Molecular Docking Against Covid-19 and HIV, and the Role of Catalysis in Stereoselective Cycloaddition Reactions: A Theoretical Investigation of $TiCl_4$-Promoted Reactions between Cyclopenta-1,3-Diene and Benzyl Acrylate/Benzyl 2-Fluoroacrylate

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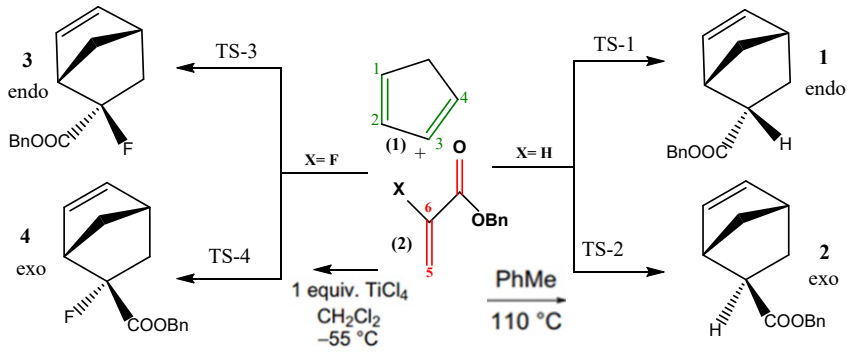

Scheme S1. Cycloaddition Reaction Pathways of Cyclopenta-1,3-Diene with Benzyl-acrylate and Benzyl-2-Fluoroacrylate with and without catalyst

Table S1. The total and relative (E, H, and G in a.u.) and relatives in kcal/mol, plus total and relative entropies S (cal/mol.K), at the computational level DFT/SDD, (cpcm,solvent=dichloromethane) temperature=408

System	E	ΔE	H	ΔH	G	ΔG	S	ΔS
1	-194,073490869		-193,977753		-194,002314		63.423	
2-H	-462,220602241		-462,029634		-462,105428		116.572	
1+2-H	-656,29409311	-----	-656,007387	-----	-656,107742	-----	179,995	-----
Ts-1	-656.263771177	19.0	-655.969134	24.0	-656.061287	29.1	141.734	-38.261
1	-656.320410548	-16.5	-656.021917	-9.1	-656.111217	-2.1	137.345	-42.650
Ts-2	-656.269610071	15.3	-655.974705	20.5	-656.067987	24.9	143.469	-36.526
2	-656.323390824	-18.3	-656.024658	-10.8	-656.114003	-3.9	137.413	-42582

Table S2. The total and relative (E, H, and G in a.u.) and relatives in kcal/mol, plus total and relative entropies S (cal/mol.K), at the computational level DFT/SDD, (cpcm,solvent=dichloromethane) temperature=408

System	E	ΔE	H	ΔH	G	ΔG	S	ΔS
1	-194,073490869		-193,977753		-194,002314		63.423	
2-F	-561,464447071		-561,280549		-561,359746		121.805	
1+2-F	-755,53793794		-755,258302		-755,36206		185,228	
Ts-3	-755.506517986	19,7	-755,218829	24,7	-755,314616	29,7	147,323	-37,905
3	-755.568904456	-19,4	-755,277690	-12,1	-755,370410	-5,2	142,605	-42,623
Ts-4	-755.515426123	14,1	-755,227562	19,2	-755,323455	24,2	147,486	-37,742
4	-755.573132078	-22,0	-755,281709	-14,6	-755,374411	-7,7	142,578	-42,65

Table S3. The total and relative (E, H, and G in a.u.) and relatives in kcal/mol, plus total and relative entropies S (cal/mol.K), at the computational level DFT/SDD, (cpcm,solvent=dichloromethane) temperature=243 with catalyzer

System	E	ΔE	H	ΔH	G	ΔG	S	ΔS
1	-194,074505507		-193,971663		-194,019191		73.100	
2-H-Cat	-2361,54811174		-2361,360345		-2361,402154		107.965	
1+2-H-Cat	-2555,622617247		-2555,332008		-2555,421345		181.065	
MC-H	-2555,69170783		-2555,399288		-2555,462821		164,065	
Ts-1-Cat	-2555,69124571	0,28	-2555,398939	0,21	-2555,458773	2,54	154.514	-9.551
1+Cat	-2555,716693272	-15,67	-2555,419988	-12,98	-2555,476409	-8,52	145,701	-18,364
Ts-2-Cat	-2555,67678199	9,36	-2555,384243	9,44	-2555,443941	11,84	154,161	-9,904
2+Cat	-2555,71285214	-13,26	-2555,416047	-10,51	-2555,472878	-6,31	146,757	-17.308

Table S4. The total and relative (E, H, and G in a.u.) and relatives in kcal/mol, plus total and relative entropies S (cal/mol.K), at the computational level DFT/SDD, (cpcm,solvent=dichloromethane) temperature=243 with catalyzer

System	E	ΔE	H	ΔH	G	ΔG	S	ΔS
1	-194,074505507		-193,971663		-194,019191		73,100	
2-F	-561,467961228		-561,295934		-561,334462		+99,491	
Cat	-1899,36386592		-1899,352355		-1899,387959		+91,941	
1+2-F+Cat	-2654,906332655		-2654,619952		-2654,741612		264,532	
MC-F	-2654,92981441		-2654,645320		-2654,709277		165,161	
Ts-3-Cat	-2654,92857076	0,78	-2654,644370	0,59	-2654,706081	2,00	159,361	-5.8
3+Cat	-2654,938287874	-5,31	-2654,65231	-4,38	-2654,730926	-13,58	203,014	38,093
Ts-4-Cat	-2654,92813909	1,05	-2654,644180	0,71	-2654,706237	1,90	160,254	-4.907
4+Cat	-2654,933914596	-2,57	-2654,64858	-2,04	-2654,725101	-9,92	197,602	32,441

Table S5. Values of basins between atoms involved in the formation of new bonds during the cycloaddition reaction cyclopenta-1,3-diene with benzyl none catalysis

Basin	1-H	2-H	3-H	4-H	5-H	6-H	7-H	8-H	9-H
V(C1,C2)	3.19	3.05	2.93	2.77	2.68	2.39	2.20	2.12	2.00
V(C3,C4)	3.17	3.01	2.71	2.48	2.31	2.14	2.05	2.02	1.99
V(C1,C4)	2.29	2.43	2.58	2.77	2.92	3.15	1.68	1.71	1.73
V'(C1,C4)	-----	-----	-----	-----	-----	-----	1.68	1.64	1.69
V(C10,C11)	3.19	3.09	2.82	2.50	2.32	2.12	2.01	1.96	1.87
V(C3)	-----	-----	0.28	0.49	-----	-----	-----	-----	-----
V(C11)	-----	-----	0.21	0.42	-----	-----	-----	-----	-----
V(C3, C11)	-----	-----	-----	-----	1.20	1.48	1.64	1.72	1.76
V(C2)	-----	-----	-----	-----	-----	0.20	-----	-----	-----
V(C10)	-----	-----	-----	-----	-----	0.47	-----	-----	-----
V(C2, C10)	-----	-----	-----	-----	-----	-----	1.10	1.29	1.66

Table S6. Values of basins between atoms involved in the formation of new bonds during the cycloaddition reaction cyclopenta-1,3-diene with benzyl-2-fluoro acrylate none catalysis

Basin	**1-F**	**2-F**	**3-F**	**4-F**	**5-F**	**6-F**	**7-F**	**8-F**	**9-F**
V(C1,C2)	3.27	3.12	2.94	2.84	2.71	2.64	2.28	2.15	2.06
V(C3,C4)	3.27	3.06	2.70	2.54	2.31	2.21	2.09	2.05	2.00
V(C1,C4)	2.23	2.35	2.57	2.68	2.90	3.00	3.19	1.68	1.70
V'(C1,C4)	-----	-----	-----	-----	-----	-----	-----	1.61	1.66
V(C10,C11)	1.78	3.44	2.95	2.73	2.41	2.29	2.16	2.09	2.03
V'(C10,C11)	1.74	-----	-----	-----	-----	-----	-----	-----	-----
V(C3)	-----	-----	0.27	0.40	-----	-----	-----	-----	-----
V(C11)	-----	-----	0.26	0.39	-----	-----	-----	-----	-----
V(C3, C11)	-----	-----	-----	-----	1.21	1.39	1.59	1.67	1.74
V(C2)	-----	-----	-----	-----	-----	-----	0.30	-----	-----
V(C10)	-----	-----	-----	-----	0.54	0.68	0.89	-----	-----
V(C2, C10)	-----	-----	-----	-----	-----	-----		1.46	1.67

Table S7. Values of basins between atoms involved in the formation of new bonds during the cycloaddition reaction cyclopenta-1,3-diene with benzyl acrylate catalyzed by $TiCl_4$

Basin	1-H-Cat	2-H-Cat	3-H-Cat	4-H-Cat	5-H-Cat	6-H-Cat
V(C1,C2)	3.21	2.76	2.62	2.53	2.33	2.18
V(C3,C4)	3.19	2.46	2.27	2.19	2.10	2.05
V(C1,C4)	2.25	2.68	2.84	2.94	3.11	3.25
V(C10,C11)	3.10	2.46	2.26	2.18	2.06	1.97
V'(C10,C11)	1.41	-----	-----	-----	-----	-----
V(C3)	-----	0.45	-----	-----	-----	-----
V(C11)	-----	0.33	-----	-----	-----	-----
V(C3, C11)	-----	-----	1.18	1.37	1.57	1.66
V(C2)	-----	-----	-----	-----	0.16	-----
V(C10)	-----	-----	-----		0.50	-----
V(C2, C10)	-----	-----	-----	-----	-----	1.02

Table S8. Values of basins between atoms involved in the formation of new bonds during the reaction cyclopenta-1,3-diene with benzyl-2-fluoro acrylate catalyzed by $TiCl_4$

Basin	1-F-Cat	2-F-Cat	3-F-Cat	4-F-Cat	5-F-Cat	6-F-Cat
V(C1,C2)	3.18	2.76	2.63	2.55	2.35	2.19
V(C3,C4)	3.17	2.44	2.26	2.18	2.09	2.05
V(C1,C4)	2.26	2.65	2.81	2.90	3.09	3.21
V'(C1,C4)	-----	-----	-----	-----	-----	-----
V(C10,C11)	1.79	2.59	2.37	2.28	2.16	2.09
V'(C10,C11)	1.61	-----	-----	-----	-----	-----
V(C3)	-----	0.43	-----	-----	-----	-----
V(C11)	-----	0.38	-----	-----	-----	-----
V(C3, C11)	-----	-----	1.20	1.38	1.57	1.65
V(C2)	-----	-----	-----	-----	0.16	-----
V(C10)	-----	-----	-----	0.53	0.82	-----
V(C2, C10)	-----	-----	-----	-----	-----	1.31