		Energy	FCI Error	Qiskit-NWQSim	# Params	# Iters	Time (min)	Optimizer	Termination
H4 H-H = 1.0 A	FCI (Qiskit/PySCF)	-2.166387449	/	/	/	/	/	/	/
	Qiskit	**-2.166307982**	**-7.9466E-05**	**/**	**26**	**575**	**0.91**	**COBYLA**	Normal return
	NWQSim, Sym 0	-2.166305451	-8.1998E-05	-2.5316E-06	48	445	0.12	LN_NEWUOA	Function tol. reached (abstol 1e-8)
	NWQSim, Sym 1	-2.166305682	-8.1767E-05	-2.3004E-06	44	338	0.09	LN_NEWUOA	Function tol. reached (abstol 1e-8)
	NWQSim, Sym 2	-2.166304945	-8.2504E-05	-3.0373E-06	40	551	0.14	LN_NEWUOA	Function tol. reached (abstol 1e-8)
	NWQSim, Sym 3	-2.166306236	-8.1213E-05	-1.7467E-06	28	398	0.10	LN_NEWUOA	Function tol. reached (abstol 1e-8)
	NWQSim, Sym 4	-2.166102989	-2.8446E-04	-2.0499E-04	14	322	0.08	LN_NEWUOA	Function tol. reached (abstol 1e-8)
	NWQSim, Qiskit Recon	**-2.166306231**	**-8.1217E-05**	**-1.7510E-06**	**26**	**183**	0.03	LN_NEWUOA	Function tol. reached (abstol 1e-8)
	NWQSim, Qiskit Recon	**-2.166307806**	**-7.9643E-05**	**-1.7671E-07**	**26**	**1019**	0.16	COBYLA	Function tol. reached (abstol 1e-8)

		Energy	FCI Error	Qiskit-NWQSim	# Params	# Iters	Time (min)	Optimizer	Termination
H4 H-H = 1.5 A	FCI (Qiskit/PySCF)	-1.996150326	/	/	/	/	/	/	/
	Qiskit	**-1.994783573**	**-1.3668E-03**	**/**	**26**	**794**	**1.23**	**COBYLA**	Normal return
	NWQSim, Sym 0	-1.994760857	-1.3895E-03	-2.2716E-05	48	504	0.13	LN_NEWUOA	Function tol. reached (abstol 1e-8)
	NWQSim, Sym 1	-1.994739575	-1.4108E-03	-4.3998E-05	44	390	0.10	LN_NEWUOA	Function tol. reached (abstol 1e-8)
	NWQSim, Sym 2	-1.994762244	-1.3881E-03	-2.1329E-05	40	521	0.14	LN_NEWUOA	Function tol. reached (abstol 1e-8)
	NWQSim, Sym 3	-1.994760049	-1.3903E-03	-2.3524E-05	28	398	0.11	LN_NEWUOA	Function tol. reached (abstol 1e-8)
	NWQSim, Sym 4	-1.994570829	-1.5795E-03	-2.1274E-04	14	303	0.08	LN_NEWUOA	Function tol. reached (abstol 1e-8)
	NWQSim, Qiskit Recon	**-1.994776167**	**-1.3742E-03**	**-7.4061E-06**	**26**	**303**	**0.05**	**LN_NEWUOA**	Function tol. reached (abstol 1e-8)
	NWQSim, Qiskit Recon	**-1.994777398**	**-1.3729E-03**	**-6.1752E-06**	**26**	**1641**	**0.24**	**COBYLA**	Function tol. reached (abstol 1e-8)

-2.166307275	-8.0173E-05
-1.994758938	-1.3914E-03

Qis	0	1	2	3

54.6	0.09495652
6.9864	0.01569978
5.3	0.01568047
8.6778	0.01574918
6.07	0.01525126
4.9137	0.01525994
1.63	0.0089071
9.51287	0.0093355

7.9294	0.01573294
6.1596	0.01579385
8.2	0.01573896
6.5	0.01633166
4.64	0.01531353
2.7014	0.00891551
14.5	0.00883608

H6, H-H=1.8 Angstrom

	UCCSD						
	Paper	NWQSim (Qis)	NWQSim (Sym 4)	NWQSim (Sym 3)	NWQSim (Sym 2)	NWQSim (Sym 1)	NWQSim (Sym 0)
Grpund-State Energy	-2.8777405997697	-2.8778341145832	-2.8706552807833	-2.8291462833120	-2.8417944878183	-2.8763459300478	-2.8763503594566
Diff with Paper UCCSD	/	9.351E-05	7.085E-03	4.859E-02	3.595E-02	1.395E-03	1.390E-03
Diff with FCI	9.829E-03	9.735E-03	1.691E-02	5.842E-02	4.577E-02	1.122E-02	1.122E-02

H6, H-H=1.8 Angstrom

	FCI	
	Paper	Qiskit/PySCF
Grpund-State Energy	-2.8875693743860	-2.8875693764358
Diff with Paper FCI	/	2.050E-09

H6, H-H=1.8 Angstrom

UCCSD Method	# Param	# Gate	# Iters	Time	Optimizer	Termination
NWQSim (Qis)	117	20898	2409	23 mins 14 secs	LN_NEWUOA	Func tol reached (--atol 1e-10)
NWQSim (Sym 4)	54	47178	1910	33 mins 48 secs	LN_NEWUOA	Func tol reached (--atol 1e-10)
NWQSim (Sym 3)	180	47178	2432	42 mins 08 secs	LN_NEWUOA	Func tol reached (--atol 1e-10)
NWQSim (Sym 2)	234	47178	2731	47 mins 42 secs	LN_NEWUOA	Func tol reached (--atol 1e-10)
NWQSim (Sym 1)	243	47178	3714	(inaccurate)	LN_NEWUOA	Func tol reached (--atol 1e-10)
NWQSim (Sym 0)	252	47178	3830	66 mins 32 secs	LN_NEWUOA	Func tol reached (--atol 1e-10)

H6_3au_DUCC3_6-electrons_6-Orbitals

Note: all energy data do NOT include the shift -0.004911582601

	FCI	UCCSD		
	Qiskit/PySCF	NWQSim (Qis)	NWQSim (Sym 4)	NWQSim (Sym 0)
Grpund-State Energy	-3.1747723379967	-3.1740027185315	-3.1569880904336	-3.1739732621868
Diff with FCI	/	7.696E-04	1.778E-02	7.991E-04

H6_3au_DUCC3_6-electrons_6-Orbitals

UCCSD Method	# Param	# Gate	# Iters	Time	Optimizer	Termination
NWQSim (Qis)	117	20898	1580	22 mins 57 secs	LN_NEWUOA	Func tol reached (--atol 1e-10)
NWQSim (Sym 4)	54	47178	1478	32 mins 41secs	LN_NEWUOA	Func tol reached (--atol 1e-10)
NWQSim (Sym 0)	252	47178	2572	56 mins 33 secs	LN_NEWUOA	Func tol reached (--atol 1e-10)

	Paper UCCSD	QFlow UCCSD			VQE UCCSD		
		Sym 4	Sym 3	Qis	Sym 4	Sym 3	Qis
Energy	-2.8777406	-2.876006742	-2.876363301	-2.877828737	-2.811243274	-2.829182432	-2.877834536
Diff to paper	/	-1.734E-03	-1.377E-03	8.814E-05	-6.650E-02	-4.856E-02	9.394E-05
# Operators	/	252	252	117	252	252	117
# Params	/	54	180	117	54	180	117
# Iters	/	**2925**	**1782**	**1116**	**1745**	**3278**	**2405**
# Gates	/	47,178	47,178	20,898	47,178	47,178	20,898
Time	/	62 mins 22 secs	38 mins 41 secs	14 mins 41 secs	36 mins 53 secs	69 mins 23 secs	31 mins 48 secs
Optimizer	/	LN_NEWUOA	LN_NEWUOA	LN_NEWUOA	LN_NEWUOA	LN_NEWUOA	LN_NEWUOA
Termination	/	**Func tol 1e-10**	**Func tol 1e-10**	**Func tol 1e-10**	**Func tol 1e-10**	**Func tol 1e-10**	**Func tol 1e-10**

H6, H-H=1.8 Angstrom						
	UCCSD					
	Paper	NWQSim (Qis)	NWQSim (Sym 4, Old)	NWQSim (Sym 0, Old)	NWQSim (QisSym)	
Grpund-State Energy	-2.8777405997697	-2.8778341145832	-2.8706552807833	-2.8763503594566	-2.8677034317583	
Diff with Paper UCCSD	/	9.351E-05	7.085E-03	1.390E-03	1.004E-02	2.878E+00
Diff with FCI	9.829E-03	9.735E-03	1.691E-02	1.122E-02	1.987E-02	2.888E+00

H6, H-H=1.8 Angstrom		
	FCI	
	Paper	Qiskit/PySCF
Grpund-State Energy	-2.8875693743860	-2.8875693764358
Diff with Paper FCI	/	2.050E-09

H6, H-H=1.8 Angstrom						
UCCSD Method	# Param	# Gate	# Iters	Time	Optimizer	Termination
NWQSim (Qis)	117	20898	2409	23 mins 14 secs	LN_NEWUOA	Func tol reached (--atol 1e-10)
NWQSim (Sym 4, Old)	54	47178	1910	33 mins 48 secs	LN_NEWUOA	Func tol reached (--atol 1e-10)
NWQSim (Sym 0, Old)	252	47178	3830	66 mins 32 secs	LN_NEWUOA	Func tol reached (--atol 1e-10)
NWQSim (QisSym)					LN_NEWUOA	Func tol reached (--atol 1e-10)
0						

H6_3au_DUCC3_6-electrons_6-Orbitals	Note: all energy data do NOT include the shift -0.004911582601					
	FCI	UCCSD				
	Qiskit/PySCF	NWQSim (Qis)	NWQSim (Sym 4, Old)	NWQSim (Sym 0, Old)	NWQSim (Sym 4, New)	NWQSim (Sym 0, New)
Grpund-State Energy	-3.1747723379967	-3.1740027185315	-3.1569880904336	-3.1739732621868		
Diff with FCI	/	7.696E-04	1.778E-02	7.991E-04	3.175E+00	3.175E+00

H6_3au_DUCC3_6-electrons_6-Orbitals						
UCCSD Method	# Param	# Gate	# Iters	Time	Optimizer	Termination
NWQSim (Qis)	117	20898	1580	22 mins 57 secs	LN_NEWUOA	Func tol reached (--atol 1e-10)
NWQSim (Sym 4, Old)	54	47178	1478	32 mins 41secs	LN_NEWUOA	Func tol reached (--atol 1e-10)
NWQSim (Sym 0, Old)	252	47178	2572	56 mins 33 secs	LN_NEWUOA	Func tol reached (--atol 1e-10)
NWQSim (QisSym)					LN_NEWUOA	Func tol reached (--atol 1e-10)