Supplementary Information

Theoretical investigation on NiF_2/picolinic acid-catalyzed chemoselective coupling–cyclization of 2-iodobenzamide and malonate to furnish homophthalimide

Nan Lu[1]

[1] *College of Chemistry and Material Science, Shandong Agricultural University, Taian City 271018, Shandong Prov., P.R. China.*

Table of Contents **Pages**

Table S1. Calculated relative energies (all in kcal mol^{-1}, relative to isolated species) for the ZPE-corrected Gibbs free energies (ΔG_{gas}), Gibbs free energies for all species in solution phase (ΔG_{sol}) at 373 K by B3LYP/6-311++G(d,p)//B3LYP/6-31G(d) method and difference between absolute energy.

Species	ΔG_{gas}	$\Delta G_{sol(THF)}$
nif2+pica	0.00	0.00
i1	-169.80	-156.24
ts-i12	-163.17	-145.22
i2	-179.39	-157.12
nif2+pica-hf	0.00	0.00
i3	-139.74	-129.88
nif2+pica-hf+2	0.00	0.00
i4	-266.87	-243.94
ts-i45	-249.92	-225.13
i5	-272.24	-248.16
nif2+pica-2hf+2	0.00	0.00
i6	-264.27	-245.40
nif2+pica-2hf+2-2-h	0.00	0.00
A	-62.41	-62.21
A+1	0.00	0.00
B	-15.27	-10.17
ts-BC1	-9.44	-6.06
C1	-26.18	-18.85
ts-C12	-11.56	-4.15
C2	-36.94	-32.92
A+1-I+2-h	0.00	0.00
D	-157.23	-141.44
ts-Di7	-150.36	-131.96
i7	-183.21	-165.19
1-I+2-h	0.00	0.00
E	29.26	20.41
ts-Ei8	58.05	44.79
i8	20.08	15.17
1-I+2-h-meoh	0.00	0.00
3	19.19	10.21

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-i12 (358i)	6.62	11.02
ts-i45 (712i)	16.95	18.81
ts-BC1 (62i)	5.83	4.10
ts-C12 (48i)	14.62	14.70
ts-Di7 (209i)	6.86	9.48
ts-Ei8 (1441i)	28.79	24.38

Figure S1. Evolution of bond lengths along the IRC for (a) **ts-i12** (b) **ts-i45** (c) **ts-Di7** (d) **ts-Ei8** at B3LYP/6-311++G(d,p) level.