

Table 1: Groupings of full Hamiltonian (1 and 2 body terms).

Systems	N	Total	QWC	FC	SVD	CSA
H ₂	4	15	3	2	4	3
LiH	12	631	142	36	22	9
BeH ₂	14	666	172	35	29	13
H ₂ O	14	1086	313	55	28	11
NH ₃	16	3609	1272	153	37	13

Table 2: HF $\sum_i \sqrt{var_i}$

Systems	H	QWC	FC	SVD	CSA	GCSA	VCSA
H ₂	0.197	0.197	0.197	0.197	0.197	0.197	0.197
LiH	0.141	1.857	0.895	1.929	5.537	1.850	1.581
BeH ₂	0.218	3.164	1.876	1.338	4.944	1.135	...
H ₂ O	0.323	9.276	5.701	8.877	20.749	8.268	...
NH ₃	0.364	15.531	5.796	8.734	21.194

Table 3: FCI $\sum_i \sqrt{var_i}$

Systems	QWC	FC	SVD	CSA	GCSA	VCSA
H ₂	0.369	0.369	0.370	0.351	0.369	0.369
LiH	2.416	1.196	1.778	5.335	1.731	1.634
BeH ₂	3.713	2.277	1.365	4.964	1.213	...
H ₂ O	11.560	6.806	7.647	19.716
NH ₃	18.735	6.151	7.620

Table 4: Energies

Systems	HF	FCI
H ₂	-1.0661	-1.1012
LiH	-7.7673	-7.7845
BeH ₂	-15.4557	-15.4817
H ₂ O	-74.9630	-75.0177
NH ₃	-55.4523	...