

Supplementary Materials

Density Functional Theory Analysis of the Copolymerization of Cyclopropenone with Ethylene Using a Palladium Catalyst

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Table S1: Energies of all the structures.Gibbs free energies (G) (in *a.u.*) of all the structures for the main text

CatA	C ₂ H ₄	cIM1 _A	cTS1 _A	cPR1 _A	tIM1 _A
-2055.81925	-78.53930	-2134.356108	-2134.335544	-2134.383986	-2134.36715
tTS1 _A	tPR1 _A				
-2134.323624	-2134.35961				
1a	TS1 _A	2A	TS2 _A	4A	TS3 _A
-652.54106	-2786.88886	-2786.90273	-2786.88677	-2786.96061	-2786.85778
3A	TS4 _A				
-2786.90367	-2786.89978				
IM _{AE1}	TS _{AE1}	PR _{AE1}	IM _{AE2}	TS _{AE2}	PR _{AE2}
-2865.49355	-2865.47984	-2865.50651	-2944.04813	-2944.02047	-2944.06330
TS1 _{1a}	IM1 _{1a}	TS2 _{1a}	CO	C ₂ Ph ₂	
-652.48383	-652.48756	-652.48584	-113.32316	-539.23344	
TS1 _{AEtCO}	IM1 _{AEtCO}	TS2 _{AEtCO}	IM2 _{AEtCO}	TS3 _{AEtCO}	PR _{AEtCO}
-2786.88988	-2786.96727	-2786.95583	-2786.96417	-2786.94115	-2673.62738
TS1 _{ACOEt}	IM1 _{ACOEt}	TS2 _{ACOEt}			
-2786.84846	-2673.60987	-2673.56727			
IM _{ACO}	TS _{ACO}	PR _{ACO}	IM _{ACOE}	TS _{ACOE}	PR _{ACOE}
-3057.39288	-3057.37072	-3057.37892	-3135.93311	-3135.91842	-3135.95968
TS _{21AAc}	PR _{21AAc}	TS _{12AAc}	PR _{12AAc}		
-3289.68602	-3289.73392	-3289.68655	-3289.73224		

Table S2: Additional computational details and detailed data of Fukui functions values for some molecules.

(A) Additional computational details:

The global reactivity index and Fukui functions values were performed using the Multiwfn program [1,2]. The calculations also used a mixed basis set (SDD for Pd and 6-31G(d) for other non-metal atoms).

Vertical ionization potential: $VIP = E_{N-1} - E_N$,

Vertical electron affinity: $VEA = E_N - E_{N+1}$,

where N denotes the number of electrons for a stable system.

Mulliken electronegativity: $\chi = \frac{VIP + VEA}{2}$,

Chemical potential: $\mu = -\chi$,

Chemical hardness: $\eta = VIP - VEA$ [3],

Electrophilicity index [4]: $\omega = \frac{\mu^2}{2\eta}$,

Nucleophilicity index: $N_{Nu} = E_{HOMO}(Nu) - E_{HOMO}(TCE)$, where Nu refers to nucleophile and TCE denotes tetracyanoethylene [5].

The Fukui function is defined as follows [6,7], where N denotes the number of electrons, the term v is external potential.

$$f(r) = \left[\frac{\partial \rho(r)}{\partial N} \right]_v$$

Nucleophilic attack: $f^+(r) = \rho_{N+1}(r) - \rho_N(r)$,

Electrophilic attack: $f^-(r) = \rho_N(r) - \rho_{N-1}(r)$.

(B) Detailed data of Fukui functions values for some molecules

CatA				1a		C ₂ H ₄	
Atom	f ⁺	Atom	f ⁺	Atom	f ⁺	Atom	f ⁺
1(P)	0.073	26(H)	0.0159	1(C)	0.0586	1(C)	0.3128
2(C)	-0.0003	27(H)	0.0136	2(C)	0.0565	2(H)	0.0936
3(C)	0.0036	28(H)	0.0204	3(C)	0.0586	3(H)	0.0936
4(S)	0.0151	29(C)	-0.0048	4(O)	0.1881	4(C)	0.3128
5(O)	0.0148	30(C)	0.0067	5(C)	0.0248	5(H)	0.0936
6(O)	0.0115	31(C)	0.0009	6(C)	0.0623	6(H)	0.0936
7(O)	0.0329	32(C)	0.0172	7(C)	0.0291		
8(C)	0.016	33(C)	0.0134	8(C)	0.0303		
9(C)	0.0284	34(H)	0.0048	9(C)	0.0328	AAc	
10(C)	0.0219	35(C)	0.0241	10(C)	0.0341	Atom	f ⁺
11(C)	0.012	36(H)	0.0142	11(H)	0.0135	1(C)	0.1160
12(H)	0.0123	37(H)	0.0127	12(H)	0.014	2(C)	0.1670

13(H)	0.0187	38(H)	0.017	13(H)	0.0242	3(H)	0.0507
14(H)	0.017	39(O)	-0.0041	14(H)	0.0243	4(H)	0.0570
15(H)	0.0071	40(O)	-0.0015	15(H)	0.0296	5(C)	0.0244
16(C)	0.0724	41(C)	0.0049	16(C)	0.0248	6(H)	0.0379
17(H)	0.0499	42(C)	0.0052	17(C)	0.0291	7(H)	0.026
18(H)	0.0296	43(H)	0.0102	18(C)	0.0341	8(O)	0.0593
19(C)	-0.0027	44(H)	0.0056	19(C)	0.0623	9(C)	0.0638
20(C)	0.0148	45(H)	0.0052	20(C)	0.0328	10(O)	0.2079
21(C)	0.0082	46(H)	0.0055	21(C)	0.0304	11(C)	0.0444
22(C)	0.0189	47(H)	0.0069	22(H)	0.0135	12(H)	0.0348
23(H)	0.0065	48(H)	0.0114	23(H)	0.0243	13(H)	0.0363
24(C)	0.0162	49(H)	0.0327	24(H)	0.0296	14(H)	0.0302
25(C)	0.0349	50(Pd)	0.2283	25(H)	0.0242	15(H)	0.0442
				26(H)	0.014		

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