Features	Definition	Access
$B_{C-H}(Biaryl_{CH}^{R})$	The Wiberg bond index of the reacting C–H bond of biaryl derived from (*R*)-C–H bond activation	DFT calculation based on xTB optimized geometries
$B_{C-H}(Biaryl_{CH}^{S})$	The Wiberg bond index of the reacting C–H bond of biaryl derived from (*S*)-C–H bond activation	DFT calculation based on xTB optimized geometries
$B_{C-H}(Biaryl_{GS})$	The Wiberg bond index of the reacting C–H bond of ground state biaryl	DFT calculation based on xTB optimized geometries
$d_{C-H}(Biaryl_{GS})$	The bond length of the reacting C–H bond of ground state biaryl	Calculation based on xTB optimized geometries
$D_{C-H}(Biaryl_{CH}^{R})$	The homolytic bond dissociation energy of the reacting C–H bond of biaryl derived from (*R*)-C–H bond activation	DFT calculation based on xTB optimized geometries
$D_{C-H}(Biaryl_{CH}^{S})$	The homolytic bond dissociation energy of the reacting C–H bond of biaryl derived from (*S*)-C–H bond activation	DFT calculation based on xTB optimized geometries
$D_{C-H}(Biaryl_{GS})$	The homolytic bond dissociation energy of the reacting C–H bond of ground state biaryl	DFT calculation based on xTB optimized geometries
$D_{C^-H^+}(Biaryl_{CH}^{R})$	The heterolytic bond dissociation energy of the reacting C–H bond of biaryl derived from (*R*)-C–H bond activation	DFT calculation based on xTB optimized geometries
$D_{C^-H^+}(Biaryl_{CH}^{S})$	The heterolytic bond dissociation energy of the reacting C–H bond of biaryl derived from (*S*)-C–H bond activation	DFT calculation based on xTB optimized geometries
$D_{C^-H^+}(Biaryl_{GS})$	The heterolytic bond dissociation energy of the reacting C–H bond of ground state biaryl	DFT calculation based on xTB optimized geometries
$\pi_{C=C}^{HOMO}(Olefin_{AI}^{R})$	The energy of π occupied molecular orbital of the C=C bond of olefin derived from (*R*)-alkene insertion TS	NBO calculation based on DFT optimized geometries
$\pi_{C=C}^{LUMO}(Olefin_{AI}^{R})$	The energy of π unoccupied molecular orbital of the C=C bond of olefin derived from (*R*)-alkene insertion TS	NBO calculation based on DFT optimized geometries
$\pi_{C1-HOMO}^{Coef}(Olefin_{AI}^{R})$	The coefficient of π occupied molecular orbital of terminal carbon in the NAO basis	NBO calculation based on DFT optimized geometries
$\pi_{C1-LUMO}^{Coef}(Olefin_{AI}^{R})$	The coefficient of π unoccupied molecular orbital of terminal carbon in the NAO basis	NBO calculation based on DFT optimized geometries
$\pi_{C2-HOMO}^{Coef}(Olefin_{AI}^{R})$	The coefficient of π occupied molecular orbital of substituted carbon in the NAO basis	NBO calculation based on DFT optimized geometries
$\pi_{C2-LUMO}^{Coef}(Olefin_{AI}^{R})$	The coefficient of π unoccupied molecular orbital of substituted carbon in the NAO basis	NBO calculation based on DFT optimized geometries
$\pi_{C=C}^{HOMO}(Olefin_{AI}^{S})$	The energy of π occupied molecular orbital of the C=C bond of olefin derived from (*S*)-alkene insertion TS	NBO calculation based on DFT optimized geometries
$\pi_{C=C}^{LUMO}(Olefin_{AI}^{S})$	The energy of π unoccupied molecular orbital of the C=C bond of olefin derived from (*S*)-alkene insertion TS	NBO calculation based on DFT optimized geometries
$\pi_{C1-HOMO}^{Coef}(Olefin_{AI}^{S})$	The coefficient of π occupied molecular orbital of terminal carbon in the NAO basis	NBO calculation based on DFT optimized geometries
$\pi_{C1-LUMO}^{Coef}(Olefin_{AI}^{S})$	The coefficient of π unoccupied molecular orbital of terminal carbon in the NAO basis	NBO calculation based on DFT optimized geometries
$\pi_{C2-HOMO}^{Coef}(Olefin_{AI}^{S})$	The coefficient of π occupied molecular orbital of substituted carbon in the NAO basis	NBO calculation based on DFT optimized geometries
$\pi_{C2-LUMO}^{Coef}(Olefin_{AI}^{S})$	The coefficient of π unoccupied molecular orbital of	NBO calculation based on DFT

	substituted carbon in the NAO basis	optimized geometries
$\pi_{C=C}^{HOMO}(Olefin_{GS})$	The energy of π occupied molecular orbital of the C=C bond of ground state olefin	NBO calculation based on DFT optimized geometries
$\pi_{C=C}^{LUMO}(Olefin_{GS})$	The energy of π unoccupied molecular orbital of the C=C bond of ground state olefin	NBO calculation based on DFT optimized geometries
$\pi_{C1-HOMO}^{Coef}(Olefin_{GS})$	The coefficient of π occupied molecular orbital of terminal carbon in the NAO basis	NBO calculation based on DFT optimized geometries
$\pi_{C1-LUMO}^{Coef}(Olefin_{GS})$	The coefficient of π unoccupied molecular orbital of terminal carbon in the NAO basis	NBO calculation based on DFT optimized geometries
$\pi_{C2-HOMO}^{Coef}(Olefin_{GS})$	The coefficient of π occupied molecular orbital of substituted carbon in the NAO basis	NBO calculation based on DFT optimized geometries
$\pi_{C2-LUMO}^{Coef}(Olefin_{GS})$	The coefficient of π unoccupied molecular orbital of substituted carbon in the NAO basis	NBO calculation based on DFT optimized geometries
$B_{C=C}(Olefin_{AI}^{R})$	The Wiberg bond index of the C=C bond of olefin derived from (*R*)-alkene insertion	DFT calculation based on xTB optimized geometries
$B_{C=C}(Olefin_{AI}^{S})$	The Wiberg bond index of the C=C bond of olefin derived from (*S*)-alkene insertion	DFT calculation based on xTB optimized geometries
$B_{C=C}(Olefin_{GS})$	The Wiberg bond index of the C=C bond of ground state olefin	DFT calculation based on xTB optimized geometries
$d_{C=C}(Olefin_{GS})$	The bond length of the C=C bond of ground state biaryl	Based on xTB optimized geometries
$B_{Pd-O1}(TDG_{CH}^{R})$	The Wiberg bond index of the Pd-O1 bond of palladium complex from (*R*)-C–H bond activation (site 1 of oxygen at base part)	DFT calculation based on xTB optimized geometries
$B_{Pd-O1}(TDG_{CH}^{S})$	The Wiberg bond index of the Pd-O1 bond of palladium complex from (*S*)-C–H bond activation (site 1 of oxygen at base part)	DFT calculation based on xTB optimized geometries
$B_{Pd-O1}(TDG_{GS}^{b})$	The Wiberg bond index of the Pd-O1 bond of ground state palladium complex (site 1 of oxygen at base part)	DFT calculation based on xTB optimized geometries
$B_{C-O1}(TDG_{CH}^{R})$	The Wiberg bond index of the C–O1 bond at base part of palladium complex from (*R*)-C–H bond activation	DFT calculation based on xTB optimized geometries
$B_{C-O1}(TDG_{CH}^{S})$	The Wiberg bond index of the C–O1 bond at base part of palladium complex from (*S*)-C–H bond activation	DFT calculation based on xTB optimized geometries
$B_{C-O1}(TDG_{GS}^{b})$	The Wiberg bond index of the C–O1 bond at base part of ground state palladium complex	DFT calculation based on xTB optimized geometries
$B_{C-O2}(TDG_{CH}^{R})$	The Wiberg bond index of the C–O2 bond at base part of palladium complex from (*R*)-C–H bond activation	DFT calculation based on xTB optimized geometries
$B_{C-O2}(TDG_{CH}^{S})$	The Wiberg bond index of the C–O2 bond at base part of palladium complex from (*S*)-C–H bond activation	DFT calculation based on xTB optimized geometries
$B_{C-O2}(TDG_{GS}^{b})$	The Wiberg bond index of the C–O2 bond at base part of ground state palladium complex	DFT calculation based on xTB optimized geometries
$d_{Pd-O1}(TDG_{GS}^{b})$	The bond length of the Pd–O1 bond of ground state palladium complex (site 1 of oxygen at base part)	Based on xTB optimized geometries
$d_{C-O1}(TDG_{GS}^{b})$	The bond length of the C–O1 bond at base part of ground state	Based on xTB optimized

	palladium complex	geometries
$d_{C-O2}(TDG_{GS}^{b})$	The bond length of the C–O2 bond at base part of ground state palladium complex	Based on xTB optimized geometries
$d_{Pd-O3}(TDG_{GS}^{b})$	The bond length of the Pd–O3 bond at ligand part of ground state palladium complex with base fragment	Based on xTB optimized geometries
$d_{Pd-N}(TDG_{GS}^{b})$	The bond length of the Pd–N bond at ligand part of ground state palladium complex with base fragment	Based on xTB optimized geometries
$d_{Pd-O3}(TDG_{GS})$	The bond length of the Pd–O3 bond at ligand part of ground state palladium complex without base fragment	Based on xTB optimized geometries
$d_{Pd-N}(TDG_{GS})$	The bond length of the Pd–N bond at ligand part of ground state palladium complex without base fragment	Based on xTB optimized geometries