Features	Definition	Access
$q_C^N(Biaryl_{CH}^R)$	The Hirshfeld charge of the reacting carbon atom of neutral	DFT calculation based on xTB
$q_C(Btaryt_{CH})$	imine derived from (R)-C-H bond activation TS	optimized geometries
	The Hirshfeld charge of the reacting carbon atom of imine	DFT calculation based on xTB
$q_C^{N+1}(Biaryl_{CH}^R)$	derived from (R)-C-H bond activation TS with one positive	optimized geometries
	charge	optimized geometries
	The Hirshfeld charge of the reacting carbon atom of imine	DFT calculation based on xTB
$q_C^{N-1}(Biaryl_{CH}^R)$	derived from (R)-C-H bond activation TS with one negative	optimized geometries
	charge	optimized geometries
$q_C^N(Biaryl_{CH}^S)$	The Hirshfeld charge of the reacting carbon atom of neutral	DFT calculation based on xTB
$q_C(Dtaryt_{CH})$	imine derived from (S)-C-H bond activation TS	optimized geometries
	The Hirshfeld charge of the reacting carbon atom of imine	DFT calculation based on xTB
$q_C^{N+1}(Biaryl_{CH}^S)$	derived from (S)-C-H bond activation TS with one positive	
	charge	optimized geometries
	The Hirshfeld charge of the reacting carbon atom of imine	DFT calculation based on xTB
$q_C^{N-1}(Biaryl_{CH}^S)$	derived from (S)-C-H bond activation TS with one negative	
	charge	optimized geometries
N.CD.	The Hirshfeld charge of the reacting carbon atom of neutral	DFT calculation based on xTB
$q_C^N(Biaryl_{GS})$	ground state imine	optimized geometries
N+1 (D: 1)	The Hirshfeld charge of the reacting carbon atom of ground state	DFT calculation based on xTB
$q_C^{N+1}(Biaryl_{GS})$	imine with one positive charge	optimized geometries
N-1 (D: 1)	The Hirshfeld charge of the reacting carbon atom of ground state	DFT calculation based on xTB
$q_C^{N-1}(Biaryl_{GS})$	imine with one negative charge	optimized geometries
N co. 1D	The Hirshfeld charge of the reacting carbon atom of neutral	DFT calculation based on xTB
$q_C^N(Biaryl_{AI}^R)$	imine derived from (R)-alkene insertion TS	optimized geometries
N+1 (D)	The Hirshfeld charge of the reacting carbon atom of imine	DFT calculation based on xTB
$q_C^{N+1}(Biaryl_{AI}^R)$	derived from (R)-alkene insertion TS with one positive charge	optimized geometries
N-1 (D) IP	The Hirshfeld charge of the reacting carbon atom of imine	DFT calculation based on xTB
$q_C^{N-1}(Biaryl_{AI}^R)$	derived from (R)-alkene insertion TS with one negative charge	optimized geometries
N	The Hirshfeld charge of the reacting carbon atom of neutral	DFT calculation based on xTB
$q_C^N(Biaryl_{AI}^S)$	imine derived from (S)-alkene insertion TS	optimized geometries
N. I. A	The Hirshfeld charge of the reacting carbon atom of imine	DFT calculation based on xTB
$q_C^{N+1}(Biaryl_{AI}^S)$	derived from (S)-alkene insertion TS with one positive charge	optimized geometries
N. 1	The Hirshfeld charge of the reacting carbon atom of imine	DFT calculation based on xTB
$q_C^{N-1}(Biaryl_{AI}^S)$	derived from (S)-alkene insertion TS with one negative charge	optimized geometries
N	The Hirshfeld charge of the reacting carbon atom of neutral	DFT calculation based on xTB
$q_C^N(Biaryl_{GS})$	ground state imine	optimized geometries
Wid	The Hirshfeld charge of the reacting carbon atom of ground state	DFT calculation based on xTB
$q_C^{N+1}(Biaryl_{GS})$	imine with one positive charge	optimized geometries
	The Hirshfeld charge of the reacting carbon atom of ground state	DFT calculation based on xTB
$q_C^{N-1}(Biaryl_{GS})$	imine with one negative charge	optimized geometries
	The Hirshfeld charge of the reacting hydrogen atom of neutral	DFT calculation based on xTB
$q_H^N(Biaryl_{CH}^R)$	imine derived from (<i>R</i>)-C–H bond activation TS	optimized geometries
	(1)	1 6

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

$f_C^+(Biaryl_{AI}^S)$ The condensed-to-atom Fukui function of the reacting carbon atom of imine derived from (S)-alkene insertion TS The condensed-to-atom Fukui function of the reacting carbon	$c_{C} = \frac{q_{C}^{N-1} - q_{C}^{N+1}}{2}$ $c_{C}^{+} = q_{C}^{N} - q_{C}^{N+1}$
$f_C^+(Biaryl_{AI}^S)$ atom of imine derived from (S)-alkene insertion TS The condensed-to-atom Fukui function of the reacting carbon $f_C^-(Biaryl_{AI}^S)$	$f_C^+ = q_C^N - q_C^{N+1}$
$f_{c}^{-}(Biaryl_{M}^{2})$	
atom of minic derived from (3)-airche insertion 13	$f_C^- = q_C^{N-1} - q_C^N$
$f_{c}^{0}(Biaryl_{GS})$ The condensed-to-atom Fukui function of the reacting carbon atom of ground state imine	$c_{C}^{0} = \frac{q_{C}^{N-1} - q_{C}^{N+1}}{2}$
$f_C^+(Biaryl_{GS})$ 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	$_{H}^{0}=\frac{q_{H}^{N-1}-q_{H}^{N+1}}{2}$
The condensed-to-atom Fukui function of the reacting hydrogen $f_H^+(Biaryl_{CH}^R)$ 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	$_{H}^{0} = \frac{q_{H}^{N-1} - q_{H}^{N+1}}{2}$
$f_H^+(Biaryl_{CH}^S)$ 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	$_{H}^{0}=\frac{q_{H}^{N-1}-q_{H}^{N+1}}{2}$
$f_H^+(Biaryl_{GS})$ 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	$\frac{f_{\overline{c}}}{\eta}$ (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)
The condensed local softnesses of the reacting carbon atom of imine derived from (S)-C–H bond activation TS 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)
	$\frac{f\bar{c}}{n}$ (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	η

$s_{C}^{+}(Biaryl_{GS})$	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	$\frac{f\bar{c}}{\eta}$ (η : Hardness)
$s_C^0(Biaryl_{AI}^R)$	The condensed local softnesses of the reacting carbon atom of imine derived from (R)-alkene insertion TS	$\frac{f_c^0}{\eta}$ (η : Hardness)
$s_{\mathcal{C}}^{+}(Biaryl_{AI}^{R})$	The condensed local softnesses of the reacting carbon atom of imine derived from (R) -alkene insertion TS	$\frac{f_c^+}{\eta}$ (η : Hardness)
$s_{\mathcal{C}}^{-}(Biaryl_{AI}^{R})$	The condensed local softnesses of the reacting carbon atom of imine derived from (R) -alkene insertion TS	$\frac{f_{\overline{c}}}{\eta}$ (η : Hardness)
$s_{\mathcal{C}}^{0}(Biaryl_{AI}^{S})$	The condensed local softnesses of the reacting carbon atom of imine derived from (S)-alkene insertion TS	$\frac{f_c^0}{\eta}$ (η : Hardness)
$s_{\scriptscriptstyle C}^+(Biaryl_{\scriptscriptstyle AI}^S)$	The condensed local softnesses of the reacting carbon atom of imine derived from (S)-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 (S)-alkene insertion TS	$\frac{f_c^-}{\eta}$ (η : Hardness)
$s_{\mathcal{C}}^{0}(Biaryl_{GS})$	The condensed local softnesses of the reacting carbon atom of ground state imine	$\frac{f_c^0}{\eta}$ (η : Hardness)
$s_{\mathcal{C}}^{+}(Biaryl_{GS})$	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	$\frac{f_{\overline{c}}^{-}}{\eta}$ (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	$\frac{f_{\overline{H}}}{\eta}$ (η : Hardness)
$s_H^0(Biaryl_{CH}^S)$	The condensed local softnesses of the reacting hydrogen atom of imine derived from (S)-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 (S)-C—H bond activation TS	$\frac{f_H^{\dagger}}{\eta}$ (η : Hardness)
$s_H^-(Biaryl_{CH}^S)$	The condensed local softnesses of the reacting hydrogen atom of imine derived from (S)-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	$\omega f_C^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{C}(Biaryl_{CH}^{R})$	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	$N_{Nu}f_C^ (E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{\mathcal{C}}(Biaryl_{GS})$	The condensed local electrophilicity index of the reacting carbon atom of ground state imine	$\omega f_C^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{C}(Biaryl_{GS})$	The condensed local nucleophilicity index of the reacting carbon atom of ground state imine	$N_{Nu}f_C^ (E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{C}(Biaryl_{AI}^{R})$	The condensed local electrophilicity index of the reacting carbon atom of imine derived from (<i>R</i>)-alkene insertion TS	$\omega f_C^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{\mathcal{C}}(Biaryl_{AI}^{R})$	The condensed local nucleophilicity index of the reacting carbon atom of imine derived from (<i>R</i>)-alkene insertion TS	$N_{Nu}f_C^ (E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{c}(Biaryl_{AI}^{S})$	The condensed local electrophilicity index of the reacting carbon atom of imine derived from (S)-alkene insertion TS	$\omega f_C^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{\mathcal{C}}(Biaryl_{AI}^{\mathcal{S}})$	The condensed local nucleophilicity index of the reacting carbon atom of imine derived from (S)-alkene insertion TS	$N_{Nu}f_C^ (E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{\mathcal{C}}(Biaryl_{GS})$	The condensed local electrophilicity index of the reacting carbon atom of ground state imine	$\omega f_C^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{C}(Biaryl_{GS})$	The condensed local nucleophilicity index of the reacting carbon atom of ground state imine	$N_{Nu}f_c^ (E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^H(Biaryl^R_{CH})$	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 (<i>R</i>)-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	$\omega f_H^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N^H_{Nu}(Biaryl^S_{CH})$	The condensed local nucleophilicity index of the reacting hydrogen atom of imine derived from (S)-C–H bond activation TS	$N_{Nu}f_{H}^{-}$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^H(Biaryl_{GS})$	The condensed local electrophilicity index of the reacting hydrogen atom of ground state imine	$\omega f_H^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{H}(Biaryl_{GS})$	The condensed local nucleophilicity index of the reacting hydrogen atom of ground state imine	$N_{Nu}f_H^ (E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$q_{C1}^N(Olefin_{AI}^R)$	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
$q_{\mathcal{C}1}^{N+1}(Olefin_{AI}^R)$	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
$q_{C1}^{N-1}(Olefin_{AI}^R)$	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 (S)-alkene insertion TS	DFT calculation based on xTB optimized geometries
$q_{C1}^{N+1}(Olefin_{Al}^S)$	The Hirshfeld charge of the reacting terminal carbon atom of olefin derived from (S)-alkene insertion TS with one positive charge	DFT calculation based on xTB optimized geometries
$q_{C1}^{N-1}(Olefin_{Al}^S)$	The Hirshfeld charge of the reacting terminal carbon atom of olefin derived from (S)-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 (R) -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 (R) -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	DFT calculation based on xTB
102() - AI)	neutral olefin from (S)-alkene insertion TS	optimized geometries
$q_{C2}^{N+1}(Olefin_{AI}^S)$	neutral olefin from (S)-alkene insertion TS The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (S)-alkene insertion TS with one positive charge	optimized geometries DFT calculation based on xTB optimized geometries
	The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (S)-alkene insertion TS with one positive	DFT calculation based on xTB
$q_{C2}^{N+1}(Olefin_{AI}^S)$	The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (S)-alkene insertion TS with one positive charge The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (S)-alkene insertion TS with one negative	DFT calculation based on xTB optimized geometries DFT calculation based on xTB
$q_{C2}^{N+1}(Olefin_{AI}^S)$ $q_{C2}^{N-1}(Olefin_{AI}^S)$	The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (S)-alkene insertion TS with one positive charge The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (S)-alkene insertion TS with one negative charge The Hirshfeld charge of the reacting substituted carbon atom of	DFT calculation based on xTB optimized geometries DFT calculation based on xTB optimized geometries DFT calculation based on xTB
$q_{C2}^{N+1}(Olefin_{AI}^S)$ $q_{C2}^{N-1}(Olefin_{AI}^S)$ $q_{C2}^{N}(Olefin_{GS}^S)$	The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (S)-alkene insertion TS with one positive charge The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (S)-alkene insertion TS with one negative charge The Hirshfeld charge of the reacting substituted carbon atom of neutral ground state olefin The Hirshfeld charge of the reacting substituted carbon atom of	DFT calculation based on xTB optimized geometries DFT calculation based on xTB optimized geometries DFT calculation based on xTB optimized geometries DFT calculation based on xTB
$q_{C2}^{N+1}(Olefin_{AI}^S)$ $q_{C2}^{N-1}(Olefin_{AI}^S)$ $q_{C2}^{N}(Olefin_{GS})$ $q_{C2}^{N+1}(Olefin_{GS})$	The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (S)-alkene insertion TS with one positive charge The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (S)-alkene insertion TS with one negative charge The Hirshfeld charge of the reacting substituted carbon atom of neutral ground state olefin The Hirshfeld charge of the reacting substituted carbon atom of ground state olefin with one positive charge The Hirshfeld charge of the reacting substituted carbon atom of	DFT calculation based on xTB optimized geometries DFT calculation based on xTB
$q_{C2}^{N+1}(Olefin_{AI}^S)$ $q_{C2}^{N-1}(Olefin_{AI}^S)$ $q_{C2}^{N}(Olefin_{GS})$ $q_{C2}^{N+1}(Olefin_{GS})$ $q_{C2}^{N-1}(Olefin_{GS})$	The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (S)-alkene insertion TS with one positive charge The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (S)-alkene insertion TS with one negative charge The Hirshfeld charge of the reacting substituted carbon atom of neutral ground state olefin The Hirshfeld charge of the reacting substituted carbon atom of ground state olefin with one positive charge The Hirshfeld charge of the reacting substituted carbon atom of ground state olefin with one negative charge The condensed-to-atom Fukui function of the terminal carbon	DFT calculation based on xTB optimized geometries
$q_{C2}^{N+1}(Olefin_{AI}^S)$ $q_{C2}^{N-1}(Olefin_{AI}^S)$ $q_{C2}^{N}(Olefin_{GS})$ $q_{C2}^{N+1}(Olefin_{GS})$ $q_{C2}^{N-1}(Olefin_{GS})$ $f_{C1}^{0}(Olefin_{AI}^R)$	The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (S)-alkene insertion TS with one positive charge The Hirshfeld charge of the reacting substituted carbon atom of olefin derived from (S)-alkene insertion TS with one negative charge The Hirshfeld charge of the reacting substituted carbon atom of neutral ground state olefin The Hirshfeld charge of the reacting substituted carbon atom of ground state olefin with one positive charge The Hirshfeld charge of the reacting substituted carbon atom of ground state olefin with one negative charge The condensed-to-atom Fukui function of the terminal carbon atom of olefin derived from (R)-alkene insertion TS The condensed-to-atom Fukui function of the terminal carbon	DFT calculation based on xTB optimized geometries DFT calculation based on xTB optimized geometries $f_{C1}^{0} = \frac{q_{C1}^{N-1} - q_{C1}^{N+1}}{2}$

$f_{C1}^+(Olefin_{AI}^S)$	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	$f_{C1}^0 = \frac{q_{C1}^{N-1} - q_{C1}^{N+1}}{2}$
	The condensed-to-atom Fukui function of the terminal carbon	
$f_{C1}^+(Olefin_{GS})$	atom of ground state olefin	$f_{C1}^+ = q_{C1}^N - q_{C1}^{N+1}$
	The condensed-to-atom Fukui function of the terminal carbon	V 4 V
$f_{C1}^-(Olefin_{GS})$	atom of ground state olefin	$f_{C1}^- = q_{C1}^{N-1} - q_{C1}^N$
-0	The condensed-to-atom Fukui function of the substituted carbon	$a_{c2}^{N-1} - a_{c2}^{N+1}$
$f_{C2}^0(Olefin_{AI}^R)$	atom of olefin derived from (R) -alkene insertion TS	$f_{C2}^0 = \frac{q_{C2}^{N-1} - q_{C2}^{N+1}}{2}$
	The condensed-to-atom Fukui function of the substituted carbon	
$f_{C2}^+(Olefin_{AI}^R)$	atom of olefin derived from (R) -alkene insertion TS	$f_{C2}^+ = q_{C2}^N - q_{C2}^{N+1}$
	The condensed-to-atom Fukui function of the substituted carbon	
$f_{C2}^-(Olefin_{AI}^R)$	atom of olefin derived from (R)-alkene insertion TS	$f_{C2}^- = q_{C2}^{N-1} - q_{C2}^N$
	The condensed-to-atom Fukui function of the substituted carbon	a^{N-1} a^{N+1}
$f_{C2}^0(Olefin_{AI}^S)$	atom of olefin derived from (S)-alkene insertion TS	$f_{C2}^0 = \frac{q_{C2}^{N-1} - q_{C2}^{N+1}}{2}$
	The condensed-to-atom Fukui function of the substituted carbon	
$f_{C2}^+(Olefin_{AI}^S)$	atom of olefin derived from (S)-alkene insertion TS	$f_{C2}^+ = q_{C2}^N - q_{C2}^{N+1}$
	The condensed-to-atom Fukui function of the substituted carbon	
$f_{C2}^-(Olefin_{AI}^S)$	atom of olefin derived from (S)-alkene insertion TS	$f_{C2}^- = q_{C2}^{N-1} - q_{C2}^N$
	The condensed-to-atom Fukui function of the substituted carbon	~N-1 ~N+1
$f_{C2}^0(Olefin_{GS})$	atom of ground state olefin	$f_{C2}^0 = \frac{q_{C2}^{N-1} - q_{C2}^{N+1}}{2}$
	The condensed-to-atom Fukui function of the substituted carbon	2
$f_{C2}^+(Olefin_{GS})$	atom of ground state olefin	$f_{C2}^+ = q_{C2}^N - q_{C2}^{N+1}$
	The condensed-to-atom Fukui function of the substituted carbon	
$f_{C2}^{-}(Olefin_{GS})$	atom of ground state olefin	$f_{C2}^- = q_{C2}^{N-1} - q_{C2}^N$
	The condensed local softnesses of the terminal carbon atom of	
$s_{C1}^0(Olefin_{AI}^R)$	olefin derived from (R)-alkene insertion TS	$\frac{f_{c_1}^n}{\eta}$ (η: Hardness)
	The condensed local softnesses of the terminal carbon atom of	
$s_{C1}^+(Olefin_{AI}^R)$	olefin derived from (R)-alkene insertion TS	$\frac{f_{C_1}^+}{\eta}$ (η : Hardness)
	The condensed local softnesses of the terminal carbon atom of	
$s_{C1}^{-}(Olefin_{AI}^{R})$	olefin derived from (R)-alkene insertion TS	$\frac{f_{C_1}^-}{\eta}$ (η : Hardness)
	The condensed local softnesses of the terminal carbon atom of	
$s_{C1}^0(Olefin_{AI}^S)$	olefin derived from (S)-alkene insertion TS	$\frac{f_{C1}^0}{\eta}$ (η : Hardness)
	The condensed local softnesses of the terminal carbon atom of	,
$s_{C1}^+(Olefin_{AI}^S)$	olefin derived from (S)-alkene insertion TS	$\frac{f_{C1}^+}{\eta}$ (η : Hardness)
	The condensed local softnesses of the terminal carbon atom of	,
$s_{C1}^-(Olefin_{AI}^S)$		$\frac{f_{C1}^-}{\eta}$ (η : Hardness)
	olefin derived from (S)-alkene insertion TS The condensed local softnesses of the terminal carbon atom of	
$s_{C1}^0(Olefin_{GS})$	The condensed local softnesses of the terminal carbon atom of	$\frac{f_{C1}^0}{\eta}$ (η : Hardness)
	ground state olefin	,
$s_{C1}^+(Olefin_{GS})$	The condensed local softnesses of the terminal carbon atom of ground state olefin	$\frac{f_{C1}^+}{\eta}$ (η : Hardness)

$s_{C1}^{-}(Olefin_{GS})$		
01() 03/	The condensed local softnesses of the terminal carbon atom of ground state olefin	$\frac{f\bar{c_1}}{\eta}$ (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 (R)-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 (S)-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 (S)-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 (S)-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	$\omega f_{C1}^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{C1}(Olefin_{AI}^R)$	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 (S)-alkene insertion TS	$\omega f_{C1}^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{C1}(Olefin_{AI}^S)$	The condensed local nucleophilicity index of the terminal carbon atom of olefin derived from (S)-alkene insertion TS	$N_{Nu}f_{C1}^{-}$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
C1	The condensed local electrophilicity index of the terminal carbon	
$\omega^{C1}(Olefin_{GS})$	atom of ground state olefin	$\omega f_{C1}^+ \ (\omega = \frac{\mu^2}{2\eta})$
$\omega^{c1}(Olefin_{GS})$ $N_{Nu}^{c1}(Olefin_{GS})$	atom of ground state olefin The condensed local nucleophilicity index of the terminal carbon atom of ground state olefin	$\omega f_{C1}^+ \ (\omega = \frac{\mu^2}{2\eta})$ $N_{Nu} f_{C1}^- $ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
	The condensed local nucleophilicity index of the terminal carbon	$N_{Nu}f_{C1}^{-}$
$N_{Nu}^{C1}(Olefin_{GS})$	The condensed local nucleophilicity index of the terminal carbon atom of ground state olefin The condensed local electrophilicity index of the substituted	$N_{Nu}f_{C1}^{-1}$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$N_{Nu}^{C1}(Olefin_{GS})$ $\omega^{C2}(Olefin_{AI}^R)$	The condensed local nucleophilicity index of the terminal carbon atom of ground state olefin The condensed local electrophilicity index of the substituted carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS The condensed local nucleophilicity index of the substituted	$N_{Nu}f_{C1}^{-}$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$ $\omega f_{C2}^{+} \ (\omega = \frac{\mu^{2}}{2\eta})$ $N_{Nu}f_{C2}^{-}$
$N_{Nu}^{C1}(Olefin_{GS})$ $\omega^{C2}(Olefin_{AI}^R)$ $N_{Nu}^{C2}(Olefin_{AI}^R)$	The condensed local nucleophilicity index of the terminal carbon atom of ground state olefin The condensed local electrophilicity index of the substituted carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS The condensed local nucleophilicity index of the substituted carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS The condensed local electrophilicity index of the substituted	$N_{Nu}f_{C1}^{-1}$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$ $\omega f_{C2}^{+} \ (\omega = \frac{\mu^{2}}{2\eta})$ $N_{Nu}f_{C2}^{-1}$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$N_{Nu}^{C1}(Olefin_{GS})$ $\omega^{C2}(Olefin_{AI}^R)$ $N_{Nu}^{C2}(Olefin_{AI}^R)$ $\omega^{C2}(Olefin_{AI}^S)$	The condensed local nucleophilicity index of the terminal carbon atom of ground state olefin The condensed local electrophilicity index of the substituted carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS The condensed local nucleophilicity index of the substituted carbon atom of olefin derived from (<i>R</i>)-alkene insertion TS The condensed local electrophilicity index of the substituted carbon atom of olefin derived from (<i>S</i>)-alkene insertion TS The condensed local nucleophilicity index of the substituted	$N_{Nu}f_{C1}^{-1}$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$ $\omega f_{C2}^{+} \ (\omega = \frac{\mu^{2}}{2\eta})$ $N_{Nu}f_{C2}^{-}$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$ $\omega f_{C2}^{+} \ (\omega = \frac{\mu^{2}}{2\eta})$ $N_{Nu}f_{C2}^{-}$

$q_{Pd}^N(TDG_{CH}^R)$	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 (R) -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 (R) -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 (S)-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 (S)-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 (R) -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 (R) -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 (R) -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 (S)-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 (S) -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 (S)-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
$q_{01}^{N-1}(TDG_{CH}^R)$	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
$q_{01}^{N-1}(TDG_{CH}^S)$	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 (<i>R</i>)-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

$q_{02}^{N+1}(TDG_{GS}^b)$	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
$q_{02}^{N-1}(TDG_{GS}^b)$	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 (<i>R</i>)-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 (<i>R</i>)-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 (<i>R</i>)-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 (<i>R</i>)-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 (<i>R</i>)-C–H activation TS	$f_{Pd}^{-} = q_{Pd}^{N-1} - q_{Pd}^{N}$
	TI 1 14 4 T 1 1 C 41 C 11 11 11 4 C	
$f_{Pd}^0(TDG_{CH}^S)$	The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (S)-C–H activation TS	$f_{Pd}^0 = \frac{q_{Pd}^{N-1} - q_{Pd}^{N+1}}{2}$
$f_{Pd}^{0}(TDG_{CH}^{S})$ $f_{Pd}^{+}(TDG_{CH}^{S})$		$f_{Pd}^{0} = \frac{q_{Pd}^{N-1} - q_{Pd}^{N+1}}{2}$ $f_{Pd}^{+} = q_{Pd}^{N} - q_{Pd}^{N+1}$
	palladium complex derived from (S)-C–H activation TS The condensed-to-atom Fukui function of the palladium atom of	_
$f_{Pd}^+(TDG_{CH}^S)$	palladium complex derived from (S)-C—H activation TS The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (S)-C—H activation TS The condensed-to-atom Fukui function of the palladium atom of	$f_{Pd}^{+} = q_{Pd}^{N} - q_{Pd}^{N+1}$
$f_{Pd}^{+}(TDG_{CH}^{S})$ $f_{Pd}^{-}(TDG_{CH}^{S})$	palladium complex derived from (S)-C-H activation TS The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (S)-C-H activation TS The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (S)-C-H activation TS The condensed-to-atom Fukui function of the palladium atom of	$f_{Pd}^{+} = q_{Pd}^{N} - q_{Pd}^{N+1}$ $f_{Pd}^{-} = q_{Pd}^{N-1} - q_{Pd}^{N}$

$f_{Pd}^{-}(TDG_{GS}^{b})$	The condensed-to-atom Fukui function of the palladium atom of	$f_{Pd}^{-} = q_{Pd}^{N-1} - q_{Pd}^{N}$
)Pu (G3)	ground state palladium complex with base fragment	Tra rra rra
$f_{Pd}^0(TDG_{AI}^R)$	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	$f_{Pd}^{+} = q_{Pd}^{N} - q_{Pd}^{N+1}$
$f_{Pd}^-(TDG_{AI}^R)$	The condensed-to-atom Fukui function of the palladium atom of palladium complex derived from (<i>R</i>)-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	$f_{Pd}^{-} = q_{Pd}^{N-1} - q_{Pd}^{N}$
$f_{\mathcal{O}1}^0(TDG_{CH}^R)$	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 (<i>R</i>)-C–H bond activation TS (site 1 at base part)	$f_{O1}^+ = q_{O1}^N - q_{O1}^{N+1}$
$f_{01}^-(TDG_{CH}^R)$	The condensed-to-atom Fukui function of the oxygen atom of palladium complex derived from (<i>R</i>)-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)	$f_{01}^0 = \frac{q_{01}^{N-1} - q_{01}^{N+1}}{2}$
$f_{o1}^+(TDG_{CH}^S)$	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)	$f_{O1}^+ = q_{O1}^N - q_{O1}^{N+1}$
$f_{01}^-(TDG_{CH}^S)$	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 (<i>R</i>)-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 (<i>R</i>)-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 (<i>R</i>)-C–H bond activation TS (site 2 at base part)	$f_{02}^{-} = q_{02}^{N-1} - q_{02}^{N}$
$f_{O2}^0(TDG_{CH}^S)$	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)	$f_{02}^{-} = q_{02}^{N-1} - q_{02}^{N}$
$f_{O2}^0(TDG_{GS}^b)$	The condensed-to-atom Fukui function of the oxygen atom of ground state palladium complex with base fragment (site 2 at base part)	$f_{O2}^0 = \frac{q_{O2}^{N-1} - q_{O2}^{N+1}}{2}$
$f_{02}^+(TDG_{GS}^b)$	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)	$f_{02}^{-} = q_{02}^{N-1} - q_{02}^{N}$
$f_C^0(TDG_{CH}^R)$	The condensed-to-atom Fukui function of the carbon atom of palladium complex derived from (<i>R</i>)-C–H bond activation TS	$f_C^0 = \frac{q_C^{N-1} - q_C^{N+1}}{2}$
$f_C^+(TDG_{CH}^R)$	The condensed-to-atom Fukui function of the carbon atom of palladium complex derived from (<i>R</i>)-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 (<i>R</i>)-C–H bond activation TS	$f_C^- = q_C^{N-1} - q_C^N$
$f_{\mathcal{C}}^{0}(TDG_{CH}^{S})$	The condensed-to-atom Fukui function of the carbon atom of palladium complex derived from (S)-C–H bond activation TS	$f_C^0 = \frac{q_C^{N-1} - q_C^{N+1}}{2}$
$f_{\mathcal{C}}^+(TDG_{CH}^S)$	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 (<i>R</i>)-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)
$s_{Pd}^0(TDG_{AI}^R)$	The condensed local softnesses of the palladium atom of palladium complex derived from (R) -alkene insertion TS	$\frac{f_{Pd}^0}{\eta}$ (η : Hardness)
$s_{Pd}^+(TDG_{AI}^R)$	The condensed local softnesses of the palladium atom of palladium complex derived from (R) -alkene insertion TS	$\frac{f_{Pd}^+}{\eta}$ (η : Hardness)
$s_{Pd}^{-}(TDG_{AI}^{R})$	The condensed local softnesses of the palladium atom of palladium complex derived from (R) -alkene insertion TS	$\frac{f_{Pd}^{-}}{\eta}$ (η : Hardness)
$s_{Pd}^0(TDG_{AI}^S)$	The condensed local softnesses of the palladium atom of palladium complex derived from (S) -alkene insertion TS	$\frac{f_{Pd}^0}{\eta}$ (η : Hardness)
$s_{Pd}^+(TDG_{AI}^S)$	The condensed local softnesses of the palladium atom of palladium complex derived from (S)-alkene insertion TS	$\frac{f_{Pd}^+}{\eta}$ (η : Hardness)
$s_{Pd}^-(TDG_{AI}^S)$	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 (<i>R</i>)-C–H bond activation TS (site 1 at base part)	$\frac{f_{01}^0}{\eta}$ (η : Hardness)

$s_{O1}^+(TDG_{CH}^R)$	The condensed local softnesses of the oxygen atom of palladium complex derived from (<i>R</i>)-C–H bond activation TS (site 1 at base part)	$\frac{f_{01}^+}{\eta}$ (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)	$\frac{f_{01}^-}{\eta}$ (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)	$\frac{f_{01}^0}{\eta}$ (η: Hardness)
$s_{01}^+(TDG_{CH}^S)$	The condensed local softnesses of the oxygen atom of palladium complex derived from (S) -C-H bond activation TS (site 1 at base part)	$\frac{f_{01}^+}{\eta}$ (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)	$\frac{f_{01}^{-}}{\eta}$ (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)	$\frac{f_{01}^0}{\eta}$ (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)	$\frac{f_{01}^+}{\eta}$ (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)	$\frac{f_{01}^-}{\eta}$ (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)	$\frac{f_{02}^0}{\eta}$ (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)	$\frac{f_{02}^+}{\eta}$ (η : Hardness)
$s_{02}^-(TDG_{CH}^R)$	The condensed local softnesses of the oxygen atom of palladium complex derived from (<i>R</i>)-C–H bond activation TS (site 2 at base part)	$\frac{f_{02}^-}{\eta}$ (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)	$\frac{f_{02}^0}{\eta}$ (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)	$\frac{f_{02}^+}{\eta}$ (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)	$\frac{f\bar{o_2}}{\eta}$ (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)	$\frac{f_{02}^0}{\eta}$ (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)	$\frac{f_{02}^+}{\eta}$ (η: Hardness)

$s_{02}^-(TDG_{GS}^b)$	The condensed local softnesses of the oxygen atom of ground state palladium complex with base fragment (site 2 at base part)	$\frac{f\bar{o}_2}{\eta}$ (η : Hardness)
$s_C^0(TDG_{CH}^R)$	The condensed local softnesses of the carbon atom of palladium complex derived from (<i>R</i>)-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 (<i>R</i>)-C–H bond activation TS	$\frac{f_{\overline{c}}}{\eta}$ (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	$\frac{f_{\overline{C}}}{\eta}$ (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	$\frac{f_{\mathcal{C}}^+}{\eta}$ (η : Hardness)
$s_C^-(TDG_{GS}^b)$	The condensed local softnesses of the carbon atom of ground state palladium complex with base fragment	$\frac{f\bar{c}}{\eta}$ (η : Hardness)
$\omega^{Pd}(TDG_{CH}^R)$	The condensed local electrophilicity index of the palladium atom of palladium complex derived from (<i>R</i>)-C–H bond activation TS	$\omega f_{Pd}^{+} \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{Pd}(TDG_{CH}^{R})$	The condensed local nucleophilicity index of the palladium atom of palladium complex derived from (<i>R</i>)-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	$\omega f_{Pd}^{+} \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{Pd}(TDG_{CH}^S)$	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	$\omega f_{Pd}^{+} \ (\omega = \frac{\mu^{2}}{2\eta})$
$N_{Nu}^{Pd}(TDG_{GS}^b)$	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 (<i>R</i>)-alkene insertion TS	$\omega f_{Pd}^{+} \ (\omega = \frac{\mu^{2}}{2\eta})$
$N_{Nu}^{Pd}(TDG_{AI}^{R})$	The condensed local nucleophilicity index of the palladium atom of palladium complex derived from (<i>R</i>)-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	$\omega f_{Pd}^{+} \ (\omega = \frac{\mu^{2}}{2\eta})$
$N_{Nu}^{Pd}(TDG_{AI}^S)$	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	$\omega f_{Pd}^{+} \ (\omega = \frac{\mu^{2}}{2\eta})$
$N_{Nu}^{Pd}(TDG_{GS})$	The condensed local nucleophilicity index of the palladium atom of ground state palladium complex	$N_{Nu}f_{Pd}^{-}$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE)$
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$\omega^{O1}(TDG^R_{CH})$	The condensed local electrophilicity index of the oxygen atom of palladium complex derived from (<i>R</i>)-C–H bond activation (site 1 at base part)	$\omega f_{O1}^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{O1}(TDG_{CH}^{R})$	The condensed local nucleophilicity index of the oxygen atom of palladium complex derived from (R) -C-H bond activation (site 1 at base part)	$N_{Nu}f_{O1}^{-}$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{O1}(TDG_{CH}^S)$	The condensed local electrophilicity index of the oxygen atom of palladium complex derived from (S)-C–H bond activation (site 1 at base part)	$\omega f_{O1}^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{O1}(TDG_{CH}^{S})$	The condensed local nucleophilicity index of the oxygen atom of palladium complex derived from (S)-C–H bond activation (site 1 at base part)	$N_{Nu}f_{O1}^{-}$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{o1}(TDG_{GS}^b)$	The condensed local electrophilicity index of the oxygen atom of ground state palladium complex with base fragment (site 1 at base part)	$\omega f_{O1}^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{O1}(TDG_{GS}^{b})$	The condensed local nucleophilicity index of the oxygen atom of ground state palladium complex with base fragment (site 1 at base part)	$N_{Nu}f_{O1}^{-}$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{O2}(TDG_{CH}^R)$	The condensed local electrophilicity index of the oxygen atom of palladium complex derived from (R) -C—H bond activation (site 2 at base part)	$\omega f_{O2}^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{O2}(TDG_{CH}^{R})$	The condensed local nucleophilicity index of the oxygen atom of palladium complex derived from (R) -C—H bond activation (site 2 at base part)	$N_{Nu}f_{O2}^{-}$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{O2}(TDG_{CH}^S)$	The condensed local electrophilicity index of the oxygen atom of palladium complex derived from (S)-C–H bond activation (site 2 at base part)	$\omega f_{02}^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{O2}(TDG_{CH}^{S})$	The condensed local nucleophilicity index of the oxygen atom of palladium complex derived from (S)-C-H bond activation (site 2 at base part)	$N_{Nu}f_{O2}^{-}$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{O2}(TDG_{GS}^b)$	The condensed local electrophilicity index of the oxygen atom of ground state palladium complex with base fragment (site 2 at base part)	$\omega f_{O2}^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{O2}(TDG_{GS}^{b})$	The condensed local nucleophilicity index of the oxygen atom of ground state palladium complex with base fragment (site 2 at base part)	$N_{Nu}f_{O2}^{-}$ $(E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{C}(TDG_{CH}^{R})$	The condensed local electrophilicity index of the carbon atom of palladium complex derived from (<i>R</i>)-C–H bond activation	$\omega f_C^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{C}(TDG_{CH}^{R})$	The condensed local nucleophilicity index of the carbon atom of palladium complex derived from (<i>R</i>)-C–H bond activation	$N_{Nu}f_C^ (E_{HOMO}(Nu) - E_{HOMO}(TCE))$
$\omega^{c}(TDG_{CH}^{S})$	The condensed local electrophilicity index of the carbon atom of palladium complex derived from (S)-C–H bond activation	$\omega f_C^+ \ (\omega = \frac{\mu^2}{2\eta})$
$N_{Nu}^{C}(TDG_{CH}^{S})$	The condensed local nucleophilicity index of the carbon atom of palladium complex derived from (S)-C–H bond activation	$N_{Nu}f_C^ (E_{HOMO}(Nu) - E_{HOMO}(TCE))$

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