

RLF was used for grouping QWC and FC.

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

Systems	N	Total	QWC	FC	GFC	SVD	CSA	GCSA	VGCSA	VCSA
H ₂	4	15	3	2	2	4	3	3	3	3
LiH	12	631	142	26	42	22	9	78	97	...
BeH ₂	14	666	172	29	36	29	13	118	129	...
H ₂ O	14	1086	311	38	50	29	11	119	148	...
NH ₃	16	3609	1262	121	122	37	13	187	208	...
N ₂	74	52

Table 2: FCI. $(\sum_i \sqrt{\text{var}_i})^2$

Systems	QWC	FC	GFC	SVD	CSA	GCSA	VGCSA	VCSA
H ₂	0.14	0.14	0.14	0.14	0.12	0.14	0.14	0.14
LiH	4.63	1.02	0.88	3.16	28.46	2.71	2.26	7
BeH ₂	14.78	3.68	1.11	1.86	24.64	1.47	0.851	9
H ₂ O	128.76	25.97	7.59	58.48	388.73	49.4	46.2	100
NH ₃	332.79	53.60	18.8	58.07	402.28	47.0	42.2	100
N ₂	8.83	10.5

Table 3: Groupings of full Hamiltonian (1 and 2 body terms).

Systems	GCSA FC	GCSA CSA
H ₂	3	3
LiH	71	24
BeH ₂	61	27
H ₂ O	82	32
NH ₃	...	34
N ₂

Table 4: FCI. $(\sum_i \sqrt{var_i})^2$

Systems	GCSA FC	GCSA CSA
H ₂	0.14	0.14
LiH	2.65	2.66
BeH ₂	1.45	1.34
H ₂ O	50.57	49.8
NH ₃	...	47.8

Table 5: FCI. $M \sum_{i=1}^M \text{var}_i$. Deprecated.

Systems	QWC	FC	SVD	CSA	GCSA FC	VGCSA
H ₂	0.15	0.14	0.26	0.17	0.19	
LiH	10.41	1.48	21.49	30.61	71.14	
BeH ₂	25.85	4.74	8.67	25.69	17.88	
H ₂ O	434.38	46.72	625.90	441.66	1688.74	
NH ₃	1685.01	103.66	742.37	453.13		

Table 6: 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	...