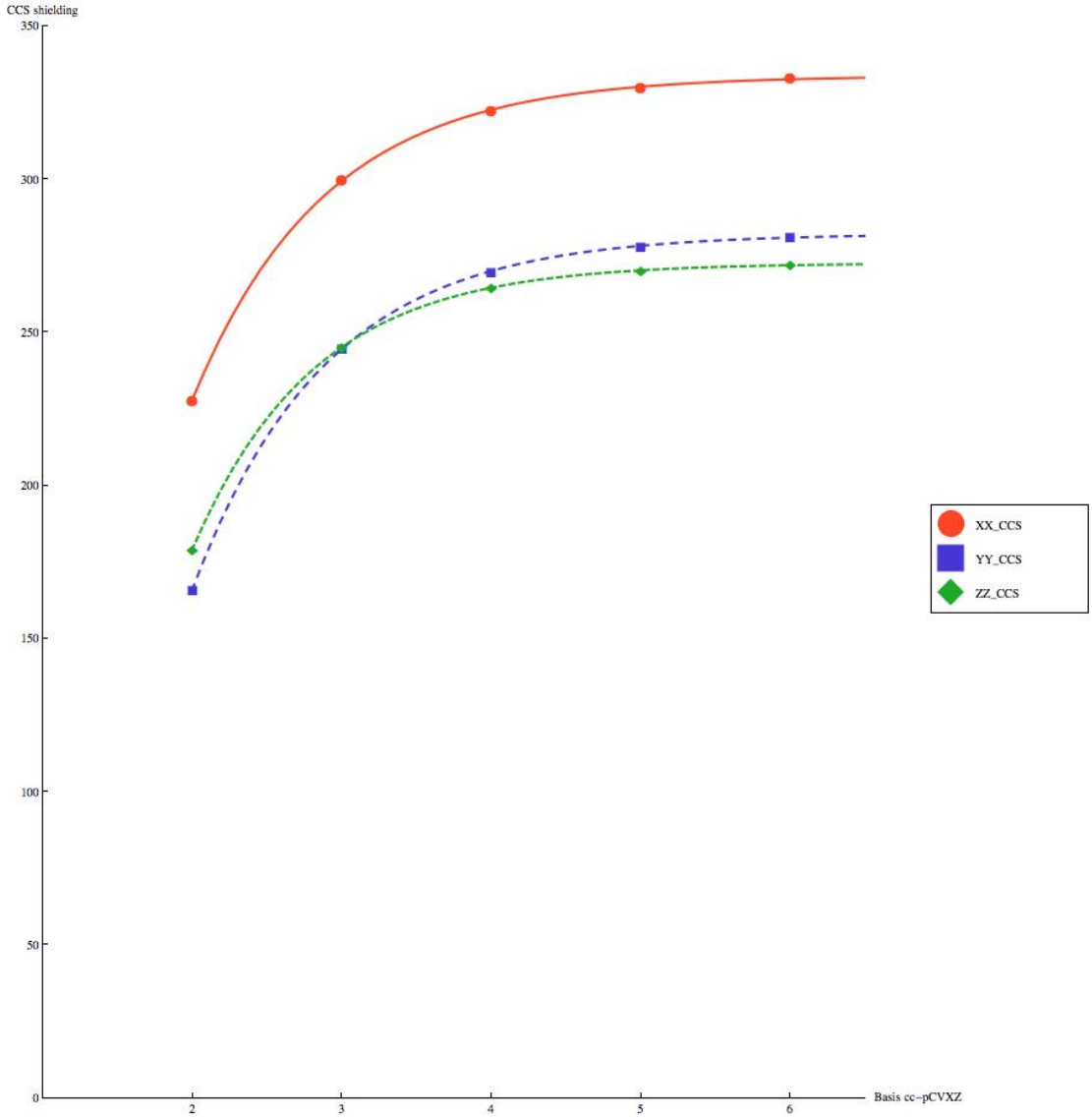

Fig S-1. Variation with the basis set of the different elements of the ^{17}O-NMR shielding tensor in H_2O calculated at the CCS level.