1. **Supplementary Materials S1.** The QTAIM \( \{q,q'\} \) path-packets of the cyclazine molecular graph for the \( S_1 \) and \( T_1 \) states without and with an applied electric (E)-field.

2. **Supplementary Materials S2.** The QTAIM \( \{p,p'\} \) path-packets of the cyclazine molecular graph for the \( S_1 \) and \( T_1 \) states without and with an applied electric (E)-field.

3. **Supplementary Materials S3.** The values of the precession \( \mathbb{K} \) along the C3-C5 \( BCP \) bond-paths for the \( S_1 \) and \( T_1 \) states
1. Supplementary Materials S1.

For the precession of the \( \{q,q'\} \) path-packet, defined by the \( e_2 \) eigenvector, about the bond-path, \( \beta = (\pi/2 - \alpha) \) and \( \alpha \) is defined by equation (2) and the right panel of Scheme 1 of the main text, we can write an expression \( K' \) for the bond-path-flexibility:

\[
K' = 1 - \cos^2 \beta, \quad \text{where} \quad \cos \beta = e_2 \cdot u, \quad \beta = (\pi/2 - \alpha) \quad \text{and} \quad 0 \leq K' \leq 1 \quad (2)
\]

For \( K' = 0 \) we have a maximum degree of facile character and for \( K = 1 \) we have the minimum degree of facile character and values of \( K' = 0 \) and \( K' = 1 \) therefore indicate bond-paths with the lowest and highest tendencies towards bond-path-flexibility respectively.
Figure S1(I). The QTAIM \{q,q'\} path-packets of the cyclazine molecular graph corresponding to the $S_1$ (left panel) and $T_1$ (right panel) states of the unchirped pulse 30 fs, 40 fs, 50 fs and 75 fs with a positive energy gap $\Delta E(S_1-T_1) > 0$ are presented in each of sub-figures (a-d) respectively.
Figure S1(II). The QTAIM \{q,q'\} path-packets of the cyclazine molecular graph corresponding to the S₁ (left panel) and T₁ (right panel) states of the unchirped pulse 5fs, 10fs, 60fs and 65fs with a negative energy gap $\Delta E(S₁-T₁) < 0$ are presented in each of sub-figures (a-d) respectively.
Figure S1(III). The QTAIM $\{q,q'\}$ path-packets of the cyclazine molecular graph corresponding to the $S_1$ (left panel) and $T_1$ (right panel) states of the chirped pulse 10 fs, 45 fs, 67 fs and 90 fs with a positive energy gap $\Delta E(S_1-T_1) > 0$ are presented in each of sub-figures (a-d) respectively.
Figure S1(IV). The QTAIM \{q,q'\} path-packets of the cyclazine molecular graph corresponding to the S_1 (left panel) and T_1 (right panel) states of the chirped pulse 5fs, 30fs, 78fs and 100fs with a negative energy gap $\Delta E(S_1-T_1) < 0$ are presented in each of sub-figures (a-d) respectively.
Figure S1(V). The QTAIM \{q,q'\} path-packets of the cyclazine molecular graph corresponding to the \(S_1\) (left panel) and \(T_1\) (right panel) states of an applied electric(E)-field = \(\pm 0.2\) a.u are presented in each of sub-figures (a-b) respectively.
2. Supplementary Materials S2.
Figure S2(I). The QTAIM \{p, p'\} path-packets of the cyclazine molecular graph corresponding to the $S_1$ (left panel) and $T_1$ (right panel) states of the unchirped pulse 30 fs, 40 fs, 50 fs and 75 fs with a positive energy gap $\Delta E(S_1-T_1) > 0$ are presented in each of sub-figures (a-d) respectively.
The QTAIM \{p,p'\} path-packets of the cyclazine molecular graph corresponding to the S\(_1\) (left panel) and T\(_1\) (right panel) states of the unchirped pulse 5fs, 10fs, 60fs and 65fs with a negative energy gap \(\Delta E(S_1-T_1) < 0\) are presented in each of sub-figures (a-d) respectively.
Figure S2(III). The QTAIM \{p,p'\} path-packets of the cyclazine molecular graph corresponding to the $S_1$ (left panel) and $T_1$ (right panel) states of the chirped pulse 10 fs, 45 fs, 67 fs and 90 fs with a positive energy gap $\Delta E(S_1-T_1) > 0$ are presented in each of sub-figures (a-d) respectively.
Figure S2(IV). The QTAIM \{p,p'\} path-packets of the cyclazine molecular graph corresponding to the $S_1$ (left panel) and $T_1$ (right panel) states of the chirped pulse 5fs, 30fs, 78fs and 100fs with a negative energy gap $\Delta E(S_1-T_1) < 0$ are presented in each of sub-figures (a-d) respectively.
Figure S2(V). The QTAIM \(\{p,p'\}\) path-packets of the cyclazine molecular graph corresponding to the \(S_1\) (left panel) and \(T_1\) (right panel) states of an applied electric\((E)\)-field = \(\pm 0.2\) a.u are presented in each of sub-figures (a-b) respectively.
Figure S3(1). The values of the precession $K$ along the C7-N9 BCP bond-paths for the $S_1$ and $T_1$ states of the unchirped pulse with a positive energy gap $\Delta E(S_1-T_1) > 0$ (top-left) of sub-figure, the unchirped pulse with a negative energy gap $\Delta E(S_1-T_1) < 0$ (top-right) of sub-figure. The chirped pulse with $\Delta E(S_1-T_1) > 0$ (bottom-left) of sub-figure and the chirped pulses with $\Delta E(S_1-T_1) < 0$ (bottom-right) of sub-figure.
Figure S3(I). The values of the precession $\mathcal{K}$ along the C13-N9 BCP bond-paths for the $S_1$ and $T_1$ states of the unchirped pulse with a positive energy gap $\Delta E(S_1-T_1) > 0$ (top-left) of sub-figure, the unchirped pulse with a negative energy gap $\Delta E(S_1-T_1) < 0$ (top-right) of sub-figure. The chirped pulse with $\Delta E(S_1-T_1) > 0$ (bottom-left) of sub-figure and the chirped pulses with $\Delta E(S_1-T_1) < 0$ (bottom-right) of sub-figure.
The profiles of the $\mathbf{K}$ for the C10-C2 BCP with the unchirped laser pulse corresponding to a $S_1$ state at a given time with $\Delta E(S_1-T_1) > 0$ responding less than the corresponding $T_1$ state the same time, see the top-left panel of Figure S3(III). The corresponding $\mathbf{K}$ for the C10-C2 BCP with $\Delta E(S_1-T_1) < 0$ and unchirped pulse result in a mixing of the $\mathbf{K}$ profiles of the $S_1$ and $T_1$ states, see the top-right panel of Figure S3(III). The effect of the chirped laser pulse on the $\mathbf{K}$ profiles with a positive energy gap $\Delta E(S_1-T_1) > 0$ is to spread out the $\mathbf{K}$ profiles of the $S_1$ and $T_1$ states, see the bottom-left panel of Figure S3(III). Conversely, the effect of the chirped pulse on negative energy gap $\Delta E(S_1-T_1) < 0$ is to contract the $\mathbf{K}$ profiles corresponding to the $S_1$ and $T_1$ states to closer together, see the bottom-right panel of Figure S3(III).

Figure S3(III). The values of the precession $\mathbf{K}$ along the C10-C2 BCP bond-paths for the $S_1$ and $T_1$ states of the unchirped pulse with a positive energy gap $\Delta E(S_1-T_1) > 0$ (top-left) of sub-figure, the unchirped pulse with a negative energy gap $\Delta E(S_1-T_1) < 0$ (top-right) of sub-figure. The chirped pulse with $\Delta E(S_1-T_1) > 0$ (bottom-left) of sub-figure and the chirped pulse $s$ with $\Delta E(S_1-T_1) < 0$ (bottom-right) of sub-figure.
Figure S3(IV). The values of the precession $\vec{K}$ along the C3-C5 BCP bond-paths for the $S_1$ and $T_1$ states of the unchirped pulse with a positive energy gap $\Delta E(S_1-T_1) > 0$ (top-left) of sub-figure, the unchirped pulse with a negative energy gap $\Delta E(S_1-T_1) < 0$ (top-right) of sub-figure. The chirped pulse with $\Delta E(S_1-T_1) > 0$ (bottom-left) of sub-figure and the chirped pulse with $\Delta E(S_1-T_1) < 0$ (bottom-right) of sub-figure.
Figure S3(V). The values of the precession $\mathbf{K}$ along the C13-C16 BCP bond-paths for the $S_1$ and $T_1$ states of the unchirped pulse with a positive energy gap $\Delta E(S_1-T_1) > 0$ (top-left) of sub-figure, the unchirped pulse with a negative energy gap $\Delta E(S_1-T_1) < 0$ (top-right) of sub-figure. The chirped pulse with $\Delta E(S_1-T_1) > 0$ (bottom-left) of sub-figure and the chirped pulse with $\Delta E(S_1-T_1) < 0$ (bottom-right) of sub-figure.