ELECTRONIC SUPPLEMENTARY INFORMATION

Workflow for practical quantum chemical calculations with quantum phase estimation algorithm: electronic ground and π–π* excited states of benzene and its derivatives

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1. Cartesian coordinates of LiH, benzene, chlorobenzene, nitrobenzene

Table S.1.1 Cartesian coordinates of LiH molecule in the unit of $\mathring{A}$, optimized at the B3LYP/6-31+G(d) level of theory.

Atom	x	y	z
H	0	0	-1.1443
Li	0	0	0.3814

Table S.1.2 Cartesian coordinates of benzene in the unit of $\mathring{A}$, optimized at the B3LYP/6-311G(d) level of theory.

Atom	x	y	z
C	0.0000	-1.3966	0.0000
C	-1.2095	-0.6983	0.0000
C	1.2095	-0.6983	0.0000
C	1.2095	0.6983	0.0000
C	-1.2095	0.6983	0.0000
C	0.0000	1.3966	0.0000
H	0.0000	-2.4837	0.0000
H	2.1509	-1.2418	0.0000
H	2.1509	1.2418	0.0000
H	-2.1509	-1.2418	0.0000
H	-2.1509	1.2418	0.0000
H	0.0000	2.4837	0.0000

Table S.1.3 Cartesian coordinates of chlorobenzene in the unit of $\mathring{A}$, optimized at the B3LYP/6-311G(d) level of theory.

Atom	x	y	z
C	0.0000	-1.2163	-0.1783
C	0.0000	0.0000	0.5034
C	0.0000	-1.2076	-1.5743
C	0.0000	0.0000	-2.2745
C	0.0000	1.2163	-0.1783
C	0.0000	1.2076	-1.5743
H	0.0000	-2.1514	-2.1128
H	0.0000	0.0000	-3.3607
H	0.0000	-2.1495	0.3749
H	0.0000	2.1495	0.3749
H	0.0000	2.1514	-2.1128
Cl	0.0000	0.0000	2.2644

Table S.1.4 Cartesian coordinates of nitrobenzene in the unit of $\mathring{A}$, optimized at the B3LYP/6-311G(d) level of theory.

Atom	x	y	z
C	0.0000	0.0000	-0.2450
C	0.0000	-1.2207	0.4278
C	0.0000	1.2207	0.4278
C	0.0000	1.2123	1.8209
C	0.0000	-1.2123	1.8209
C	0.0000	0.0000	2.5164
H	0.0000	2.1429	-0.1400
H	0.0000	2.1532	2.3631
H	0.0000	-2.1429	-0.1400
H	0.0000	-2.1532	2.3631
H	0.0000	0.0000	3.6028
N	0.0000	0.0000	-1.7179
O	0.0000	-1.0898	-2.2898
O	0.0000	1.0898	-2.2898

2. Active orbitals used for the CAS-CI calculations of Benzene, Chlorobenzene, Nitrobenzene

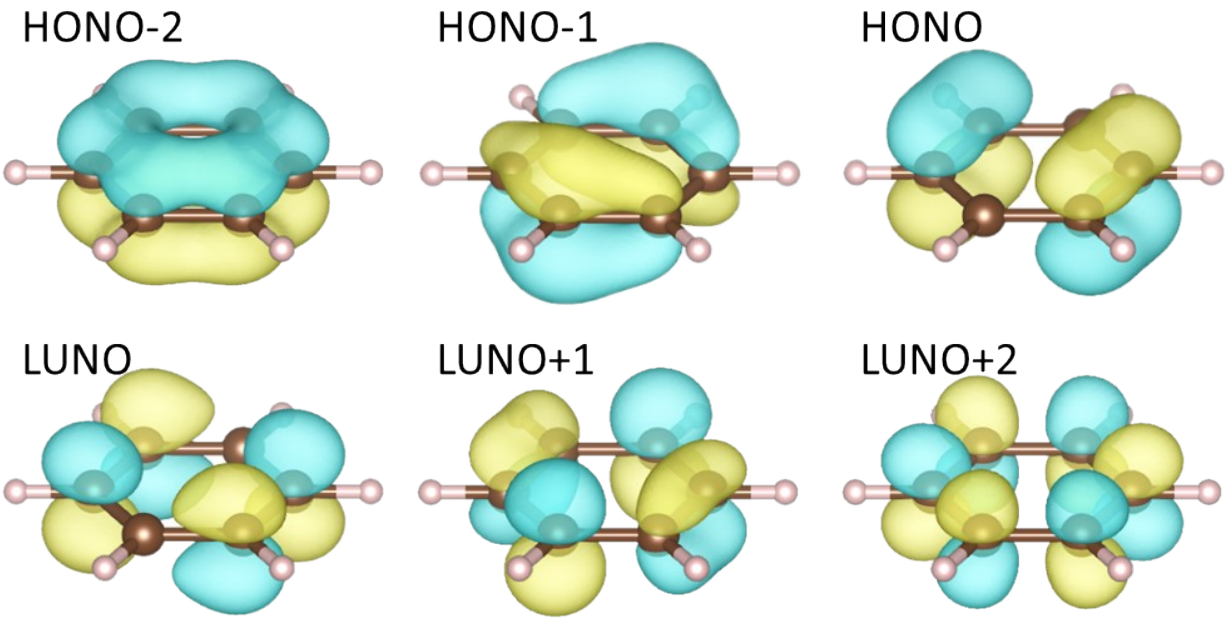

Figure S.2.1. Active orbitals used for the CAS-CI calculations of benzene. Label at the upper left of each orbital refers to the index of the pseudo-natural orbitals constructed from the MP2 calculation.

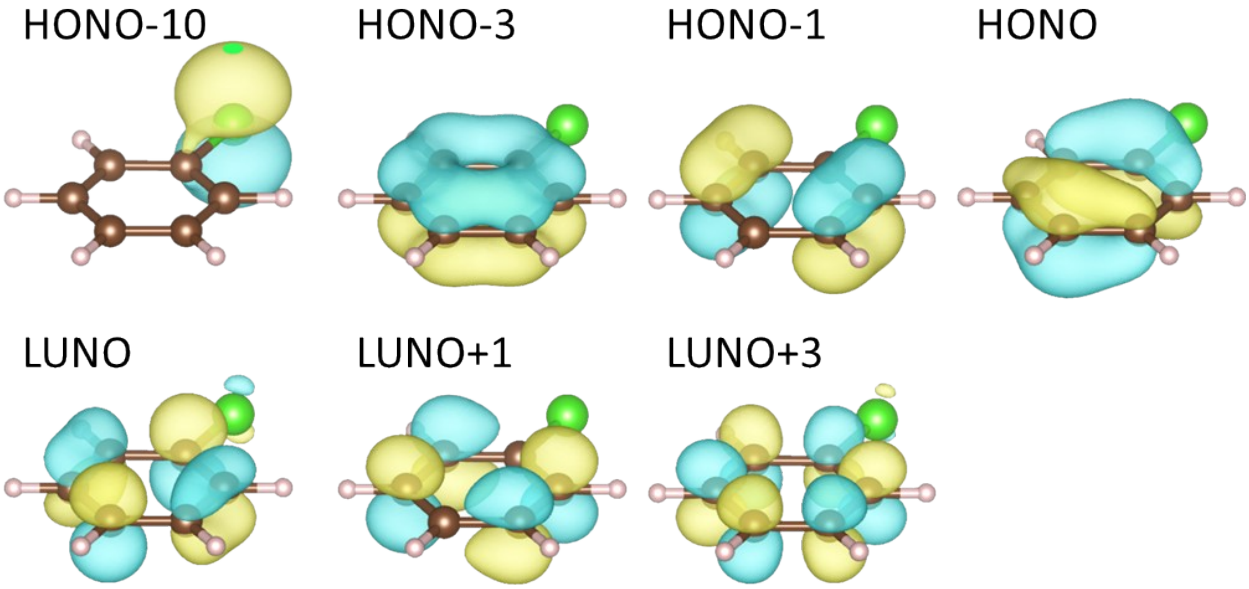

Figure S.2.2. Active orbitals used for the CAS-CI calculations of chlorobenzene. Label at the upper left of each orbital refers to the index of the pseudo-natural orbitals constructed from the MP2 calculation.

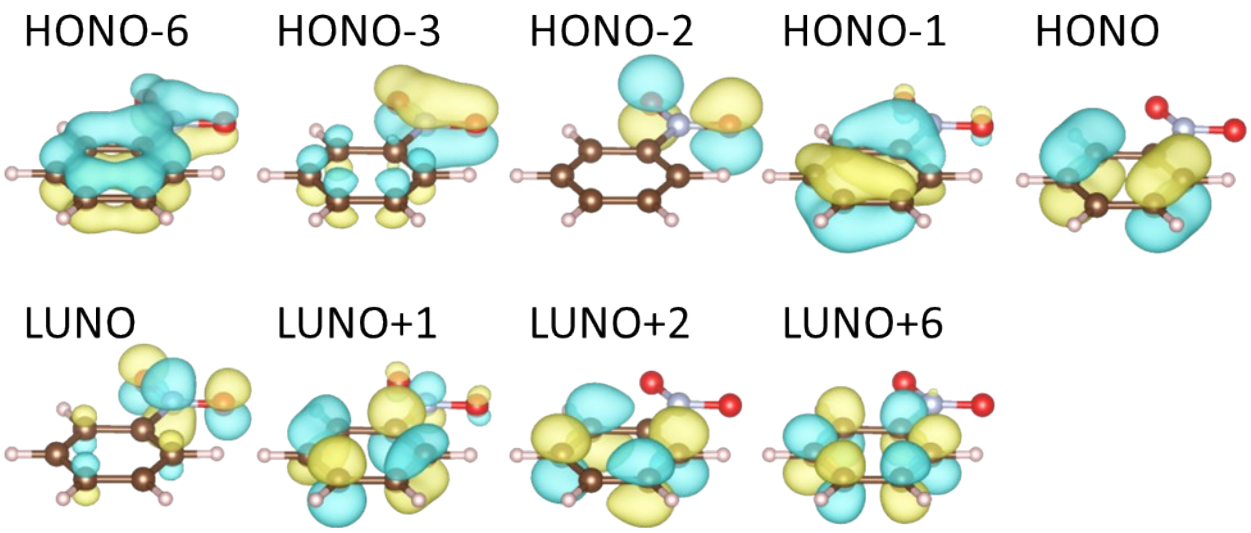

Figure S.2.3. Active orbitals used for the CAS-CI calculations of nitrobenzene. Label at the upper left of each orbital refers to the index of the pseudo-natural orbitals constructed from the MP2 calculation.

3. Details of quantum phase estimation

Table S.3.1 The detail of Hamiltonian and quantum phase estimation for LiH.

Number of qubits	13	15	17	19	21
Number of electrons	4	4	4	4	4
Number of atoms	2	2	2	2	2
Number of active spin-orbitals	12	14	16	18	20
Number of one-electron integrals	36	54	76	78	80
Number of two-electron integrals	1824	3732	6944	9012	11168
Number of quantum gates (for determining the whole 4 digits)	3888	9348	19684	26304	33884

Table S.3.2 The detail of Hamiltonian and quantum phase estimation for benzene, chlorobenzene, nitrobenzene

	Benzene	Chlorobenzene	Nitrobenzene
Number of electrons	42	58	64
Number of atoms	12	12	14
Number of active spin-orbitals	12	14	18
Number of one-electron integrals	16	58	90
Number of two-electron integrals	1184	4964	23284
Number of qubits	13	15	19
Number of quantum gates (for determining the whole 10 digits)	2420	12624	42156

4. Quantum Circuits used for the preparation of the excited state approximate wave function.

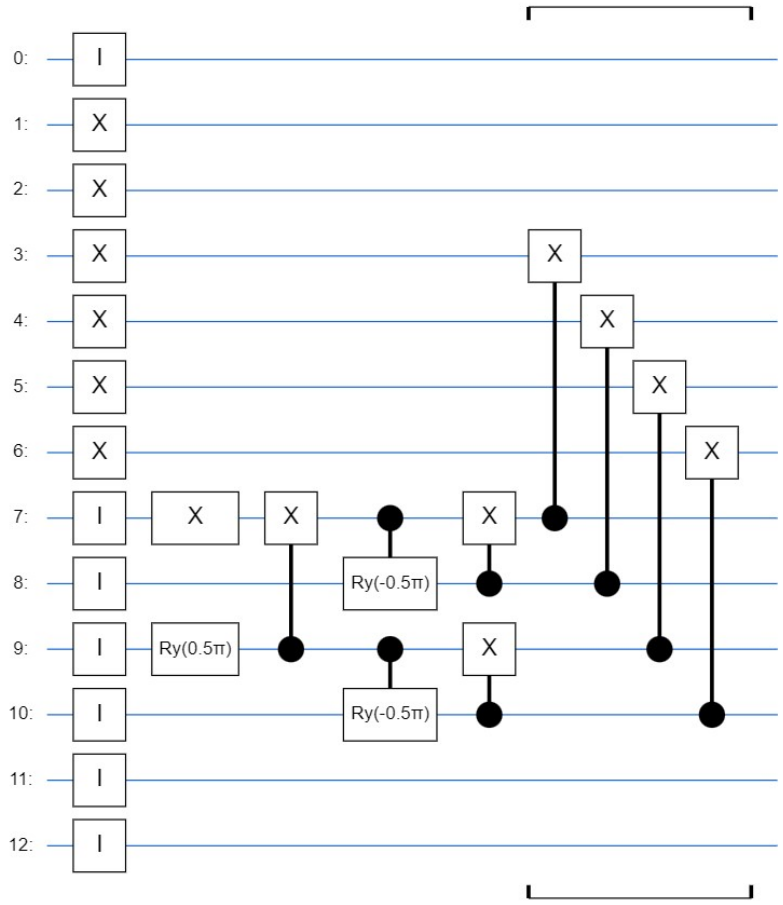

Figure S.4.1 Quantum circuit used for the preparation of the excited state approximate wave function of benzene.

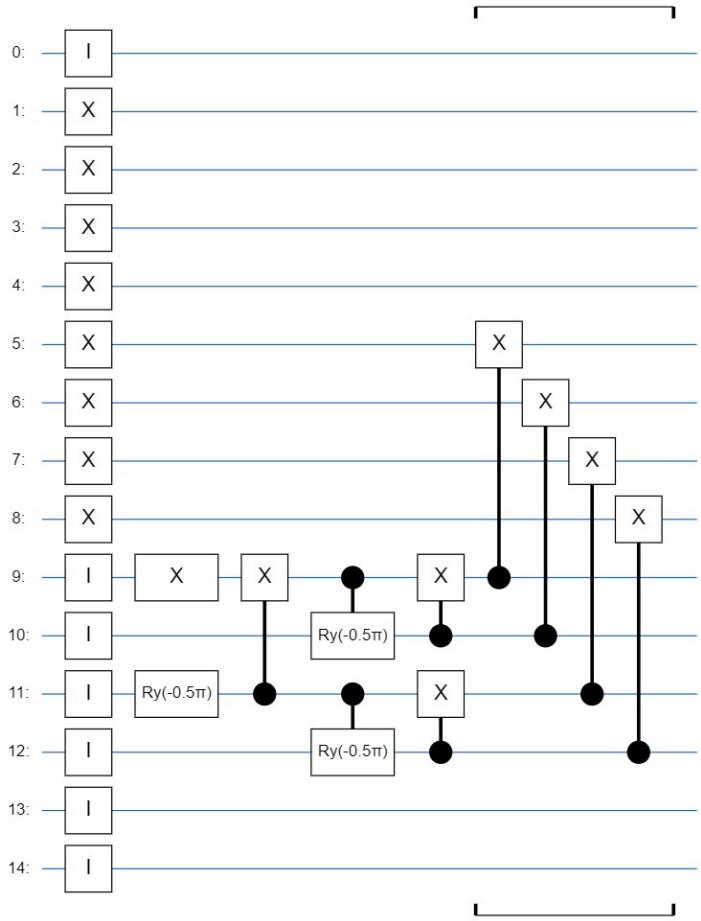

Figure S.4.2 Quantum circuit used for the preparation of the excited state approximate wave function of chlorobenzene.

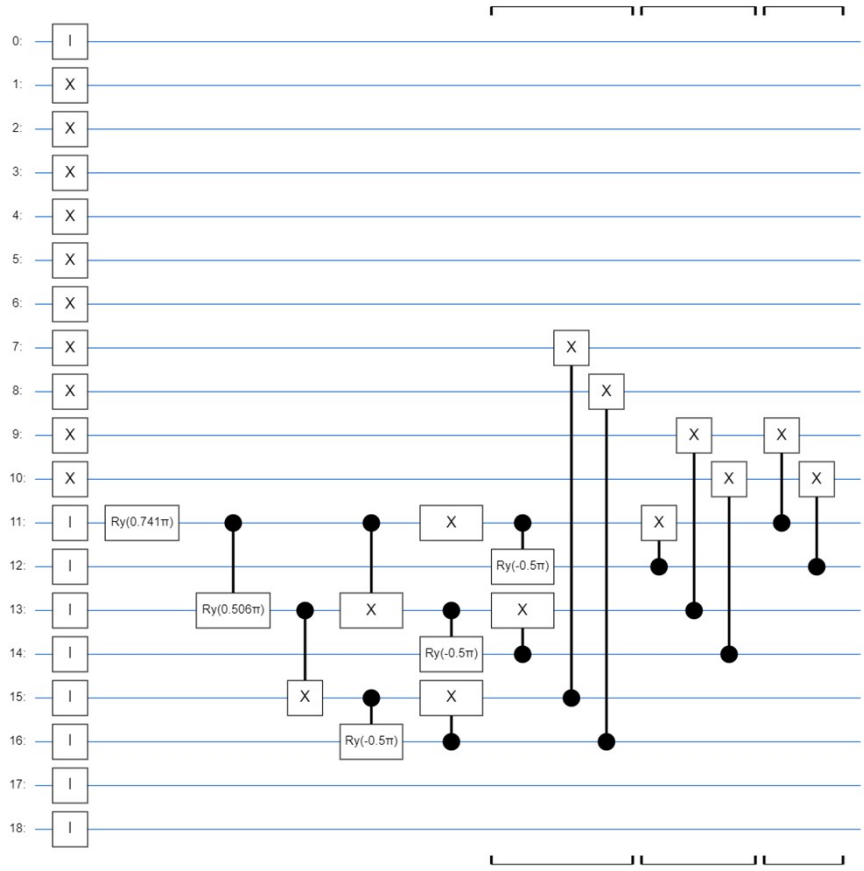

Figure S.4.3 Quantum circuit used for the preparation of the excited state approximate wave function of benzene.