Theoretical studies of the long lifetimes of the $6d\,{}^2D_{3/2,5/2}$ states in Fr: Implications for parity nonconservation measurements

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The lifetimes of the $6d\,{}^2D_{3/2}$ and $6d\,{}^2D_{5/2}$ states in Fr are estimated to be $540(10)$ ns and $1704(32)$ ns respectively. They are determined by calculating the radiative transition amplitudes of the allowed electric dipole (E1) and the forbidden electric quadrupole (E2) and magnetic dipole (M1) channels using the second order many-body perturbation theory (MBPT(2)) and the coupled-cluster (CC) method at different levels of approximation in the relativistic framework. These long lifetimes and the large electric dipole parity non conserving amplitudes of $7s\,{}^2S_{1/2} \rightarrow 6d\,{}^2D_{3/2,5/2}$ transitions strongly favour Fr as a leading candidate for the measurement of parity nonconservation arising from the neutral current weak interaction and the nuclear anapole moment.

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Francium (Fr) is considered to be a promising candidate for the measurements of the electric dipole moment (EDM) arising due to the violations of parity and time reversal symmetries [1, 2], parity nonconservation (PNC) effects due to the neutral weak interaction [2, 3] and the nuclear anapole moment [4, 5] as it is the heaviest alkali metal atom. The focus of all the ongoing Fr PNC experiments is the $7\,{}^sS_{1/2}$ metal atom. The focus of all the ongoing Fr PNC experiments is the $7s\,{}^2S_{1/2} \rightarrow 8s\,{}^2S_{1/2}$ transition [2, 3, 5]; which is largely inspired by the Cs PNC experiment [6]. However, relativistic many-body calculations show that the PNC amplitudes in the $7s\,{}^2S_{1/2} \rightarrow 6d\,{}^2D_{3/2,5/2}$ transition amplitudes in Fr are about three times larger than that of the $7s\,{}^2S_{1/2} \rightarrow 8s\,{}^2S_{1/2}$ transition [7, 8]. The $S - D$ PNC transitions in the singly ionized Ba, Ra and Yb have been the subject of theoretical investigations [9–11] and the principle of their measurements has been discussed [12, 13]. It has also been highlighted that the PNC measurements for the $S - D_{5/2}$ transitions in these ions would provide unambiguous signatures of the existence of the nuclear anapole moment (NAM) [14, 15], which is still an open question [16]. Apart from exhibiting large PNC effects, another important aspect of these transitions is that the excited $D$ states in these ions are metastable, and they provide long inter- rogation times which enhances the precision of the measurement of the small PNC effects [12]. In this Rapid Communication, we present the results of our theoretical studies on the lifetimes the $6d\,{}^2D_{3/2}$ and $6d\,{}^2D_{5/2}$ states in Fr, which were undertaken to assess the feasibility of the measurement of PNC in this atom using the $7s\,{}^2S_{1/2} \rightarrow 6d\,{}^2D_{3/2,5/2}$ transitions.

An electron from the $6d\,{}^2D_{3/2}$ state can decay to its low-lying $7p\,{}^2P_{1/2}$ and $7p\,{}^2P_{3/2}$ states by the electric dipole (E1) and forbidden magnetic octupole (M3) transitions and to the ground state by the forbidden magnetic dipole (M1) and electric quadrupole (E2) transitions. We neglect contributions due to the M3 transition as the corresponding transition probability is very weak owing to its inversely proportional to seventh power of transition wavelength. Similarly, an electron from the $6d\,{}^2D_{5/2}$ state can decay to its fine-structure partner $6d\,{}^2D_{3/2}$ state via both the M1 and E2 transitions while to the low-lying $7p\,{}^2P_{3/2}$ state by the E1 transition and to the ground state by the E2 transition. In this case too, we have omitted contributions due to the M3 transition. The transition probabilities due to the above E1, E2 and M1 channels for a transition, say, $|\Psi_i\rangle \rightarrow |\Psi_f\rangle$ are given by

\[
A_{ij}^{E1} = \frac{2.0261 \times 10^{-6}}{\lambda_{ij}^3 g_i} S_{ij}^{E1},
\]

\[
A_{ij}^{E2} = \frac{1.1195 \times 10^{-22}}{\lambda_{ij}^5 g_i} S_{ij}^{E2},
\]

\[
A_{ij}^{M1} = \frac{2.6971 \times 10^{-11}}{\lambda_{ij}^3 g_i} S_{ij}^{M1},
\]

where the quantity $S_{ij}^O = |\langle \Psi_i | O | \Psi_f \rangle|^2$ is known as the line strength for the corresponding reduced matrix element $|\langle \Psi_i | O | \Psi_f \rangle|^2$ of a transition operator $O$. These
quantities are later given in atomic unit (a.u.). In the 
above expressions, \( g_i = 2J_i + 1 \) is the degeneracy factor 
of the state \( |\Psi_i\rangle \) with the angular momentum \( J_i \) and the 
transition wavelength (\( \lambda_{ij} \)) is used in nm which when 
substituted, the transition probabilities (\( A_{ij}^{(n)} \)) are 
obtained in \( s^{-1} \). The lifetime (\( \tau \)) of the atomic state \( |\Psi_i\rangle \) is 
determined by taking the reciprocal of the total emission 
transition probabilities involving all the possible spontaneous 
transition channels (in \( s \)). i.e.

\[
\tau_i = \frac{1}{\sum_{O,f} A_{ij}^{(n)}} 
\]

where the summations over \( O \) and \( f \) correspond to all 
probable decay channels and all the lower states respectively. 
We have attempted to obtain accurate results for the transition probabilities, hence the lifetimes of the 
atomic states by performing relativistic many-body calculations of the line strengths and using wavelengths that 
are determined from the experimental transition energies 
given in the National Institute of Science and Technology 
(NIST) database [19].

To investigate the role of the electron correlation effects 
in the evaluation of the radiative transition amplitudes, we 
employ the second order many-body perturbation theory 
(MBPT(2)) and the coupled-cluster (CC) method in the 
relativistic framework. Further, we take different lev-
els of approximation in the CC method to see the conver-
genence in the results. We give below a brief description of 
these methods using Bloch’s prescription [20], in which 
atomic wave function of state \( |\Psi_n\rangle \) is expressed as 

\[
|\Psi_n\rangle = \Omega_n|\Phi_n\rangle, 
\]

where \( \Omega_n \) and \( |\Phi_n\rangle \) are known as the wave operator and 
reference state respectively. The ground and the consid-
ered excited 6d states of Fr have the electronic configurations 
as \[ 6p^67s^22^3S_{1/2} \] and \[ 6p^67d^22^3D_{3/2,5/2} \] respectively. 
To reduce the computational effort, we construct these 
states by creating a common reference state function \( |\Phi_e\rangle \) with the \( 6p^6 \) configuration using the 
Dirac-Hartree-Fock (DHF) method. In this approach the atomic Hamiltonian 
(\( H \)) in the Dirac-Coulomb interaction approximation is 
divided as DHF Hamiltonian \( H_0 \) and residual Coulomb 
interaction \( V_r \). For the calculation of the exact states 
with a valence orbital, we define new working reference 
states as \( |\Phi_n\rangle = a_n^\dagger |\Phi_c\rangle \). Here \( a_n^\dagger \) appends an electron 
from the respective valence orbital denoted by an index 
\( n \). As a consequence \( \Omega_n \) can now be divided as 

\[
\Omega_n = 1 + \chi_c + \chi_n, 
\]

where \( \chi_c \) and \( \chi_n \) are responsible for carrying out excitations 
(generating configuration state functions) from \( |\Phi_c\rangle \) and 
\( |\Phi_n\rangle \), respectively, due to \( V_r \). In a perturbative series 
expansion, we have 

\[
\chi_c = \sum_k \chi_c^{(k)} \quad \text{and} \quad \chi_n = \sum_k \chi_n^{(k)}. 
\]

In these expressions, the superscripts imply number of \( V_r \) 
considered in the calculations and represents order of perturbation; e.g. MBPT(2) method bears terms up to 
two \( V_r \) \((k = 2)\).

Using the generalized Bloch’s equation, \( k \)th order am-
plitudes for the \( \chi_c \) and \( \chi_n \) operators are obtained by [20]

\[
[\chi_c^{(k)}, H_0]P = QV_r(1 + \chi_c^{(k-1)})P, 
\]

and 

\[
[\chi_n^{(k)}, H_0]P = QV_r(1 + \chi_c^{(k-1)} + \chi_n^{(k-1)})P - \sum_{m=1}^{k-1} \chi_n^{(k-m)} 
\times PV_r(1 + \chi_c^{(m-1)} + \chi_n^{(m-1)})P, 
\]

where the projection operators \( P = |\Phi_e\rangle \langle \Phi_e| \) and \( Q = 1 - 
P \) describe the model space and the orthogonal space of 
the Hamiltonian \( H_0 \) respectively. Note that here \( \chi_c^{(0)} = 0 \) 
and \( \chi_n^{(0)} = 0 \). Using these amplitudes, the energy of the state \( |\Psi_n\rangle \) is evaluated by using an effective Hamiltonian 

\[
H_n^{eff} = PH\Omega_n P. 
\]

Using the CC ansatz, the above expressions can be put 
together to construct a wave operator to infinite order as 

\[
|\Psi_n\rangle = \Omega_n|\Phi_n\rangle = e^{T(1 + S_n)}|\Phi_c\rangle, 
\]

such that \( \chi_c = e^{T} - 1 \) and \( \chi_n = e^{S_n} - 1 \). Here the 
\( T \) and \( S_n \) are the CC excitation operators that excite 
electrons from the core and core along with the valence orbital 
respectively. In this work, we have only accounted 
the singly and doubly excited states denoting the CC 
operators by subscripts 1 and 2 respectively as 

\[
T = T_1 + T_2 \quad \text{and} \quad S_n = S_{1n} + S_{2n}. 
\]

This is referred to as the CCSD method in the literature. 
When only the linear terms are retain in Eq. (11) with 
singles and doubles approximation, it is referred to as 
the LCCSD method. The amplitudes of the \( T \) and \( S_n \) 
operators are determined using the expressions 

\[
H_N\chi_c P = QH_N P 
\]

and 

\[
H_N\chi_n P = QH_N(1 + \chi_c)P - \chi_n H_N^{eff} 
\]

where we have defined normal order Hamiltonian \( H_N = 
H - PHP \) and the effective Hamiltonian to evaluate ion-
ization potential (IP) of an electron from the valence 
orbital \( n \) of the respective state is given by \( H_N^{eff} = 
PH_N(1 + \chi_c + \chi_n)P \). We have also included contribu-
tions from important triples excitations perturbatively 
from \( \chi_c^{(2)} \) and \( \chi_n^{(2)} \) in the construction of \( H_N^{eff} \) and the 
approach is referred to as the CCSD(T) method.
After obtaining amplitudes using the above equations, the transition matrix element of an operator $O$ between the states $|\Psi_i\rangle$ and $|\Psi_f\rangle$ is evaluated using the expression

$$\frac{\langle\Psi_f|O|\Psi_i\rangle}{\langle\Psi_f|\Psi_f\rangle^{1/2}} = \frac{\langle\Phi_f|\Omega_{\Psi_f}|\Phi_i\rangle}{\langle\Phi_f|\Omega_{\Psi_f}|\Phi_f\rangle^{1/2}}$$  \hspace{1cm} (15)$$

This gives rise to a finite number of terms for the MBPT(2) and LCCSD methods, but it involves two non-terminating series in the numerator and denominator which are $e^{T^i}Oe^{T}$ and $e^{T^i}e^{T}$ respectively in the CCSD and CCSD(T) methods. In order to evaluate all the significant contributions from these series, we have used the Wick’s generalized theorem $[20]$ to divide these terms into the effective one-body, two-body and three-body terms. The effective one-body terms are the dominant ones, they are computed first considering the CC terms with the approximations $e^{T^i}Oe^{T} \approx O + OT + T^1O + \frac{1}{2}OT^2 + \frac{1}{4}T^2O + T^1OT$ and $e^{T^i}e^{T} \approx T^1T + \frac{1}{2}T^1T^2 + \frac{1}{2}T^1T^2$. Then, they are stored and contracted with the $T_2$ and $T_2^\dagger$ operators avoiding repetitions of the diagrams in a self-consistent procedure to account for the higher order one-body terms from the non-terminating series. They are again stored as an intermediate form for the further contraction with the $S_n$ and $S_n^\dagger$ operators. Similarly the effective two-body and three-body terms are computed after contracting with the above effective one-body terms with the $T_2$ and $T_2^\dagger$ operators, but they are computed directly contracting with the $S_n$ and $S_n^\dagger$ operators. Thus, these effective two-body and three-body terms also have contributions from the non-terminating series. To see the convergence of the results with the series expansion, we present contributions with $k$ numbers of $T$ and/or $T^i$ operators from these non-terminating series, which we refer to as the CCSD$^{(k)}$ method considering terms up to $k \rightarrow \infty$ in a self-consistent procedure as described above. Our final CCSD results correspond to the CCSD$^{(\infty)}$ method. The same procedure is also adopted for the CCSD(T) method. The contribution from the normalizations of the wave functions ($C_{\text{norm}}$) is estimated explicitly using the expression

$$C_{\text{norm}} = \left[\frac{\langle\Psi_f|O|\Psi_i\rangle}{\langle\Psi_f|\Psi_f\rangle^{1/2}} - \langle\Psi_f|O|\Psi_i\rangle\right]. \hspace{1cm} (16)$$

In Table I we give the radiative transition matrix elements for all the considered channels from the DHF, MBPT(2), LCCSD, CCSD and CCSD(T) methods to analyze the propagation of the correlation effects through various levels of approximations in the many-body theories and the experimental values of the transition wavelengths from the NIST database $[19]$ that we have used later. We also give contributions from the CCSD method by truncating the non-linear terms with $k = 2$, $k = 4$ and from a self-consistent ($k = \infty$) calculation. For $k = 2$, the expression evaluating the property given by Eq. (15) has the same number of terms as does the LCCSD method. Therefore, differences in the results from the LCCSD and CCSD$^{(2)}$ methods imply the correlation contributions arising through the non-linear terms in the wave function determining equations of the CCSD method and are found to be quite large. Often, these contributions are neglected in the calculations as they require prohibitively large computational resources for their evaluation. Again, we observe from the trends that the correlation effects at the MBPT(2) method are large, and that there are strong cancellations in the LCCSD approximation and the results almost converge for $k = 4$ when non-linear terms are included in the CCSD method. The

| $J_i \rightarrow J_f$ | $\lambda_{Jf}$ | DHF | MBPT(2) | LCCSD | CCSD$^{(2)}$ | CCSD$^{(4)}$ | CCSD$^{(\infty)}$ | CCSD(T) | Uncertainties |
|----------------------|-------------|-----|--------|--------|-------------|-------------|-------------|----------|--------------|
|                      |             |     |        |        |             |             |             |          | Basis Breit QED |
| $6d^2D_{3/2} \rightarrow 7p^2P_{1/2}$ | 2504.7 | 9.22 | 7.73   | 6.81   | 7.46        | 7.47        | 7.47        | 7.43     | 0.05 -0.01 0.001 |
| $6d^2D_{3/2} \rightarrow 7p^2P_{3/2}$ | 4336.7 | 4.28 | 3.57   | 3.12   | 3.44        | 3.45        | 3.45        | 3.42     | 0.02 -0.01 0.001 |
| $6d^2D_{3/2} \rightarrow 7p^2P_{1/2}$ | 3991.0 | 12.80| 10.83  | 9.68   | 10.54       | 10.55       | 10.55       | 10.51    | 0.07 -0.02 0.001 |

TABLE I: Magnitudes of the reduced matrix elements $\langle J_i|O|J_f \rangle$ of transition operators (Os) given in a.u. from different many-body methods. Uncertainties from the finite size basis set, non-inclusion of the Breit interaction and due to QED effects are quoted using the MBPT(2) method. Wavelengths $(\lambda_{Jf})$ from the NIST database $[19]$ are quoted in nm for the respective transitions.
discrepancy in the results of the CCSD(4) and CCSD(∞) methods is beyond second significant digit implying that the results have converged within the precision of our interest. The valence triple excitations seem to change the results slightly. We also give uncertainties associated with these results by estimating contributions due to the finite size of our basis set, neglected contributions from the Breit interaction and corrections from the quantum electrodynamics (QED). These estimates are carried out using the MBPT(2) method which gives the largest correlation effects.

After analyzing the trends in the correlation effects at different levels of approximation, we now focus on the contributions from different terms in the CCSD method. We present these results in Table II along with the contributions from $C_{norm}$. Contributions from the corresponding radiative operator $O$ are the DHF results, $OT_1$ and its complex conjugate terms give core-valence correlations, $OS_{1f}$ and $S_{1f}^\dagger O$ give the pair correlation effects involving the valence orbitals, $OS_{2f}$ and $S_{2f}^\dagger O$ give the core-polarization correlation effects involving the valence orbitals, etc. Contributions from the other non-linear terms such as representing the core pair correlation effects coming through the $T_{3f}^d$ matrix element are not given explicitly in the above table, however their contributions can be obtained by taking the differences of the contributions given in Table III and the final CCSD results given in Table I. As can be seen from Table III, core-valence correlations are small and the largest correlation effects come through the pair correlation effects in the E1 and E2 matrix element calculations. Nevertheless, the core-polarization effects are also very significant and are the dominant ones in the calculations of the M1 matrix elements. We also find contributions from $C_{norm}$ to be fairly large.

We now use the matrix elements from the CCSD(T) method and the experimental wavelengths mentioned in Table I to evaluate the transition probabilities due to different radiative decay channels from the $6d \rightarrow 3/2$ and $6d \rightarrow 5/2$ states. These values are given in Table III along with their branching ratios for the individual transitions. As can be seen from this table that branching ratios are dominated by the E1 transitions and they are entirely responsible for determining the lifetimes of the $6d \rightarrow 3/2$ and $6d \rightarrow 5/2$ states. Using these transition probabilities, we estimate the lifetimes of the $6d \rightarrow 3/2$ and $6d \rightarrow 5/2$ states as $\tau_{6d3/2} = 540(10)$ ns and $\tau_{6d5/2} = 1704(32)$ ns, respectively. These values are very large compared to the other low-lying excited $7p \rightarrow 2P_{1/2}$, $8s \rightarrow 2S_{1/2}$, $7p \rightarrow 2P_{1/2,3/2}$, $7d \rightarrow 2D_{3/2,5/2}$ and $9s \rightarrow 2S_{1/2}$ states of Fr which are measured till date as $\tau_{7pl_1/2} = 29.45(11)$ ns, $\tau_{7pl_3/2} = 21.02(15)$ ns, $\tau_{7sl_1/2} = 53.30(44)$ ns, $\tau_{7sl_3/2} = 73.6(3)$ ns and $\tau_{7dl_5/2} = 67.7(29)$ ns, $\tau_{7sp1/2} = 149.3(5)$ ns, $\tau_{7sp3/2} = 83.5(1.5)$ ns and $\tau_{9sl_1/2} = 107.53(90)$ ns respectively [21].

Table II: Contributions to the reduced matrix elements $\langle J_i | O | J_f \rangle$ from various terms of the CCSD method (in a.u.). Differences between these values from the CCSD results are quoted in Table II correspond to those non-linear terms that are not mentioned explicitly here.

| $J_i \rightarrow J_f$ | $O$ | $OT_1$ | $T_{3f}^d$ | $OS_{1f}$ | $S_{1f}^\dagger O$ | $OS_{2f}$ | $S_{2f}^\dagger O$ | $OS_{1f}^\dagger OS_{1f}$ | $S_{2f}^\dagger OS_{2f}$ | $S_{2f}^\dagger OS_{1f}$ | $C_{norm}$ |
|----------------------|-----|--------|----------------|--------|----------------|--------|----------------|----------------|----------------|----------------|--------|
| $6d \rightarrow 7p \ 2P_{1/2}$ | $E1$ | $6.306$ | $-0.003$ | $-0.002$ | $-0.001$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ |
| $6d \rightarrow 7p \ 2P_{3/2}$ | $E2$ | $6.306$ | $-0.003$ | $-0.002$ | $-0.001$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ |
| $6d \rightarrow 7s \ 2S_{1/2}$ | $M1$ | $9.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ |
| $6d \rightarrow 7s \ 2P_{1/2}$ | $E1$ | $6.306$ | $-0.003$ | $-0.002$ | $-0.001$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ |
| $6d \rightarrow 7s \ 2P_{3/2}$ | $E2$ | $6.306$ | $-0.003$ | $-0.002$ | $-0.001$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ |
| $6d \rightarrow 7s \ 2S_{1/2}$ | $M1$ | $9.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ |
| $6d \rightarrow 7s \ 2P_{1/2}$ | $E1$ | $6.306$ | $-0.003$ | $-0.002$ | $-0.001$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ |
| $6d \rightarrow 7s \ 2P_{3/2}$ | $E2$ | $6.306$ | $-0.003$ | $-0.002$ | $-0.001$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ |
| $6d \rightarrow 7s \ 2S_{1/2}$ | $M1$ | $9.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ | $-0.000$ |

Table III: Transition probabilities ($A_{O}^{E}$) due to different transition decay channels (Os) in s$^{-1}$ and their branching ratios from the $6d \rightarrow 3/2$ and $6d \rightarrow 5/2$ states of Fr. Uncertainties are quoted within the parentheses.

| $J_i \rightarrow J_f$ | $O$ | $A_{O}^{E}$ | Branching ratio |
|----------------------|-----|------------|----------------|
| $6d \rightarrow 7p \ 2P_{1/2}$ | $E1$ | $1779511(33688)$ | $0.96$ |
| $6d \rightarrow 7p \ 2P_{3/2}$ | $E1$ | $1779511(33688)$ | $0.94$ |
| $6d \rightarrow 7s \ 2S_{1/2}$ | $E2$ | $53.96(60)$ | $0.00$ |
| $6d \rightarrow 7s \ 2P_{1/2}$ | $E1$ | $58677(11219)$ | $1.00$ |
| $6d \rightarrow 7s \ 2P_{3/2}$ | $E2$ | $39.33(19)$ | $0.00$ |
| $6d \rightarrow 7s \ 2S_{1/2}$ | $M1$ | $0.00$ | $0.00$ |
| $6d \rightarrow 7s \ 2P_{1/2}$ | $E1$ | $58677(11219)$ | $1.00$ |
| $6d \rightarrow 7s \ 2P_{3/2}$ | $E2$ | $39.33(19)$ | $0.00$ |
| $6d \rightarrow 7s \ 2S_{1/2}$ | $M1$ | $0.00$ | $0.00$ |
lifetimes of the excited $6d^2D_{3/2}$ and $6d^2D_{5/2}$ states, make Fr a potentially attractive candidate for a PNC experiment.

In summary, we have performed relativistic many-body calculations of the lifetimes of the $6d^2D_{3/2}$ and $6d^2D_{5/2}$ states of Fr and they are found to be large. These results favour the measurement of PNC in the $7s^2S_{1/2} \rightarrow 6d^2D_{3/2}$ and $7s^2S_{1/2} \rightarrow 6d^2D_{5/2}$ transitions of Fr, where calculations predict large PNC effects. For the evaluation of the lifetimes, we have calculated radiative transition matrix elements using the relativistic CC method. We have also investigated the roles of the electron correlation effects in the determination of these quantities systematically by approximating many-body methods at different levels and give contributions explicitly from various CCSD terms.

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