Supplementary Tables and Figures

Theoretical investigation on $Pd(OAc)_2$-catalyzedspiro-cyclisation of sulfonamide and maleimide via γ-C(sp3)−H bond activation leading to spiropyrrolidine

Table S1: Calculated relative energies (all in kcalmol^{-1}, relative to isolated species) for the ZPE-correctedGibbs free energies(ΔG_{gas}),Gibbs free energies for all species in solution phase(ΔG_{sol}) at 378 K by B3LYP/6-311++G(d,p)//B3LYP/6-31G(d)methodanddifference between absolute energy.

Species	ΔG_{gas}	$\Delta G_{sol(EtOH)}$
pdoac2+ql	0.00	0.00
i1	-111.20	-108.38
ts-i1A	-108.26	-105.84
A	-126.28	-126.24
A+1	0.00	0.00
i2	-232.40	-210.92
ts-i23	-222.81	-201.47
i3	-241.67	-219.37
i3-AcOH	0.00	0.00
B	71.02	61.07
ts-Bi4	88.73	77.01
i4	70.63	57.54
i4-AcOH	0.00	0.00
C	65.10	54.20
C+2	0.00	0.00
i5	-105.04	-98.83
ts-i5D	-88.44	-82.42
D	-96.82	-89.53
ts-DE	-83.02	-76.15
E	-83.36	-78.27
ts-EF	-64.86	-60.67
F	-95.98	-84.12
ts-Fi6	-69.56	-59.81
i6	-117.54	-107.10

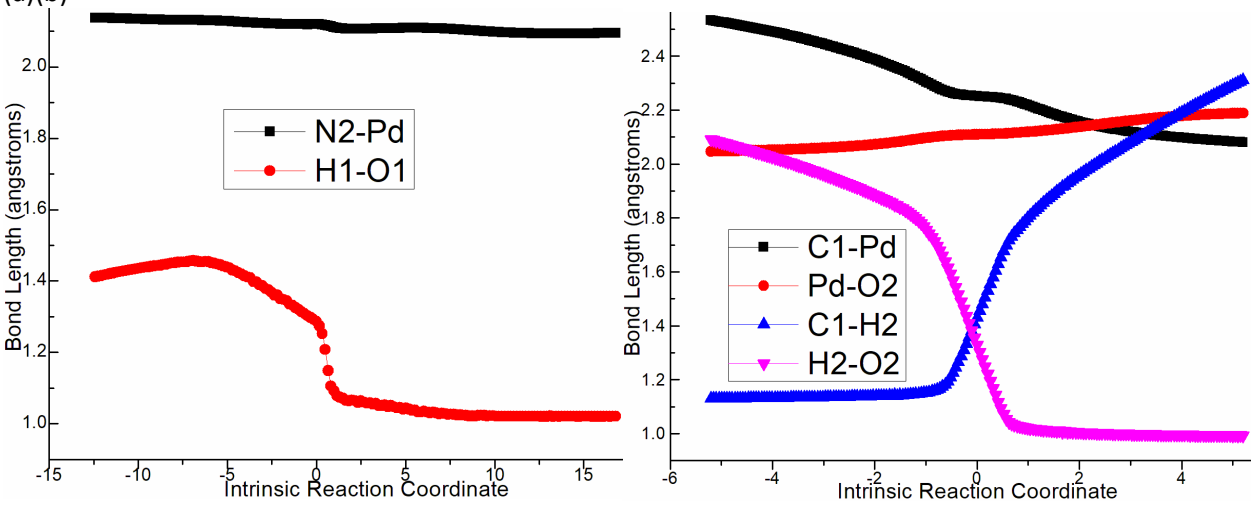
Table S2: The activation energy(local barrier) (in kcal mol^{-1}) of all reactions in the gas, solution phase calculated with B3LYP/6-311++G(d,p)//B3LYP/6-31G(d) method.

TS	$\Delta G^{\neq}_{gas}$	$\Delta G^{\neq}_{sol}$
ts-i1A(112i)	2.9	2.5
ts-i23(154i)	9.6	9.5

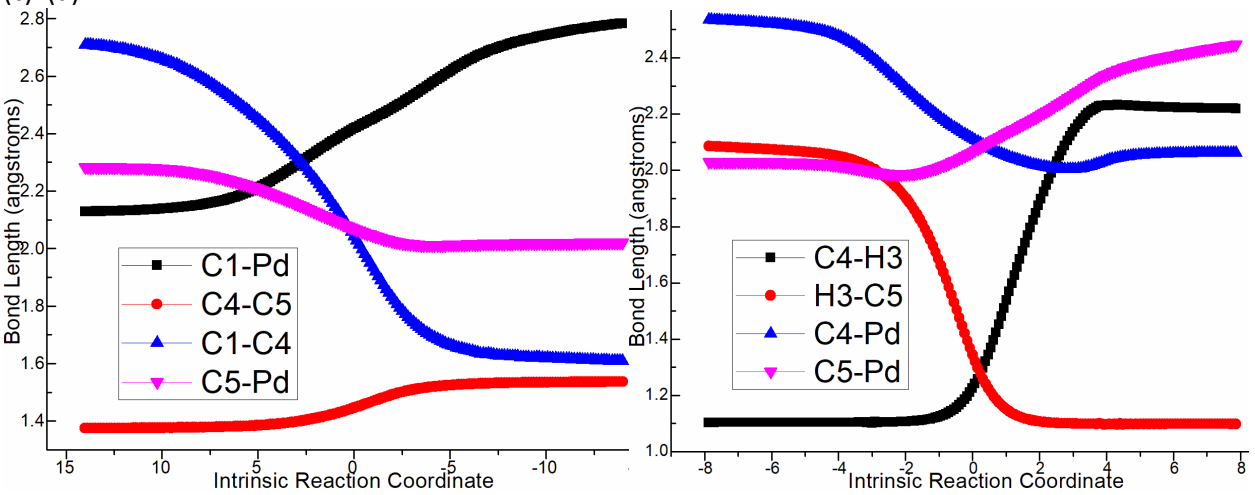
ts-Bi4(1437i)	17.7	15.9
ts-i5D(87i)	16.6	16.4
ts-DE(216i)	13.8	13.4
ts-EF(668i)	18.5	17.6
ts-Fi6(254i)	26.4	24.3

Figure S1: Evolution of bond lengths along the IRC for (a) **ts-i23**(b) **ts-Bi4**(c)**ts-DE**(d)**ts-EF**(e) **ts-Fi6**at B3LYP/6-311++G(d,p) level.

(a)(b)



(c) (d)



(e)