

Features	Definition	Access
$q_C^N(Biaryl_{CH}^R)$	The Hirshfeld charge of the reacting carbon atom of neutral imine derived from (<i>R</i>)-C–H bond activation TS	DFT calculation based on xTB optimized geometries
$q_C^{N+1}(Biaryl_{CH}^R)$	The Hirshfeld charge of the reacting carbon atom of imine derived from (<i>R</i>)-C–H bond activation TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_C^{N-1}(Biaryl_{CH}^R)$	The Hirshfeld charge of the reacting carbon atom of imine derived from (<i>R</i>)-C–H bond activation TS with one negative charge	DFT calculation based on xTB optimized geometries
$q_C^N(Biaryl_{CH}^S)$	The Hirshfeld charge of the reacting carbon atom of neutral imine derived from (<i>S</i>)-C–H bond activation TS	DFT calculation based on xTB optimized geometries
$q_C^{N+1}(Biaryl_{CH}^S)$	The Hirshfeld charge of the reacting carbon atom of imine derived from (<i>S</i>)-C–H bond activation TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_C^{N-1}(Biaryl_{CH}^S)$	The Hirshfeld charge of the reacting carbon atom of imine derived from (<i>S</i>)-C–H bond activation TS with one negative charge	DFT calculation based on xTB optimized geometries
$q_C^N(Biaryl_{GS})$	The Hirshfeld charge of the reacting carbon atom of neutral ground state imine	DFT calculation based on xTB optimized geometries
$q_C^{N+1}(Biaryl_{GS})$	The Hirshfeld charge of the reacting carbon atom of ground state imine with one positive charge	DFT calculation based on xTB optimized geometries
$q_C^{N-1}(Biaryl_{GS})$	The Hirshfeld charge of the reacting carbon atom of ground state imine with one negative charge	DFT calculation based on xTB optimized geometries
$q_C^N(Biaryl_{AI}^R)$	The Hirshfeld charge of the reacting carbon atom of neutral imine derived from (<i>R</i>)-alkene insertion TS	DFT calculation based on xTB optimized geometries
$q_C^{N+1}(Biaryl_{AI}^R)$	The Hirshfeld charge of the reacting carbon atom of imine derived from (<i>R</i>)-alkene insertion TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_C^{N-1}(Biaryl_{AI}^R)$	The Hirshfeld charge of the reacting carbon atom of imine derived from (<i>R</i>)-alkene insertion TS with one negative charge	DFT calculation based on xTB optimized geometries
$q_C^N(Biaryl_{AI}^S)$	The Hirshfeld charge of the reacting carbon atom of neutral imine derived from (<i>S</i>)-alkene insertion TS	DFT calculation based on xTB optimized geometries
$q_C^{N+1}(Biaryl_{AI}^S)$	The Hirshfeld charge of the reacting carbon atom of imine derived from (<i>S</i>)-alkene insertion TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_C^{N-1}(Biaryl_{AI}^S)$	The Hirshfeld charge of the reacting carbon atom of imine derived from (<i>S</i>)-alkene insertion TS with one negative charge	DFT calculation based on xTB optimized geometries
$q_C^N(Biaryl_{GS})$	The Hirshfeld charge of the reacting carbon atom of neutral ground state imine	DFT calculation based on xTB optimized geometries
$q_C^{N+1}(Biaryl_{GS})$	The Hirshfeld charge of the reacting carbon atom of ground state imine with one positive charge	DFT calculation based on xTB optimized geometries
$q_C^{N-1}(Biaryl_{GS})$	The Hirshfeld charge of the reacting carbon atom of ground state imine with one negative charge	DFT calculation based on xTB optimized geometries
$q_H^N(Biaryl_{CH}^R)$	The Hirshfeld charge of the reacting hydrogen atom of neutral imine derived from (<i>R</i>)-C–H bond activation TS	DFT calculation based on xTB optimized geometries
$q_H^{N+1}(Biaryl_{CH}^R)$	The Hirshfeld charge of the reacting hydrogen atom of imine	DFT calculation based on xTB

	derived from (<i>R</i>)-C–H bond activation TS with one positive charge	optimized geometries
$q_H^{N-1}(\text{Biaryl}_{CH}^R)$	The Hirshfeld charge of the reacting hydrogen atom of imine derived from (<i>R</i>)-C–H bond activation TS with one negative charge	DFT calculation based on xTB optimized geometries
$q_H^N(\text{Biaryl}_{CH}^S)$	The Hirshfeld charge of the reacting hydrogen atom of neutral imine derived from (<i>S</i>)-C–H bond activation TS	DFT calculation based on xTB optimized geometries
$q_H^{N+1}(\text{Biaryl}_{CH}^S)$	The Hirshfeld charge of the reacting hydrogen atom of imine derived from (<i>S</i>)-C–H bond activation TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_H^{N-1}(\text{Biaryl}_{CH}^S)$	The Hirshfeld charge of the reacting hydrogen atom of imine derived from (<i>S</i>)-C–H bond activation TS with one negative charge	DFT calculation based on xTB optimized geometries
$q_H^N(\text{Biaryl}_{GS})$	The Hirshfeld charge of the reacting hydrogen atom of neutral ground state imine	DFT calculation based on xTB optimized geometries
$q_H^{N+1}(\text{Biaryl}_{GS})$	The Hirshfeld charge of the reacting hydrogen atom of ground state imine with one positive charge	DFT calculation based on xTB optimized geometries
$q_H^{N-1}(\text{Biaryl}_{GS})$	The Hirshfeld charge of the reacting hydrogen atom of ground state imine with one negative charge	DFT calculation based on xTB optimized geometries
$f_C^0(\text{Biaryl}_{CH}^R)$	The condensed-to-atom Fukui function of the reacting carbon atom of imine derived from (<i>R</i>)-C–H bond activation TS	$f_C^0 = \frac{q_C^{N-1} - q_C^{N+1}}{2}$
$f_C^+(\text{Biaryl}_{CH}^R)$	The condensed-to-atom Fukui function of the reacting carbon atom of imine derived from (<i>R</i>)-C–H bond activation TS	$f_C^+ = q_C^N - q_C^{N+1}$
$f_C^-(\text{Biaryl}_{CH}^R)$	The condensed-to-atom Fukui function of the reacting carbon atom of imine derived from (<i>R</i>)-C–H bond activation TS	$f_C^- = q_C^{N-1} - q_C^N$
$f_C^0(\text{Biaryl}_{CH}^S)$	The condensed-to-atom Fukui function of the reacting carbon atom of imine derived from (<i>S</i>)-C–H bond activation TS	$f_C^0 = \frac{q_C^{N-1} - q_C^{N+1}}{2}$
$f_C^+(\text{Biaryl}_{CH}^S)$	The condensed-to-atom Fukui function of the reacting carbon atom of imine derived from (<i>S</i>)-C–H bond activation TS	$f_C^+ = q_C^N - q_C^{N+1}$
$f_C^-(\text{Biaryl}_{CH}^S)$	The condensed-to-atom Fukui function of the reacting carbon atom of imine derived from (<i>S</i>)-C–H bond activation TS	$f_C^- = q_C^{N-1} - q_C^N$
$f_C^0(\text{Biaryl}_{GS})$	The condensed-to-atom Fukui function of the reacting carbon atom of ground state imine	$f_C^0 = \frac{q_C^{N-1} - q_C^{N+1}}{2}$
$f_C^+(\text{Biaryl}_{GS})$	The condensed-to-atom Fukui function of the reacting carbon atom of ground state imine	$f_C^+ = q_C^N - q_C^{N+1}$
$f_C^-(\text{Biaryl}_{GS})$	The condensed-to-atom Fukui function of the reacting carbon atom of ground state imine	$f_C^- = q_C^{N-1} - q_C^N$
$f_C^0(\text{Biaryl}_{Al}^R)$	The condensed-to-atom Fukui function of the reacting carbon atom of imine derived from (<i>R</i>)-alkene insertion TS	$f_C^0 = \frac{q_C^{N-1} - q_C^{N+1}}{2}$
$f_C^+(\text{Biaryl}_{Al}^R)$	The condensed-to-atom Fukui function of the reacting carbon atom of imine derived from (<i>R</i>)-alkene insertion TS	$f_C^+ = q_C^N - q_C^{N+1}$
$f_C^-(\text{Biaryl}_{Al}^R)$	The condensed-to-atom Fukui function of the reacting carbon atom of imine derived from (<i>R</i>)-alkene insertion TS	$f_C^- = q_C^{N-1} - q_C^N$

$f_C^0(Biaryl_{AI}^S)$	The condensed-to-atom Fukui function of the reacting carbon atom of imine derived from (S)-alkene insertion TS	$f_C^0 = \frac{q_C^{N-1} - q_C^{N+1}}{2}$
$f_C^+(Biaryl_{AI}^S)$	The condensed-to-atom Fukui function of the reacting carbon atom of imine derived from (S)-alkene insertion TS	$f_C^+ = q_C^N - q_C^{N+1}$
$f_C^-(Biaryl_{AI}^S)$	The condensed-to-atom Fukui function of the reacting carbon atom of imine derived from (S)-alkene insertion TS	$f_C^- = q_C^{N-1} - q_C^N$
$f_C^0(Biaryl_{GS})$	The condensed-to-atom Fukui function of the reacting carbon atom of ground state imine	$f_C^0 = \frac{q_C^{N-1} - q_C^{N+1}}{2}$
$f_C^+(Biaryl_{GS})$	The condensed-to-atom Fukui function of the reacting carbon atom of ground state imine	$f_C^+ = q_C^N - q_C^{N+1}$
$f_C^-(Biaryl_{GS})$	The condensed-to-atom Fukui function of the reacting carbon atom of ground state imine	$f_C^- = q_C^{N-1} - q_C^N$
$f_H^0(Biaryl_{CH}^R)$	The condensed-to-atom Fukui function of the reacting hydrogen atom of imine derived from (R)-C–H bond activation TS	$f_H^0 = \frac{q_H^{N-1} - q_H^{N+1}}{2}$
$f_H^+(Biaryl_{CH}^R)$	The condensed-to-atom Fukui function of the reacting hydrogen atom of imine derived from (R)-C–H bond activation TS	$f_H^+ = q_H^N - q_H^{N+1}$
$f_H^-(Biaryl_{CH}^R)$	The condensed-to-atom Fukui function of the reacting hydrogen atom of imine derived from (R)-C–H bond activation TS	$f_H^- = q_H^{N-1} - q_H^N$
$f_H^0(Biaryl_{CH}^S)$	The condensed-to-atom Fukui function of the reacting hydrogen atom of imine derived from (S)-C–H bond activation TS	$f_H^0 = \frac{q_H^{N-1} - q_H^{N+1}}{2}$
$f_H^+(Biaryl_{CH}^S)$	The condensed-to-atom Fukui function of the reacting hydrogen atom of imine derived from (S)-C–H bond activation TS	$f_H^+ = q_H^N - q_H^{N+1}$
$f_H^-(Biaryl_{CH}^S)$	The condensed-to-atom Fukui function of the reacting hydrogen atom of imine derived from (S)-C–H bond activation TS	$f_H^- = q_H^{N-1} - q_H^N$
$f_H^0(Biaryl_{GS})$	The condensed-to-atom Fukui function of the reacting carbon atom of ground state imine	$f_H^0 = \frac{q_H^{N-1} - q_H^{N+1}}{2}$
$f_H^+(Biaryl_{GS})$	The condensed-to-atom Fukui function of the reacting carbon atom of ground state imine	$f_H^+ = q_H^N - q_H^{N+1}$
$f_H^-(Biaryl_{GS})$	The condensed-to-atom Fukui function of the reacting carbon atom of ground state imine	$f_H^- = q_H^{N-1} - q_H^N$
$s_C^0(Biaryl_{CH}^R)$	The condensed local softnesses of the reacting carbon atom of imine derived from (R)-C–H bond activation TS	$\frac{f_C^0}{\eta}$ (η : Hardness)
$s_C^+(Biaryl_{CH}^R)$	The condensed local softnesses of the reacting carbon atom of imine derived from (R)-C–H bond activation TS	$\frac{f_C^+}{\eta}$ (η : Hardness)
$s_C^-(Biaryl_{CH}^R)$	The condensed local softnesses of the reacting carbon atom of imine derived from (R)-C–H bond activation TS	$\frac{f_C^-}{\eta}$ (η : Hardness)
$s_C^0(Biaryl_{CH}^S)$	The condensed local softnesses of the reacting carbon atom of imine derived from (S)-C–H bond activation TS	$\frac{f_C^0}{\eta}$ (η : Hardness)
$s_C^+(Biaryl_{CH}^S)$	The condensed local softnesses of the reacting carbon atom of imine derived from (S)-C–H bond activation TS	$\frac{f_C^+}{\eta}$ (η : Hardness)
$s_C^-(Biaryl_{CH}^S)$	The condensed local softnesses of the reacting carbon atom of imine derived from (S)-C–H bond activation TS	$\frac{f_C^-}{\eta}$ (η : Hardness)
$s_C^0(Biaryl_{GS})$	The condensed local softnesses of the reacting carbon atom of ground state imine	$\frac{f_C^0}{\eta}$ (η : Hardness)

$s_C^+(Biaryl_{GS})$	The condensed local softnesses of the reacting carbon atom of ground state imine	$\frac{f_C^+}{\eta}$ (η : Hardness)
$s_C^-(Biaryl_{GS})$	The condensed local softnesses of the reacting carbon atom of ground state imine	$\frac{f_C^-}{\eta}$ (η : Hardness)
$s_C^0(Biaryl_{AI}^R)$	The condensed local softnesses of the reacting carbon atom of imine derived from (<i>R</i>)-alkene insertion TS	$\frac{f_C^0}{\eta}$ (η : Hardness)
$s_C^+(Biaryl_{AI}^R)$	The condensed local softnesses of the reacting carbon atom of imine derived from (<i>R</i>)-alkene insertion TS	$\frac{f_C^+}{\eta}$ (η : Hardness)
$s_C^-(Biaryl_{AI}^R)$	The condensed local softnesses of the reacting carbon atom of imine derived from (<i>R</i>)-alkene insertion TS	$\frac{f_C^-}{\eta}$ (η : Hardness)
$s_C^0(Biaryl_{AI}^S)$	The condensed local softnesses of the reacting carbon atom of imine derived from (<i>S</i>)-alkene insertion TS	$\frac{f_C^0}{\eta}$ (η : Hardness)
$s_C^+(Biaryl_{AI}^S)$	The condensed local softnesses of the reacting carbon atom of imine derived from (<i>S</i>)-alkene insertion TS	$\frac{f_C^+}{\eta}$ (η : Hardness)
$s_C^-(Biaryl_{AI}^S)$	The condensed local softnesses of the reacting carbon atom of imine derived from (<i>S</i>)-alkene insertion TS	$\frac{f_C^-}{\eta}$ (η : Hardness)
$s_C^0(Biaryl_{GS})$	The condensed local softnesses of the reacting carbon atom of ground state imine	$\frac{f_C^0}{\eta}$ (η : Hardness)
$s_C^+(Biaryl_{GS})$	The condensed local softnesses of the reacting carbon atom of ground state imine	$\frac{f_C^+}{\eta}$ (η : Hardness)
$s_C^-(Biaryl_{GS})$	The condensed local softnesses of the reacting carbon atom of ground state imine	$\frac{f_C^-}{\eta}$ (η : Hardness)
$s_H^0(Biaryl_{CH}^R)$	The condensed local softnesses of the reacting hydrogen atom of imine derived from (<i>R</i>)-C–H bond activation TS	$\frac{f_H^0}{\eta}$ (η : Hardness)
$s_H^+(Biaryl_{CH}^R)$	The condensed local softnesses of the reacting hydrogen atom of imine derived from (<i>R</i>)-C–H bond activation TS	$\frac{f_H^+}{\eta}$ (η : Hardness)
$s_H^-(Biaryl_{CH}^R)$	The condensed local softnesses of the reacting hydrogen atom of imine derived from (<i>R</i>)-C–H bond activation TS	$\frac{f_H^-}{\eta}$ (η : Hardness)
$s_H^0(Biaryl_{CH}^S)$	The condensed local softnesses of the reacting hydrogen atom of imine derived from (<i>S</i>)-C–H bond activation TS	$\frac{f_H^0}{\eta}$ (η : Hardness)
$s_H^+(Biaryl_{CH}^S)$	The condensed local softnesses of the reacting hydrogen atom of imine derived from (<i>S</i>)-C–H bond activation TS	$\frac{f_H^+}{\eta}$ (η : Hardness)
$s_H^-(Biaryl_{CH}^S)$	The condensed local softnesses of the reacting hydrogen atom of imine derived from (<i>S</i>)-C–H bond activation TS	$\frac{f_H^-}{\eta}$ (η : Hardness)
$s_H^0(Biaryl_{GS})$	The condensed local softnesses of the reacting hydrogen atom of ground state imine	$\frac{f_H^0}{\eta}$ (η : Hardness)
$s_H^+(Biaryl_{GS})$	The condensed local softnesses of the reacting hydrogen atom of ground state imine	$\frac{f_H^+}{\eta}$ (η : Hardness)
$s_H^-(Biaryl_{GS})$	The condensed local softnesses of the reacting hydrogen atom of ground state imine	$\frac{f_H^-}{\eta}$ (η : Hardness)
$\omega^C(Biaryl_{CH}^R)$	The condensed local electrophilicity index of the reacting carbon atom of imine derived from (<i>R</i>)-C–H bond activation TS	ωf_C^+ ($\omega = \frac{\mu^2}{2\eta}$)
$N_{Nu}^C(Biaryl_{CH}^R)$	The condensed local nucleophilicity index of the reacting carbon atom of imine derived from (<i>R</i>)-C–H bond activation TS	$N_{Nu} f_C^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)

$\omega^C(Biaryl_{CH}^S)$	The condensed local electrophilicity index of the reacting carbon atom of imine derived from (S)-C–H bond activation TS	$\omega f_C^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^C(Biaryl_{CH}^S)$	The condensed local nucleophilicity index of the reacting carbon atom of imine derived from (S)-C–H bond activation TS	$N_{Nu}f_C^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^C(Biaryl_{GS}^S)$	The condensed local electrophilicity index of the reacting carbon atom of ground state imine	$\omega f_C^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^C(Biaryl_{GS}^S)$	The condensed local nucleophilicity index of the reacting carbon atom of ground state imine	$N_{Nu}f_C^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^C(Biaryl_{Al}^R)$	The condensed local electrophilicity index of the reacting carbon atom of imine derived from (R)-alkene insertion TS	$\omega f_C^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^C(Biaryl_{Al}^R)$	The condensed local nucleophilicity index of the reacting carbon atom of imine derived from (R)-alkene insertion TS	$N_{Nu}f_C^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^C(Biaryl_{Al}^S)$	The condensed local electrophilicity index of the reacting carbon atom of imine derived from (S)-alkene insertion TS	$\omega f_C^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^C(Biaryl_{Al}^S)$	The condensed local nucleophilicity index of the reacting carbon atom of imine derived from (S)-alkene insertion TS	$N_{Nu}f_C^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^C(Biaryl_{GS}^S)$	The condensed local electrophilicity index of the reacting carbon atom of ground state imine	$\omega f_C^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^C(Biaryl_{GS}^S)$	The condensed local nucleophilicity index of the reacting carbon atom of ground state imine	$N_{Nu}f_C^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^H(Biaryl_{CH}^R)$	The condensed local electrophilicity index of the reacting hydrogen atom of imine derived from (R)-C–H bond activation TS	$\omega f_H^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^H(Biaryl_{CH}^R)$	The condensed local nucleophilicity index of the reacting hydrogen atom of imine derived from (R)-C–H bond activation TS	$N_{Nu}f_H^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^H(Biaryl_{CH}^S)$	The condensed local electrophilicity index of the reacting hydrogen atom of imine derived from (S)-C–H bond activation TS	$\omega f_H^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^H(Biaryl_{CH}^S)$	The condensed local nucleophilicity index of the reacting hydrogen atom of imine derived from (S)-C–H bond activation TS	$N_{Nu}f_H^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^H(Biaryl_{GS}^S)$	The condensed local electrophilicity index of the reacting hydrogen atom of ground state imine	$\omega f_H^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^H(Biaryl_{GS}^S)$	The condensed local nucleophilicity index of the reacting hydrogen atom of ground state imine	$N_{Nu}f_H^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$q_{C1}^N(Olefin_{Al}^R)$	The Hirshfeld charge of the reacting terminal carbon atom of neutral olefin derived from (R)-alkene insertion TS	DFT calculation based on xTB optimized geometries
$q_{C1}^{N+1}(Olefin_{Al}^R)$	The Hirshfeld charge of the reacting terminal carbon atom of olefin derived from (R)-alkene insertion TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_{C1}^{N-1}(Olefin_{Al}^R)$	The Hirshfeld charge of the reacting terminal carbon atom of olefin derived from (R)-alkene insertion TS with one negative charge	DFT calculation based on xTB optimized geometries

$q_{C1}^N(Olefin_{AI}^S)$	The Hirshfeld charge of the reacting terminal carbon atom of neutral olefin derived from (<i>S</i>)-alkene insertion TS	DFT calculation based on xTB optimized geometries
$q_{C1}^{N+1}(Olefin_{AI}^S)$	The Hirshfeld charge of the reacting terminal carbon atom of olefin derived from (<i>S</i>)-alkene insertion TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_{C1}^{N-1}(Olefin_{AI}^S)$	The Hirshfeld charge of the reacting terminal carbon atom of olefin derived from (<i>S</i>)-alkene insertion TS with one negative charge	DFT calculation based on xTB optimized geometries
$q_{C1}^N(Olefin_{GS})$	The Hirshfeld charge of the reacting terminal carbon atom of neutral ground state olefin	DFT calculation based on xTB optimized geometries
$q_{C1}^{N+1}(Olefin_{GS})$	The Hirshfeld charge of the reacting terminal carbon atom of ground state olefin with one positive charge	DFT calculation based on xTB optimized geometries
$q_{C1}^{N-1}(Olefin_{GS})$	The Hirshfeld charge of the reacting terminal carbon atom of ground state olefin with one negative charge	DFT calculation based on xTB optimized geometries
$q_{C2}^N(Olefin_{AI}^R)$	The Hirshfeld charge of the reacting substituted carbon atom of neutral olefin derived from (<i>R</i>)-alkene insertion TS	DFT calculation based on xTB optimized geometries
$q_{C2}^{N+1}(Olefin_{AI}^R)$	The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_{C2}^{N-1}(Olefin_{AI}^R)$	The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS with one negative charge	DFT calculation based on xTB optimized geometries
$q_{C2}^N(Olefin_{AI}^S)$	The Hirshfeld charge of the reacting substituted carbon atom of neutral olefin from (<i>S</i>)-alkene insertion TS	DFT calculation based on xTB optimized geometries
$q_{C2}^{N+1}(Olefin_{AI}^S)$	The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (<i>S</i>)-alkene insertion TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_{C2}^{N-1}(Olefin_{AI}^S)$	The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (<i>S</i>)-alkene insertion TS with one negative charge	DFT calculation based on xTB optimized geometries
$q_{C2}^N(Olefin_{GS})$	The Hirshfeld charge of the reacting substituted carbon atom of neutral ground state olefin	DFT calculation based on xTB optimized geometries
$q_{C2}^{N+1}(Olefin_{GS})$	The Hirshfeld charge of the reacting substituted carbon atom of ground state olefin with one positive charge	DFT calculation based on xTB optimized geometries
$q_{C2}^{N-1}(Olefin_{GS})$	The Hirshfeld charge of the reacting substituted carbon atom of ground state olefin with one negative charge	DFT calculation based on xTB optimized geometries
$f_{C1}^0(Olefin_{AI}^R)$	The condensed-to-atom Fukui function of the terminal carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS	$f_{C1}^0 = \frac{q_{C1}^{N-1} - q_{C1}^{N+1}}{2}$
$f_{C1}^+(Olefin_{AI}^R)$	The condensed-to-atom Fukui function of the terminal carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS	$f_{C1}^+ = q_{C1}^N - q_{C1}^{N+1}$
$f_{C1}^-(Olefin_{AI}^R)$	The condensed-to-atom Fukui function of the terminal carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS	$f_{C1}^- = q_{C1}^{N-1} - q_{C1}^N$
$f_{C1}^0(Olefin_{AI}^S)$	The condensed-to-atom Fukui function of the terminal carbon atom of olefin derived from (<i>S</i>)-alkene insertion TS	$f_{C1}^0 = \frac{q_{C1}^{N-1} - q_{C1}^{N+1}}{2}$

$f_{C1}^+(Olefin_{AI}^S)$	The condensed-to-atom Fukui function of the terminal carbon atom of olefin derived from (S)-alkene insertion TS	$f_{C1}^+ = q_{C1}^N - q_{C1}^{N+1}$
$f_{C1}^-(Olefin_{AI}^S)$	The condensed-to-atom Fukui function of the terminal carbon atom of olefin derived from (S)-alkene insertion TS	$f_{C1}^- = q_{C1}^{N-1} - q_{C1}^N$
$f_{C1}^0(Olefin_{GS})$	The condensed-to-atom Fukui function of the terminal carbon atom of ground state olefin	$f_{C1}^0 = \frac{q_{C1}^{N-1} - q_{C1}^{N+1}}{2}$
$f_{C1}^+(Olefin_{GS})$	The condensed-to-atom Fukui function of the terminal carbon atom of ground state olefin	$f_{C1}^+ = q_{C1}^N - q_{C1}^{N+1}$
$f_{C1}^-(Olefin_{GS})$	The condensed-to-atom Fukui function of the terminal carbon atom of ground state olefin	$f_{C1}^- = q_{C1}^{N-1} - q_{C1}^N$
$f_{C2}^0(Olefin_{AI}^R)$	The condensed-to-atom Fukui function of the substituted carbon atom of olefin derived from (R)-alkene insertion TS	$f_{C2}^0 = \frac{q_{C2}^{N-1} - q_{C2}^{N+1}}{2}$
$f_{C2}^+(Olefin_{AI}^R)$	The condensed-to-atom Fukui function of the substituted carbon atom of olefin derived from (R)-alkene insertion TS	$f_{C2}^+ = q_{C2}^N - q_{C2}^{N+1}$
$f_{C2}^-(Olefin_{AI}^R)$	The condensed-to-atom Fukui function of the substituted carbon atom of olefin derived from (R)-alkene insertion TS	$f_{C2}^- = q_{C2}^{N-1} - q_{C2}^N$
$f_{C2}^0(Olefin_{AI}^S)$	The condensed-to-atom Fukui function of the substituted carbon atom of olefin derived from (S)-alkene insertion TS	$f_{C2}^0 = \frac{q_{C2}^{N-1} - q_{C2}^{N+1}}{2}$
$f_{C2}^+(Olefin_{AI}^S)$	The condensed-to-atom Fukui function of the substituted carbon atom of olefin derived from (S)-alkene insertion TS	$f_{C2}^+ = q_{C2}^N - q_{C2}^{N+1}$
$f_{C2}^-(Olefin_{AI}^S)$	The condensed-to-atom Fukui function of the substituted carbon atom of olefin derived from (S)-alkene insertion TS	$f_{C2}^- = q_{C2}^{N-1} - q_{C2}^N$
$f_{C2}^0(Olefin_{GS})$	The condensed-to-atom Fukui function of the substituted carbon atom of ground state olefin	$f_{C2}^0 = \frac{q_{C2}^{N-1} - q_{C2}^{N+1}}{2}$
$f_{C2}^+(Olefin_{GS})$	The condensed-to-atom Fukui function of the substituted carbon atom of ground state olefin	$f_{C2}^+ = q_{C2}^N - q_{C2}^{N+1}$
$f_{C2}^-(Olefin_{GS})$	The condensed-to-atom Fukui function of the substituted carbon atom of ground state olefin	$f_{C2}^- = q_{C2}^{N-1} - q_{C2}^N$
$s_{C1}^0(Olefin_{AI}^R)$	The condensed local softnesses of the terminal carbon atom of olefin derived from (R)-alkene insertion TS	$\frac{f_{C1}^0}{\eta}$ (η : Hardness)
$s_{C1}^+(Olefin_{AI}^R)$	The condensed local softnesses of the terminal carbon atom of olefin derived from (R)-alkene insertion TS	$\frac{f_{C1}^+}{\eta}$ (η : Hardness)
$s_{C1}^-(Olefin_{AI}^R)$	The condensed local softnesses of the terminal carbon atom of olefin derived from (R)-alkene insertion TS	$\frac{f_{C1}^-}{\eta}$ (η : Hardness)
$s_{C1}^0(Olefin_{AI}^S)$	The condensed local softnesses of the terminal carbon atom of olefin derived from (S)-alkene insertion TS	$\frac{f_{C1}^0}{\eta}$ (η : Hardness)
$s_{C1}^+(Olefin_{AI}^S)$	The condensed local softnesses of the terminal carbon atom of olefin derived from (S)-alkene insertion TS	$\frac{f_{C1}^+}{\eta}$ (η : Hardness)
$s_{C1}^-(Olefin_{AI}^S)$	The condensed local softnesses of the terminal carbon atom of olefin derived from (S)-alkene insertion TS	$\frac{f_{C1}^-}{\eta}$ (η : Hardness)
$s_{C1}^0(Olefin_{GS})$	The condensed local softnesses of the terminal carbon atom of ground state olefin	$\frac{f_{C1}^0}{\eta}$ (η : Hardness)
$s_{C1}^+(Olefin_{GS})$	The condensed local softnesses of the terminal carbon atom of ground state olefin	$\frac{f_{C1}^+}{\eta}$ (η : Hardness)

$s_{C1}^-(Olefin_{GS})$	The condensed local softnesses of the terminal carbon atom of ground state olefin	$\frac{f_{C1}^-}{\eta}$ (η : Hardness)
$s_{C2}^0(Olefin_{AI}^R)$	The condensed local softnesses of the substituted carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS	$\frac{f_{C2}^0}{\eta}$ (η : Hardness)
$s_{C2}^+(Olefin_{AI}^R)$	The condensed local softnesses of the substituted carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS	$\frac{f_{C2}^+}{\eta}$ (η : Hardness)
$s_{C2}^-(Olefin_{AI}^R)$	The condensed local softnesses of the substituted carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS	$\frac{f_{C2}^-}{\eta}$ (η : Hardness)
$s_{C2}^0(Olefin_{AI}^S)$	The condensed local softnesses of the substituted carbon atom of olefin derived from (<i>S</i>)-alkene insertion TS	$\frac{f_{C2}^0}{\eta}$ (η : Hardness)
$s_{C2}^+(Olefin_{AI}^S)$	The condensed local softnesses of the substituted carbon atom of olefin derived from (<i>S</i>)-alkene insertion TS	$\frac{f_{C2}^+}{\eta}$ (η : Hardness)
$s_{C2}^-(Olefin_{AI}^S)$	The condensed local softnesses of the substituted carbon atom of olefin derived from (<i>S</i>)-alkene insertion TS	$\frac{f_{C2}^-}{\eta}$ (η : Hardness)
$s_{C2}^0(Olefin_{GS})$	The condensed local softnesses of the substituted carbon atom of ground state olefin	$\frac{f_{C2}^0}{\eta}$ (η : Hardness)
$s_{C2}^+(Olefin_{GS})$	The condensed local softnesses of the substituted carbon atom of ground state olefin	$\frac{f_{C2}^+}{\eta}$ (η : Hardness)
$s_{C2}^-(Olefin_{GS})$	The condensed local softnesses of the substituted carbon atom of ground state olefin	$\frac{f_{C2}^-}{\eta}$ (η : Hardness)
$\omega^{C1}(Olefin_{AI}^R)$	The condensed local electrophilicity index of the terminal carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS	ωf_{C1}^+ ($\omega = \frac{\mu^2}{2\eta}$)
$N_{Nu}^{C1}(Olefin_{AI}^R)$	The condensed local nucleophilicity index of the terminal carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS	$N_{Nu}f_{C1}^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^{C1}(Olefin_{AI}^S)$	The condensed local electrophilicity index of the terminal carbon atom of olefin derived from (<i>S</i>)-alkene insertion TS	ωf_{C1}^+ ($\omega = \frac{\mu^2}{2\eta}$)
$N_{Nu}^{C1}(Olefin_{AI}^S)$	The condensed local nucleophilicity index of the terminal carbon atom of olefin derived from (<i>S</i>)-alkene insertion TS	$N_{Nu}f_{C1}^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^{C1}(Olefin_{GS})$	The condensed local electrophilicity index of the terminal carbon atom of ground state olefin	ωf_{C1}^+ ($\omega = \frac{\mu^2}{2\eta}$)
$N_{Nu}^{C1}(Olefin_{GS})$	The condensed local nucleophilicity index of the terminal carbon atom of ground state olefin	$N_{Nu}f_{C1}^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^{C2}(Olefin_{AI}^R)$	The condensed local electrophilicity index of the substituted carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS	ωf_{C2}^+ ($\omega = \frac{\mu^2}{2\eta}$)
$N_{Nu}^{C2}(Olefin_{AI}^R)$	The condensed local nucleophilicity index of the substituted carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS	$N_{Nu}f_{C2}^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^{C2}(Olefin_{AI}^S)$	The condensed local electrophilicity index of the substituted carbon atom of olefin derived from (<i>S</i>)-alkene insertion TS	ωf_{C2}^+ ($\omega = \frac{\mu^2}{2\eta}$)
$N_{Nu}^{C2}(Olefin_{AI}^S)$	The condensed local nucleophilicity index of the substituted carbon atom of olefin derived from (<i>S</i>)-alkene insertion TS	$N_{Nu}f_{C2}^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^{C2}(Olefin_{GS})$	The condensed local electrophilicity index of the substituted carbon atom of ground state olefin	ωf_{C2}^+ ($\omega = \frac{\mu^2}{2\eta}$)
$N_{Nu}^{C2}(Olefin_{GS})$	The condensed local nucleophilicity index of the substituted carbon atom of ground state olefin	$N_{Nu}f_{C2}^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)

$q_{Pd}^N(TDG_{CH}^R)$	The Hirshfeld charge of the palladium atom of neutral palladium complex derived from (<i>R</i>)-C–H bond activation TS	DFT calculation based on xTB optimized geometries
$q_{Pd}^{N+1}(TDG_{CH}^R)$	The Hirshfeld charge of the palladium atom of palladium complex derived from (<i>R</i>)-C–H bond activation TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_{Pd}^{N-1}(TDG_{CH}^R)$	The Hirshfeld charge of the palladium atom of palladium complex derived from (<i>R</i>)-C–H bond activation TS with one negative charge	DFT calculation based on xTB optimized geometries
$q_{Pd}^N(TDG_{CH}^S)$	The Hirshfeld charge of the palladium atom of neutral palladium complex derived from (<i>S</i>)-C–H bond activation TS	DFT calculation based on xTB optimized geometries
$q_{Pd}^{N+1}(TDG_{CH}^S)$	The Hirshfeld charge of the palladium atom of palladium complex derived from (<i>S</i>)-C–H bond activation TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_{Pd}^{N-1}(TDG_{CH}^S)$	The Hirshfeld charge of the palladium atom of palladium complex derived from (<i>S</i>)-C–H bond activation TS with one negative charge	DFT calculation based on xTB optimized geometries
$q_{Pd}^N(TDG_{GS}^b)$	The Hirshfeld charge of the palladium atom of neutral ground state palladium complex with base fragment	DFT calculation based on xTB optimized geometries
$q_{Pd}^{N+1}(TDG_{GS}^b)$	The Hirshfeld charge of the palladium atom of ground state palladium complex with base fragment and one positive charge	DFT calculation based on xTB optimized geometries
$q_{Pd}^{N-1}(TDG_{GS}^b)$	The Hirshfeld charge of the palladium atom of ground state palladium complex with base fragment and one negative charge	DFT calculation based on xTB optimized geometries
$q_{Pd}^N(TDG_{AI}^R)$	The Hirshfeld charge of the palladium atom of neutral palladium complex derived from (<i>R</i>)-alkene insertion TS	DFT calculation based on xTB optimized geometries
$q_{Pd}^{N+1}(TDG_{AI}^R)$	The Hirshfeld charge of the palladium atom of palladium complex derived from (<i>R</i>)-alkene insertion TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_{Pd}^{N-1}(TDG_{AI}^R)$	The Hirshfeld charge of the palladium atom of palladium complex derived from (<i>R</i>)-alkene insertion TS with one negative charge	DFT calculation based on xTB optimized geometries
$q_{Pd}^N(TDG_{AI}^S)$	The Hirshfeld charge of the palladium atom of neutral palladium complex derived from (<i>S</i>)-alkene insertion TS	DFT calculation based on xTB optimized geometries
$q_{Pd}^{N+1}(TDG_{AI}^S)$	The Hirshfeld charge of the palladium atom of palladium complex derived from (<i>S</i>)-alkene insertion TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_{Pd}^{N-1}(TDG_{AI}^S)$	The Hirshfeld charge of the palladium atom of palladium complex derived from (<i>S</i>)-alkene insertion TS with one negative charge	DFT calculation based on xTB optimized geometries
$q_{Pd}^N(TDG_{GS})$	The Hirshfeld charge of the palladium atom of neutral ground state palladium complex	DFT calculation based on xTB optimized geometries
$q_{Pd}^{N+1}(TDG_{GS})$	The Hirshfeld charge of the palladium atom of ground state palladium complex with one positive charge	DFT calculation based on xTB optimized geometries
$q_{Pd}^{N-1}(TDG_{GS})$	The Hirshfeld charge of the palladium atom of ground state palladium complex with one negative charge	DFT calculation based on xTB optimized geometries

$q_{O1}^N(TDG_{CH}^R)$	The Hirshfeld charge of the oxygen atom of neutral palladium complex derived from (R)-C–H activation TS (site 1 at base part)	DFT calculation based on xTB optimized geometries
$q_{O1}^{N+1}(TDG_{CH}^R)$	The Hirshfeld charge of the oxygen atom of palladium complex derived from (R)-C–H activation TS with one positive charge (site 1 at base part)	DFT calculation based on xTB optimized geometries
$q_{O1}^{N-1}(TDG_{CH}^R)$	The Hirshfeld charge of the oxygen atom of palladium complex derived from (R)-C–H activation TS with one negative charge (site 1 at base part)	DFT calculation based on xTB optimized geometries
$q_{O1}^N(TDG_{CH}^S)$	The Hirshfeld charge of the oxygen atom of neutral palladium complex derived from (S)-C–H activation TS (site 1 at base part)	DFT calculation based on xTB optimized geometries
$q_{O1}^{N+1}(TDG_{CH}^S)$	The Hirshfeld charge of the oxygen atom of palladium complex derived from (S)-C–H activation TS with one positive charge (site 1 at base part)	DFT calculation based on xTB optimized geometries
$q_{O1}^{N-1}(TDG_{CH}^S)$	The Hirshfeld charge of the oxygen atom of palladium complex derived from (S)-C–H activation TS with one negative charge (site 1 at base part)	DFT calculation based on xTB optimized geometries
$q_{O1}^N(TDG_{GS}^b)$	The Hirshfeld charge of the oxygen atom of neutral ground state palladium complex with base fragment (site 1 at base part)	DFT calculation based on xTB optimized geometries
$q_{O1}^{N+1}(TDG_{GS}^b)$	The Hirshfeld charge of the oxygen atom of ground state palladium complex with base fragment and one positive charge (site 1 at base part)	DFT calculation based on xTB optimized geometries
$q_{O1}^{N-1}(TDG_{GS}^b)$	The Hirshfeld charge of the oxygen atom of ground state palladium complex with base fragment and one negative charge (site 1 at base part)	DFT calculation based on xTB optimized geometries
$q_{O2}^N(TDG_{CH}^R)$	The Hirshfeld charge of the oxygen atom of neutral palladium complex derived from (R)-C–H activation TS (site 2 at base part)	DFT calculation based on xTB optimized geometries
$q_{O2}^{N+1}(TDG_{CH}^R)$	The Hirshfeld charge of the oxygen atom of palladium complex derived from (R)-C–H activation TS with one positive charge (site 2 at base part)	DFT calculation based on xTB optimized geometries
$q_{O2}^{N-1}(TDG_{CH}^R)$	The Hirshfeld charge of the oxygen atom of palladium complex derived from (R)-C–H activation TS with one negative charge (site 2 at base part)	DFT calculation based on xTB optimized geometries
$q_{O2}^N(TDG_{CH}^S)$	The Hirshfeld charge of the oxygen atom of neutral palladium complex derived from (S)-C–H activation TS (site 2 at base part)	DFT calculation based on xTB optimized geometries
$q_{O2}^{N+1}(TDG_{CH}^S)$	The Hirshfeld charge of the oxygen atom of palladium complex derived from (S)-C–H activation TS with one positive charge (site 2 at base part)	DFT calculation based on xTB optimized geometries
$q_{O2}^{N-1}(TDG_{CH}^S)$	The Hirshfeld charge of the oxygen atom of palladium complex derived from (S)-C–H activation TS with one negative charge (site 2 at base part)	DFT calculation based on xTB optimized geometries
$q_{O2}^N(TDG_{GS}^b)$	The Hirshfeld charge of the oxygen atom of neutral ground state palladium complex with base fragment (site 2 at base part)	DFT calculation based on xTB optimized geometries

$q_{O_2}^{N+1}(TDG_{GS}^b)$	The Hirshfeld charge of the oxygen atom of ground state palladium complex with base fragment and one positive charge (site 2 at base part)	DFT calculation based on xTB optimized geometries
$q_{O_2}^{N-1}(TDG_{GS}^b)$	The Hirshfeld charge of the oxygen atom of ground state palladium complex with base fragment and one negative charge (site 2 at base part)	DFT calculation based on xTB optimized geometries
$q_C^N(TDG_{CH}^R)$	The Hirshfeld charge of the carbon atom of neutral palladium complex derived from (R)-C–H bond activation TS	DFT calculation based on xTB optimized geometries
$q_C^{N+1}(TDG_{CH}^R)$	The Hirshfeld charge of the carbon atom of palladium complex derived from (R)-C–H bond activation TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_C^{N-1}(TDG_{CH}^R)$	The Hirshfeld charge of the carbon atom of palladium complex derived from (R)-C–H bond activation TS with one negative charge	DFT calculation based on xTB optimized geometries
$q_C^N(TDG_{CH}^S)$	The Hirshfeld charge of the carbon atom of neutral palladium complex derived from (S)-C–H bond activation TS	DFT calculation based on xTB optimized geometries
$q_C^{N+1}(TDG_{CH}^S)$	The Hirshfeld charge of the carbon atom of palladium complex derived from (S)-C–H bond activation TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_C^{N-1}(TDG_{CH}^S)$	The Hirshfeld charge of the carbon atom of palladium complex derived from (S)-C–H bond activation TS with one negative charge	DFT calculation based on xTB optimized geometries
$q_C^N(TDG_{GS}^b)$	The Hirshfeld charge of the carbon atom of neutral ground state palladium complex with base fragment	DFT calculation based on xTB optimized geometries
$q_C^{N+1}(TDG_{GS}^b)$	The Hirshfeld charge of the carbon atom of ground state palladium complex with base fragment and one positive charge	DFT calculation based on xTB optimized geometries
$q_C^{N-1}(TDG_{GS}^b)$	The Hirshfeld charge of the carbon atom of ground state palladium complex with base fragment and one negative charge	DFT calculation based on xTB optimized geometries
$f_{Pd}^0(TDG_{CH}^R)$	The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (R)-C–H activation TS	$f_{Pd}^0 = \frac{q_{Pd}^{N-1} - q_{Pd}^{N+1}}{2}$
$f_{Pd}^+(TDG_{CH}^R)$	The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (R)-C–H activation TS	$f_{Pd}^+ = q_{Pd}^N - q_{Pd}^{N+1}$
$f_{Pd}^-(TDG_{CH}^R)$	The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (R)-C–H activation TS	$f_{Pd}^- = q_{Pd}^{N-1} - q_{Pd}^N$
$f_{Pd}^0(TDG_{CH}^S)$	The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (S)-C–H activation TS	$f_{Pd}^0 = \frac{q_{Pd}^{N-1} - q_{Pd}^{N+1}}{2}$
$f_{Pd}^+(TDG_{CH}^S)$	The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (S)-C–H activation TS	$f_{Pd}^+ = q_{Pd}^N - q_{Pd}^{N+1}$
$f_{Pd}^-(TDG_{CH}^S)$	The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (S)-C–H activation TS	$f_{Pd}^- = q_{Pd}^{N-1} - q_{Pd}^N$
$f_{Pd}^0(TDG_{GS}^b)$	The condensed-to-atom Fukui function of the palladium atom of ground state palladium complex with base fragment	$f_{Pd}^0 = \frac{q_{Pd}^{N-1} - q_{Pd}^{N+1}}{2}$
$f_{Pd}^+(TDG_{GS}^b)$	The condensed-to-atom Fukui function of the palladium atom of ground state palladium complex with base fragment	$f_{Pd}^+ = q_{Pd}^N - q_{Pd}^{N+1}$

$f_{Pd}^-(TDG_{GS}^b)$	The condensed-to-atom Fukui function of the palladium atom of ground state palladium complex with base fragment	$f_{Pd}^- = q_{Pd}^{N-1} - q_{Pd}^N$
$f_{Pd}^0(TDG_{AI}^R)$	The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (R)-alkene insertion TS	$f_{Pd}^0 = \frac{q_{Pd}^{N-1} - q_{Pd}^{N+1}}{2}$
$f_{Pd}^+(TDG_{AI}^R)$	The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (R)-alkene insertion TS	$f_{Pd}^+ = q_{Pd}^N - q_{Pd}^{N+1}$
$f_{Pd}^-(TDG_{AI}^S)$	The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (S)-alkene insertion TS	$f_{Pd}^- = q_{Pd}^{N-1} - q_{Pd}^N$
$f_{Pd}^0(TDG_{AI}^S)$	The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (S)-alkene insertion TS	$f_{Pd}^0 = \frac{q_{Pd}^{N-1} - q_{Pd}^{N+1}}{2}$
$f_{Pd}^+(TDG_{AI}^S)$	The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (S)-alkene insertion TS	$f_{Pd}^+ = q_{Pd}^N - q_{Pd}^{N+1}$
$f_{Pd}^-(TDG_{AI}^S)$	The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (S)-alkene insertion TS	$f_{Pd}^- = q_{Pd}^{N-1} - q_{Pd}^N$
$f_{Pd}^0(TDG_{GS})$	The condensed-to-atom Fukui function of the palladium atom of ground state palladium complex	$f_{Pd}^0 = \frac{q_{Pd}^{N-1} - q_{Pd}^{N+1}}{2}$
$f_{Pd}^+(TDG_{GS})$	The condensed-to-atom Fukui function of the palladium atom of ground state palladium complex	$f_{Pd}^+ = q_{Pd}^N - q_{Pd}^{N+1}$
$f_{Pd}^-(TDG_{GS})$	The condensed-to-atom Fukui function of the palladium atom of ground state palladium complex	$f_{Pd}^- = q_{Pd}^{N-1} - q_{Pd}^N$
$f_{O1}^0(TDG_{CH}^R)$	The condensed-to-atom Fukui function of the oxygen atom of palladium complex derived from (R)-C–H bond activation TS (site 1 at base part)	$f_{O1}^0 = \frac{q_{O1}^{N-1} - q_{O1}^{N+1}}{2}$
$f_{O1}^+(TDG_{CH}^R)$	The condensed-to-atom Fukui function of the oxygen atom of palladium complex derived from (R)-C–H bond activation TS (site 1 at base part)	$f_{O1}^+ = q_{O1}^N - q_{O1}^{N+1}$
$f_{O1}^-(TDG_{CH}^R)$	The condensed-to-atom Fukui function of the oxygen atom of palladium complex derived from (R)-C–H bond activation TS (site 1 at base part)	$f_{O1}^- = q_{O1}^{N-1} - q_{O1}^N$
$f_{O1}^0(TDG_{CH}^S)$	The condensed-to-atom Fukui function of the oxygen atom of palladium complex derived from (S)-C–H bond activation TS (site 1 at base part)	$f_{O1}^0 = \frac{q_{O1}^{N-1} - q_{O1}^{N+1}}{2}$
$f_{O1}^+(TDG_{CH}^S)$	The condensed-to-atom Fukui function of the oxygen atom of palladium complex derived from (S)-C–H bond activation TS (site 1 at base part)	$f_{O1}^+ = q_{O1}^N - q_{O1}^{N+1}$
$f_{O1}^-(TDG_{CH}^S)$	The condensed-to-atom Fukui function of the oxygen atom of palladium complex derived from (S)-C–H bond activation TS (site 1 at base part)	$f_{O1}^- = q_{O1}^{N-1} - q_{O1}^N$
$f_{O1}^0(TDG_{GS}^b)$	The condensed-to-atom Fukui function of the oxygen atom of ground state palladium complex with base fragment (site 1 at base part)	$f_{O1}^0 = \frac{q_{O1}^{N-1} - q_{O1}^{N+1}}{2}$
$f_{O1}^+(TDG_{GS}^b)$	The condensed-to-atom Fukui function of the oxygen atom of ground state palladium complex with base fragment (site 1 at base part)	$f_{O1}^+ = q_{O1}^N - q_{O1}^{N+1}$

$f_{O1}^{-}(TDG_{GS}^b)$	The condensed-to-atom Fukui function of the oxygen atom of ground state palladium complex with base fragment (site 1 at base part)	$f_{O1}^{-} = q_{O1}^{N-1} - q_{O1}^N$
$f_{O2}^0(TDG_{CH}^R)$	The condensed-to-atom Fukui function of the oxygen atom of palladium complex derived from (R)-C–H bond activation TS (site 2 at base part)	$f_{O2}^0 = \frac{q_{O2}^{N-1} - q_{O2}^{N+1}}{2}$
$f_{O2}^{+}(TDG_{CH}^R)$	The condensed-to-atom Fukui function of the oxygen atom of palladium complex derived from (R)-C–H bond activation TS (site 2 at base part)	$f_{O2}^{+} = q_{O2}^N - q_{O2}^{N+1}$
$f_{O2}^{-}(TDG_{CH}^R)$	The condensed-to-atom Fukui function of the oxygen atom of palladium complex derived from (R)-C–H bond activation TS (site 2 at base part)	$f_{O2}^{-} = q_{O2}^{N-1} - q_{O2}^N$
$f_{O2}^0(TDG_{CH}^S)$	The condensed-to-atom Fukui function of the oxygen atom of palladium complex derived from (S)-C–H bond activation TS (site 2 at base part)	$f_{O2}^0 = \frac{q_{O2}^{N-1} - q_{O2}^{N+1}}{2}$
$f_{O2}^{+}(TDG_{CH}^S)$	The condensed-to-atom Fukui function of the oxygen atom of palladium complex derived from (S)-C–H bond activation TS (site 2 at base part)	$f_{O2}^{+} = q_{O2}^N - q_{O2}^{N+1}$
$f_{O2}^{-}(TDG_{CH}^S)$	The condensed-to-atom Fukui function of the oxygen atom of palladium complex derived from (S)-C–H bond activation TS (site 2 at base part)	$f_{O2}^{-} = q_{O2}^{N-1} - q_{O2}^N$
$f_{O2}^0(TDG_{GS}^b)$	The condensed-to-atom Fukui function of the oxygen atom of ground state palladium complex with base fragment (site 2 at base part)	$f_{O2}^0 = \frac{q_{O2}^{N-1} - q_{O2}^{N+1}}{2}$
$f_{O2}^{+}(TDG_{GS}^b)$	The condensed-to-atom Fukui function of the oxygen atom of ground state palladium complex with base fragment (site 2 at base part)	$f_{O2}^{+} = q_{O2}^N - q_{O2}^{N+1}$
$f_{O2}^{-}(TDG_{GS}^b)$	The condensed-to-atom Fukui function of the oxygen atom of ground state palladium complex with base fragment (site 2 at base part)	$f_{O2}^{-} = q_{O2}^{N-1} - q_{O2}^N$
$f_C^0(TDG_{CH}^R)$	The condensed-to-atom Fukui function of the carbon atom of palladium complex derived from (R)-C–H bond activation TS	$f_C^0 = \frac{q_C^{N-1} - q_C^{N+1}}{2}$
$f_C^{+}(TDG_{CH}^R)$	The condensed-to-atom Fukui function of the carbon atom of palladium complex derived from (R)-C–H bond activation TS	$f_C^{+} = q_C^N - q_C^{N+1}$
$f_C^{-}(TDG_{CH}^R)$	The condensed-to-atom Fukui function of the carbon atom of palladium complex derived from (R)-C–H bond activation TS	$f_C^{-} = q_C^{N-1} - q_C^N$
$f_C^0(TDG_{CH}^S)$	The condensed-to-atom Fukui function of the carbon atom of palladium complex derived from (S)-C–H bond activation TS	$f_C^0 = \frac{q_C^{N-1} - q_C^{N+1}}{2}$
$f_C^{+}(TDG_{CH}^S)$	The condensed-to-atom Fukui function of the carbon atom of palladium complex derived from (S)-C–H bond activation TS	$f_C^{+} = q_C^N - q_C^{N+1}$
$f_C^{-}(TDG_{CH}^S)$	The condensed-to-atom Fukui function of the carbon atom of palladium complex derived from (S)-C–H bond activation TS	$f_C^{-} = q_C^{N-1} - q_C^N$
$f_C^0(TDG_{GS}^b)$	The condensed-to-atom Fukui function of the carbon atom of ground state palladium complex	$f_C^0 = \frac{q_C^{N-1} - q_C^{N+1}}{2}$

$f_C^+(TDG_{GS}^b)$	The condensed-to-atom Fukui function of the carbon atom of ground state palladium complex	$f_C^+ = q_C^N - q_C^{N+1}$
$f_C^-(TDG_{GS}^b)$	The condensed-to-atom Fukui function of the carbon atom of ground state palladium complex	$f_C^- = q_C^{N-1} - q_C^N$
$s_{Pd}^0(TDG_{CH}^R)$	The condensed local softnesses of the palladium atom of palladium complex derived from (R)-C–H bond activation TS	$\frac{f_{Pd}^0}{\eta}$ (η : Hardness)
$s_{Pd}^+(TDG_{CH}^R)$	The condensed local softnesses of the palladium atom of palladium complex derived from (R)-C–H bond activation TS	$\frac{f_{Pd}^+}{\eta}$ (η : Hardness)
$s_{Pd}^-(TDG_{CH}^R)$	The condensed local softnesses of the palladium atom of palladium complex derived from (R)-C–H bond activation TS	$\frac{f_{Pd}^-}{\eta}$ (η : Hardness)
$s_{Pd}^0(TDG_{CH}^S)$	The condensed local softnesses of the palladium atom of palladium complex derived from (S)-C–H bond activation TS	$\frac{f_{Pd}^0}{\eta}$ (η : Hardness)
$s_{Pd}^+(TDG_{CH}^S)$	The condensed local softnesses of the palladium atom of palladium complex derived from (S)-C–H bond activation TS	$\frac{f_{Pd}^+}{\eta}$ (η : Hardness)
$s_{Pd}^-(TDG_{CH}^S)$	The condensed local softnesses of the palladium atom of palladium complex derived from (S)-C–H bond activation TS	$\frac{f_{Pd}^-}{\eta}$ (η : Hardness)
$s_{Pd}^0(TDG_{GS}^b)$	The condensed local softnesses of the palladium atom of ground state palladium complex with base fragment	$\frac{f_{Pd}^0}{\eta}$ (η : Hardness)
$s_{Pd}^+(TDG_{GS}^b)$	The condensed local softnesses of the palladium atom of ground state palladium complex with base fragment	$\frac{f_{Pd}^+}{\eta}$ (η : Hardness)
$s_{Pd}^-(TDG_{GS}^b)$	The condensed local softnesses of the palladium atom of ground state palladium complex with base fragment	$\frac{f_{Pd}^-}{\eta}$ (η : Hardness)
$s_{Pd}^0(TDG_{Al}^R)$	The condensed local softnesses of the palladium atom of palladium complex derived from (R)-alkene insertion TS	$\frac{f_{Pd}^0}{\eta}$ (η : Hardness)
$s_{Pd}^+(TDG_{Al}^R)$	The condensed local softnesses of the palladium atom of palladium complex derived from (R)-alkene insertion TS	$\frac{f_{Pd}^+}{\eta}$ (η : Hardness)
$s_{Pd}^-(TDG_{Al}^R)$	The condensed local softnesses of the palladium atom of palladium complex derived from (R)-alkene insertion TS	$\frac{f_{Pd}^-}{\eta}$ (η : Hardness)
$s_{Pd}^0(TDG_{Al}^S)$	The condensed local softnesses of the palladium atom of palladium complex derived from (S)-alkene insertion TS	$\frac{f_{Pd}^0}{\eta}$ (η : Hardness)
$s_{Pd}^+(TDG_{Al}^S)$	The condensed local softnesses of the palladium atom of palladium complex derived from (S)-alkene insertion TS	$\frac{f_{Pd}^+}{\eta}$ (η : Hardness)
$s_{Pd}^-(TDG_{Al}^S)$	The condensed local softnesses of the palladium atom of palladium complex derived from (S)-alkene insertion TS	$\frac{f_{Pd}^-}{\eta}$ (η : Hardness)
$s_{Pd}^0(TDG_{GS})$	The condensed local softnesses of the palladium atom of ground state palladium complex	$\frac{f_{Pd}^0}{\eta}$ (η : Hardness)
$s_{Pd}^+(TDG_{GS})$	The condensed local softnesses of the palladium atom of ground state palladium complex	$\frac{f_{Pd}^+}{\eta}$ (η : Hardness)
$s_{Pd}^-(TDG_{GS})$	The condensed local softnesses of the palladium atom of ground state palladium complex	$\frac{f_{Pd}^-}{\eta}$ (η : Hardness)
$s_{O1}^0(TDG_{CH}^R)$	The condensed local softnesses of the oxygen atom of palladium complex derived from (R)-C–H bond activation TS (site 1 at base part)	$\frac{f_{O1}^0}{\eta}$ (η : Hardness)

$s_{O1}^+(TDG_{CH}^R)$	The condensed local softnesses of the oxygen atom of palladium complex derived from (R)-C–H bond activation TS (site 1 at base part)	$\frac{f_{O1}^+}{\eta}$ (η : Hardness)
$s_{O1}^-(TDG_{CH}^R)$	The condensed local softnesses of the oxygen atom of palladium complex derived from (R)-C–H bond activation TS (site 1 at base part)	$\frac{f_{O1}^-}{\eta}$ (η : Hardness)
$s_{O1}^0(TDG_{CH}^S)$	The condensed local softnesses of the oxygen atom of palladium complex derived from (S)-C–H bond activation TS (site 1 at base part)	$\frac{f_{O1}^0}{\eta}$ (η : Hardness)
$s_{O1}^+(TDG_{CH}^S)$	The condensed local softnesses of the oxygen atom of palladium complex derived from (S)-C–H bond activation TS (site 1 at base part)	$\frac{f_{O1}^+}{\eta}$ (η : Hardness)
$s_{O1}^-(TDG_{CH}^S)$	The condensed local softnesses of the oxygen atom of palladium complex derived from (S)-C–H bond activation TS (site 1 at base part)	$\frac{f_{O1}^-}{\eta}$ (η : Hardness)
$s_{O1}^0(TDG_{GS}^b)$	The condensed local softnesses of the oxygen atom of ground state palladium complex with base fragment (site 1 at base part)	$\frac{f_{O1}^0}{\eta}$ (η : Hardness)
$s_{O1}^+(TDG_{GS}^b)$	The condensed local softnesses of the oxygen atom of ground state palladium complex with base fragment (site 1 at base part)	$\frac{f_{O1}^+}{\eta}$ (η : Hardness)
$s_{O1}^-(TDG_{GS}^b)$	The condensed local softnesses of the oxygen atom of ground state palladium complex with base fragment (site 1 at base part)	$\frac{f_{O1}^-}{\eta}$ (η : Hardness)
$s_{O2}^0(TDG_{CH}^R)$	The condensed local softnesses of the oxygen atom of palladium complex derived from (R)-C–H bond activation TS (site 2 at base part)	$\frac{f_{O2}^0}{\eta}$ (η : Hardness)
$s_{O2}^+(TDG_{CH}^R)$	The condensed local softnesses of the oxygen atom of palladium complex derived from (R)-C–H bond activation TS (site 2 at base part)	$\frac{f_{O2}^+}{\eta}$ (η : Hardness)
$s_{O2}^-(TDG_{CH}^R)$	The condensed local softnesses of the oxygen atom of palladium complex derived from (R)-C–H bond activation TS (site 2 at base part)	$\frac{f_{O2}^-}{\eta}$ (η : Hardness)
$s_{O2}^0(TDG_{CH}^S)$	The condensed local softnesses of the oxygen atom of palladium complex derived from (S)-C–H bond activation TS (site 2 at base part)	$\frac{f_{O2}^0}{\eta}$ (η : Hardness)
$s_{O2}^+(TDG_{CH}^S)$	The condensed local softnesses of the oxygen atom of palladium complex derived from (S)-C–H bond activation TS (site 2 at base part)	$\frac{f_{O2}^+}{\eta}$ (η : Hardness)
$s_{O2}^-(TDG_{CH}^S)$	The condensed local softnesses of the oxygen atom of palladium complex derived from (S)-C–H bond activation TS (site 2 at base part)	$\frac{f_{O2}^-}{\eta}$ (η : Hardness)
$s_{O2}^0(TDG_{GS}^b)$	The condensed local softnesses of the oxygen atom of ground state palladium complex with base fragment (site 2 at base part)	$\frac{f_{O2}^0}{\eta}$ (η : Hardness)
$s_{O2}^+(TDG_{GS}^b)$	The condensed local softnesses of the oxygen atom of ground state palladium complex with base fragment (site 2 at base part)	$\frac{f_{O2}^+}{\eta}$ (η : Hardness)

$s_{O_2}^-(TDG_{GS}^b)$	The condensed local softnesses of the oxygen atom of ground state palladium complex with base fragment (site 2 at base part)	$\frac{f_{O_2}^-}{\eta}$ (η : Hardness)
$s_C^0(TDG_{CH}^R)$	The condensed local softnesses of the carbon atom of palladium complex derived from (R)-C–H bond activation TS	$\frac{f_C^0}{\eta}$ (η : Hardness)
$s_C^+(TDG_{CH}^R)$	The condensed local softnesses of the carbon atom of palladium complex derived from (R)-C–H bond activation TS	$\frac{f_C^+}{\eta}$ (η : Hardness)
$s_C^-(TDG_{CH}^R)$	The condensed local softnesses of the carbon atom of palladium complex derived from (R)-C–H bond activation TS	$\frac{f_C^-}{\eta}$ (η : Hardness)
$s_C^0(TDG_{CH}^S)$	The condensed local softnesses of the carbon atom of palladium complex derived from (S)-C–H bond activation TS	$\frac{f_C^0}{\eta}$ (η : Hardness)
$s_C^+(TDG_{CH}^S)$	The condensed local softnesses of the carbon atom of palladium complex derived from (S)-C–H bond activation TS	$\frac{f_C^+}{\eta}$ (η : Hardness)
$s_C^-(TDG_{CH}^S)$	The condensed local softnesses of the carbon atom of palladium complex derived from (S)-C–H bond activation TS	$\frac{f_C^-}{\eta}$ (η : Hardness)
$s_C^0(TDG_{GS}^b)$	The condensed local softnesses of the carbon atom of ground state palladium complex with base fragment	$\frac{f_C^0}{\eta}$ (η : Hardness)
$s_C^+(TDG_{GS}^b)$	The condensed local softnesses of the carbon atom of ground state palladium complex with base fragment	$\frac{f_C^+}{\eta}$ (η : Hardness)
$s_C^-(TDG_{GS}^b)$	The condensed local softnesses of the carbon atom of ground state palladium complex with base fragment	$\frac{f_C^-}{\eta}$ (η : Hardness)
$\omega^{Pd}(TDG_{CH}^R)$	The condensed local electrophilicity index of the palladium atom of palladium complex derived from (R)-C–H bond activation TS	ωf_{Pd}^+ ($\omega = \frac{\mu^2}{2\eta}$)
$N_{Nu}^{Pd}(TDG_{CH}^R)$	The condensed local nucleophilicity index of the palladium atom of palladium complex derived from (R)-C–H bond activation TS	$N_{Nu}f_{Pd}^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^{Pd}(TDG_{CH}^S)$	The condensed local electrophilicity index of the palladium atom of palladium complex derived from (S)-C–H bond activation TS	ωf_{Pd}^+ ($\omega = \frac{\mu^2}{2\eta}$)
$N_{Nu}^{Pd}(TDG_{CH}^S)$	The condensed local nucleophilicity index of the palladium atom of palladium complex derived from (S)-C–H bond activation TS	$N_{Nu}f_{Pd}^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^{Pd}(TDG_{GS}^b)$	The condensed local electrophilicity index of the palladium atom of ground state palladium complex with base fragment	ωf_{Pd}^+ ($\omega = \frac{\mu^2}{2\eta}$)
$N_{Nu}^{Pd}(TDG_{GS}^b)$	The condensed local nucleophilicity index of the palladium atom of ground state palladium complex with base fragment	$N_{Nu}f_{Pd}^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^{Pd}(TDG_{AI}^R)$	The condensed local electrophilicity index of the palladium atom of palladium complex derived from (R)-alkene insertion TS	ωf_{Pd}^+ ($\omega = \frac{\mu^2}{2\eta}$)
$N_{Nu}^{Pd}(TDG_{AI}^R)$	The condensed local nucleophilicity index of the palladium atom of palladium complex derived from (R)-alkene insertion TS	$N_{Nu}f_{Pd}^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^{Pd}(TDG_{AI}^S)$	The condensed local electrophilicity index of the palladium atom of palladium complex derived from (S)-alkene insertion TS	ωf_{Pd}^+ ($\omega = \frac{\mu^2}{2\eta}$)
$N_{Nu}^{Pd}(TDG_{AI}^S)$	The condensed local nucleophilicity index of the palladium atom of palladium complex derived from (S)-alkene insertion TS	$N_{Nu}f_{Pd}^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)
$\omega^{Pd}(TDG_{GS})$	The condensed local electrophilicity index of the palladium atom of ground state palladium complex	ωf_{Pd}^+ ($\omega = \frac{\mu^2}{2\eta}$)
$N_{Nu}^{Pd}(TDG_{GS})$	The condensed local nucleophilicity index of the palladium atom of ground state palladium complex	$N_{Nu}f_{Pd}^-$ ($E_{HOMO}(Nu) - E_{HOMO}(TCE)$)

$\omega^{O1}(TDG_{CH}^R)$	The condensed local electrophilicity index of the oxygen atom of palladium complex derived from (R)-C–H bond activation (site 1 at base part)	$\omega f_{O1}^+ \quad (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{O1}(TDG_{CH}^R)$	The condensed local nucleophilicity index of the oxygen atom of palladium complex derived from (R)-C–H bond activation (site 1 at base part)	$N_{Nuf_{O1}}^-$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{O1}(TDG_{CH}^S)$	The condensed local electrophilicity index of the oxygen atom of palladium complex derived from (S)-C–H bond activation (site 1 at base part)	$\omega f_{O1}^+ \quad (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{O1}(TDG_{CH}^S)$	The condensed local nucleophilicity index of the oxygen atom of palladium complex derived from (S)-C–H bond activation (site 1 at base part)	$N_{Nuf_{O1}}^-$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{O1}(TDG_{GS}^b)$	The condensed local electrophilicity index of the oxygen atom of ground state palladium complex with base fragment (site 1 at base part)	$\omega f_{O1}^+ \quad (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{O1}(TDG_{GS}^b)$	The condensed local nucleophilicity index of the oxygen atom of ground state palladium complex with base fragment (site 1 at base part)	$N_{Nuf_{O1}}^-$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{O2}(TDG_{CH}^R)$	The condensed local electrophilicity index of the oxygen atom of palladium complex derived from (R)-C–H bond activation (site 2 at base part)	$\omega f_{O2}^+ \quad (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{O2}(TDG_{CH}^R)$	The condensed local nucleophilicity index of the oxygen atom of palladium complex derived from (R)-C–H bond activation (site 2 at base part)	$N_{Nuf_{O2}}^-$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{O2}(TDG_{CH}^S)$	The condensed local electrophilicity index of the oxygen atom of palladium complex derived from (S)-C–H bond activation (site 2 at base part)	$\omega f_{O2}^+ \quad (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{O2}(TDG_{CH}^S)$	The condensed local nucleophilicity index of the oxygen atom of palladium complex derived from (S)-C–H bond activation (site 2 at base part)	$N_{Nuf_{O2}}^-$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{O2}(TDG_{GS}^b)$	The condensed local electrophilicity index of the oxygen atom of ground state palladium complex with base fragment (site 2 at base part)	$\omega f_{O2}^+ \quad (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{O2}(TDG_{GS}^b)$	The condensed local nucleophilicity index of the oxygen atom of ground state palladium complex with base fragment (site 2 at base part)	$N_{Nuf_{O2}}^-$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^C(TDG_{CH}^R)$	The condensed local electrophilicity index of the carbon atom of palladium complex derived from (R)-C–H bond activation	$\omega f_C^+ \quad (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^C(TDG_{CH}^R)$	The condensed local nucleophilicity index of the carbon atom of palladium complex derived from (R)-C–H bond activation	$N_{Nuf_C}^-$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^C(TDG_{CH}^S)$	The condensed local electrophilicity index of the carbon atom of palladium complex derived from (S)-C–H bond activation	$\omega f_C^+ \quad (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^C(TDG_{CH}^S)$	The condensed local nucleophilicity index of the carbon atom of palladium complex derived from (S)-C–H bond activation	$N_{Nuf_C}^-$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$

$\omega^c(TDG_{GS}^b)$	The condensed local electrophilicity index of the carbon atom of ground state palladium complex with base fragment	$\omega f_C^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^c(TDG_{GS}^b)$	The condensed local nucleophilicity index of the carbon atom of ground state palladium complex with base fragment	$N_{Nu} f_C^-$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$