Features	Definition	Access
$B_{C-H}(Biaryl_{CH}^R)$	The Wiberg bond index of the reacting C-H bond of biaryl	DFT calculation based on xTB
	derived from (R)-C-H bond activation	optimized geometries
$B_{C-H}(Biaryl_{CH}^S)$	The Wiberg bond index of the reacting C-H bond of biaryl	DFT calculation based on xTB
	derived from (S)-C-H bond activation	optimized geometries
$B_{C-H}(Biaryl_{GS})$	The Wiberg bond index of the reacting C-H bond of ground	DFT calculation based on xTB
	state biaryl	optimized geometries
$d_{C-H}(Biaryl_{GS})$	The bond length of the reacting C-H bond of ground state	Calculation based on xTB
	biaryl	optimized geometries
$D_{C-H}(Biaryl_{CH}^R)$	The homolytic bond dissociation energy of the reacting C–H	DFT calculation based on xTB
	bond of biaryl derived from (R)-C-H bond activation	optimized geometries
$D_{C-H}(Biaryl_{CH}^S)$	The homolytic bond dissociation energy of the reacting C–H	DFT calculation based on xTB
	bond of biaryl derived from (S)-C-H bond activation	optimized geometries
$D_{C-H}(Biaryl_{GS})$	The homolytic bond dissociation energy of the reacting C-H	DFT calculation based on xTB
$\nu_{C-H}(\mathit{biaryl}_{GS})$	bond of ground state biaryl	optimized geometries
$D_{C^{-}H^{+}}(Biaryl_{CH}^{R})$	The heterolytic bond dissociation energy of the reacting C-H	DFT calculation based on xTB
$D_{C^-H^+}(B\iota ary\iota_{CH}^*)$	bond of biaryl derived from (R)-C-H bond activation	optimized geometries
$D_{C^-H^+}(Biaryl_{CH}^S)$	The heterolytic bond dissociation energy of the reacting C-H	DFT calculation based on xTB
$D_{C^{-}H^{+}}(DtatytcH)$	bond of biaryl derived from (S)-C-H bond activation	optimized geometries
$D_{C^-H^+}(Biaryl_{GS})$	The heterolytic bond dissociation energy of the reacting C-H	DFT calculation based on xTB
$D_{C}^{-}H^{+}(Dtaryt_{GS})$	bond of ground state biaryl	optimized geometries
$\pi^{HOMO}_{C=C}(Olefin^R_{AI})$	The energy of $\boldsymbol{\pi}$ occupied molecular orbital of the C=C bond of	NBO calculation based on DFT
$n_{C=C}$ (Ote) in_{AI})	olefin derived from (R)-alkene insertion TS	optimized geometries
$\pi^{LUMO}_{C=C}(Olefin^R_{AI})$	The energy of π unoccupied molecular orbital of the C=C bond	NBO calculation based on DFT
$n_{C=C}$ (ott) m_{AI})	of olefin derived from (R)-alkene insertion TS	optimized geometries
$\pi_{C1-HOMO}^{Coef}(Olefin_{AI}^{R})$	The coefficient of $\boldsymbol{\pi}$ occupied molecular orbital of terminal	NBO calculation based on DFT
C1-HOMO(Ote) (MAI)	carbon in the NAO basis	optimized geometries
$\pi^{Coef}_{C1-LUMO}(Olefin_{AI}^R)$	The coefficient of $\boldsymbol{\pi}$ unoccupied molecular orbital of terminal	NBO calculation based on DFT
C1-LUMO (OTC) THAI)	carbon in the NAO basis	optimized geometries
$\pi^{Coef}_{C2-HOMO}(Olefin^R_{AI})$	The coefficient of π occupied molecular orbital of substituted	NBO calculation based on DFT
	carbon in the NAO basis	optimized geometries
$\pi^{Coef}_{C2-LUMO}(Olefin^R_{AI})$	The coefficient of π unoccupied molecular orbital of	NBO calculation based on DFT
	substituted carbon in the NAO basis	optimized geometries
$\pi^{HOMO}_{C=C}(Olefin^S_{AI})$	The energy of π occupied molecular orbital of the C=C bond of	NBO calculation based on DFT
	olefin derived from (S)-alkene insertion TS	optimized geometries
$\pi_{C=C}^{LUMO}(Olefin_{AI}^{S})$	The energy of π unoccupied molecular orbital of the C=C bond	NBO calculation based on DFT
C-C (STAI)	of olefin derived from (S)-alkene insertion TS	optimized geometries
$\pi^{\textit{Coef}}_{\textit{C1-HOMO}}(\textit{Olefin}_{\textit{AI}}^{\textit{S}})$	The coefficient of π occupied molecular orbital of terminal	NBO calculation based on DFT
CI-HOMO(· ··)···AI)	carbon in the NAO basis	optimized geometries
$\pi^{Coef}_{C1-LUMO}(Olefin_{AI}^S)$	The coefficient of π unoccupied molecular orbital of terminal	NBO calculation based on DFT
C1-LUMU(Coo) WAI)	carbon in the NAO basis	optimized geometries
$\pi^{Coef}_{C2-HOMO}(Olefin_{AI}^S)$	The coefficient of π occupied molecular orbital of substituted	NBO calculation based on DFT
	carbon in the NAO basis	optimized geometries
$\pi^{Coef}_{C2-LUMO}(Olefin_{AI}^S)$	The coefficient of π unoccupied molecular orbital of	NBO calculation based on DFT

	substituted carbon in the NAO basis	optimized geometries
$\pi^{HOMO}_{C=C}(Olefin_{GS})$	The energy of π occupied molecular orbital of the C=C bond of	NBO calculation based on DFT
	ground state olefin	optimized geometries
$\pi^{LUMO}_{C=C}(Olefin_{GS})$	The energy of π unoccupied molecular orbital of the C=C bond	NBO calculation based on DFT
	of ground state olefin	optimized geometries
$\pi^{Coef}_{C1-HOMO}(Olefin_{GS})$	The coefficient of $\boldsymbol{\pi}$ occupied molecular orbital of terminal	NBO calculation based on DFT
	carbon in the NAO basis	optimized geometries
$\pi^{Coef}_{C1-LUMO}(Olefin_{GS})$	The coefficient of $\boldsymbol{\pi}$ unoccupied molecular orbital of terminal	NBO calculation based on DFT
	carbon in the NAO basis	optimized geometries
$\pi^{Coef}_{C2-HOMO}(Olefin_{GS})$	The coefficient of $\boldsymbol{\pi}$ occupied molecular orbital of substituted	NBO calculation based on DFT
	carbon in the NAO basis	optimized geometries
$\pi^{Coef}_{C2-LUMO}(Olefin_{GS})$	The coefficient of π unoccupied molecular orbital of	NBO calculation based on DFT
	substituted carbon in the NAO basis	optimized geometries
$B_{C=C}(Olefin_{AI}^R)$	The Wiberg bond index of the C=C bond of olefin derived from	DFT calculation based on xTB
	(R)-alkene insertion	optimized geometries
$B_{C=C}(Olefin_{AI}^S)$	The Wiberg bond index of the C=C bond of olefin derived from	DFT calculation based on xTB
	(S)-alkene insertion	optimized geometries
$B_{C=C}(Olefin_{GS})$		DFT calculation based on xTB
	The Wiberg bond index of the C=C bond of ground state olefin	optimized geometries
		Based on xTB optimized
$d_{C=C}(Olefin_{GS})$	The bond length of the C=C bond of ground state biaryl	geometries
	The Wiberg bond index of the Pd-O1 bond of palladium	-
$B_{Pd-O1}(TDG_{CH}^R)$	complex from (R) -C—H bond activation (site 1 of oxygen at	DFT calculation based on xTB
	base part)	optimized geometries
	The Wiberg bond index of the Pd-O1 bond of palladium	
$B_{Pd-O1}(TDG_{CH}^S)$	complex from (S)-C—H bond activation (site 1 of oxygen at	DFT calculation based on xTB
$D_{Pd}-O1(IDG_{CH})$	base part)	optimized geometries
	The Wiberg bond index of the Pd-O1 bond of ground state	DFT calculation based on xTB
$B_{Pd-O1}(TDG_{GS}^b)$	palladium complex (site 1 of oxygen at base part)	optimized geometries
	The Wiberg bond index of the C–O1 bond at base part of	DFT calculation based on xTB
$B_{C-O1}(TDG_{CH}^R)$	•	optimized geometries
	palladium complex from (R)-C-H bond activation	
$B_{C-O1}(TDG_{CH}^S)$	The Wiberg bond index of the C–O1 bond at base part of	DFT calculation based on xTB
	palladium complex from (S)-C–H bond activation	optimized geometries
$B_{C-O1}(TDG_{GS}^b)$	The Wiberg bond index of the C–O1 bond at base part of	DFT calculation based on xTB
	ground state palladium complex	optimized geometries
$B_{C-O2}(TDG_{CH}^R)$	The Wiberg bond index of the C–O2 bond at base part of	DFT calculation based on xTB
	palladium complex from (R)-C-H bond activation	optimized geometries
$B_{C-O2}(TDG_{CH}^S)$	The Wiberg bond index of the C-O2 bond at base part of	DFT calculation based on xTB
0.02(palladium complex from (S)-C-H bond activation	optimized geometries
$B_{C-O2}(TDG_{GS}^b)$	The Wiberg bond index of the C-O2 bond at base part of	DFT calculation based on xTB
	ground state palladium complex	optimized geometries
$d_{Pd-O1}(TDG_{GS}^b)$	The bond length of the Pd-O1 bond of ground state palladium	Based on xTB optimized
	complex (site 1 of oxygen at base part)	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	Based on xTB optimized
$u_{C-02}(IDG_{GS})$	palladium complex	geometries
$d_{Pd-O3}(TDG_{GS}^b)$	The bond length of the Pd-O3 bond at ligand part of ground	Based on xTB optimized
	state palladium complex with base fragment	geometries
d (TDC^b)	The bond length of the Pd-N bond at ligand part of ground	Based on xTB optimized
$d_{Pd-N}(TDG_{GS}^b)$	state palladium complex with base fragment	geometries
d (TDC)	The bond length of the Pd-O3 bond at ligand part of ground	Based on xTB optimized
$d_{Pd-O3}(TDG_{GS})$	state palladium complex without base fragment	geometries
$d_{Pd-N}(TDG_{GS})$	The bond length of the Pd-N bond at ligand part of ground	Based on xTB optimized
	state palladium complex without base fragment	geometries