

Modifying catalytic sustainability: aromaticity, conceptual DFT and steric mapping

Carles Alcaide i Blaya

Supervisors:

Dr. Albert Poater Teixidor

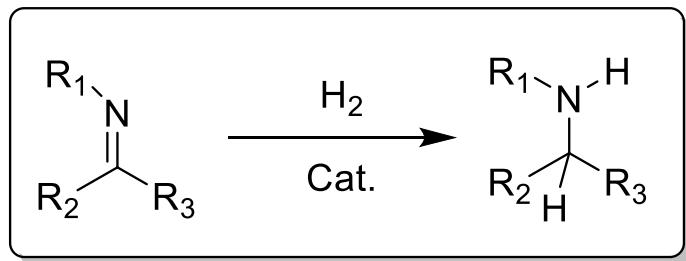
Dra. Sílvia Simon Rabaseda

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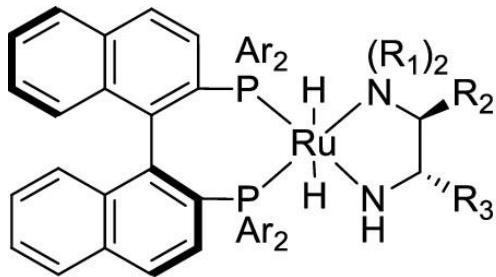
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- 2. Objectives**
- 3. Methodology**
 - i. Electronic and geometrical indices
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INTRODUCTION

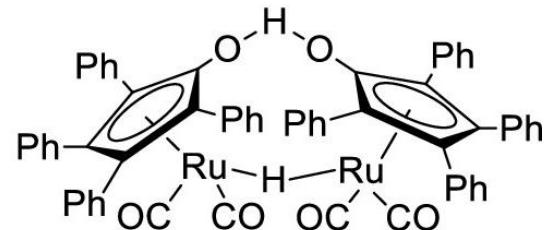
Catalytic hydrogenation



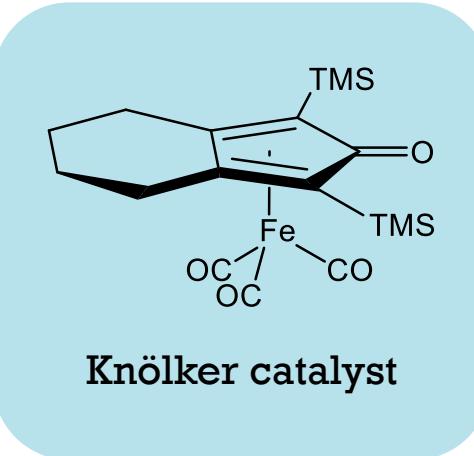
Long-established catalysts



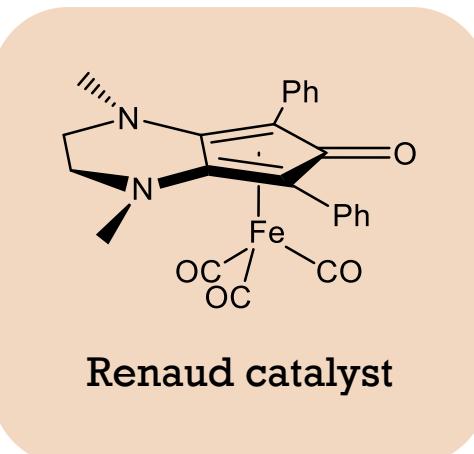
Shvo catalyst



Noyori catalyst



Knölker catalyst



Renaud catalyst

Org. Biomol. Chem., 2006, 4, 393-406

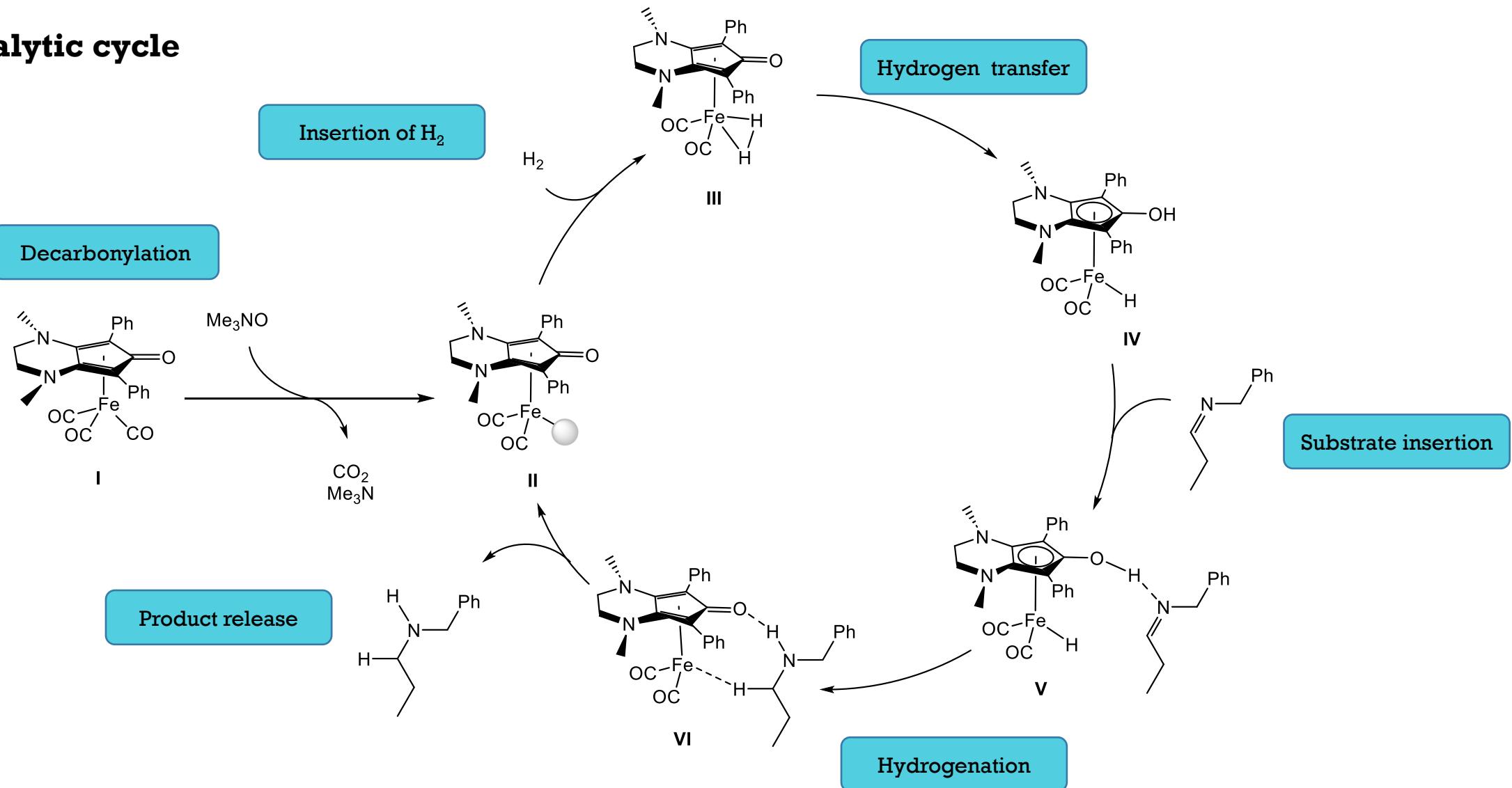
J. Am. Chem. Soc., 1986, 108, 7400-7402

Angew. Chem. Int. Ed., 1999, 38, 2064-2066

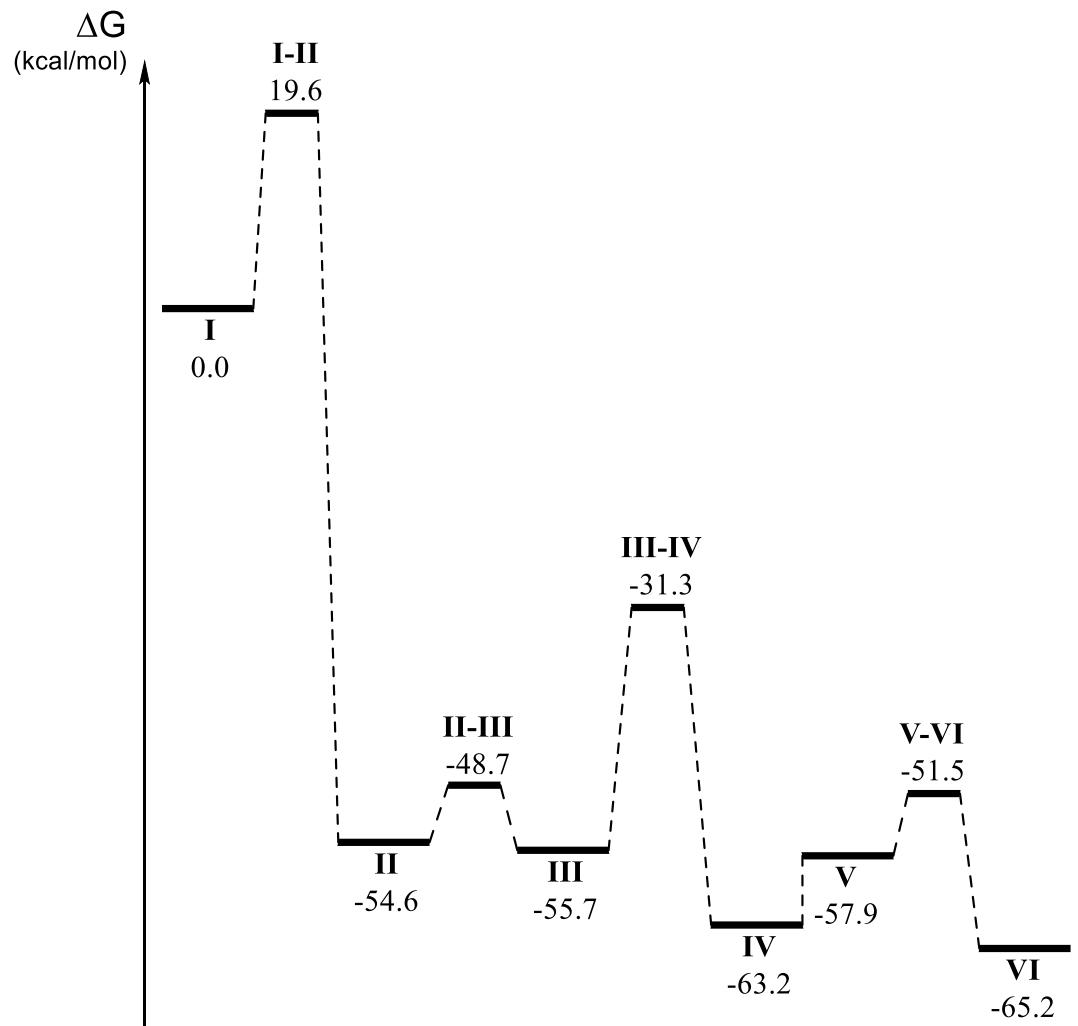
J. Am. Chem. Soc., 2009, 131, 2499-2507

INTRODUCTION

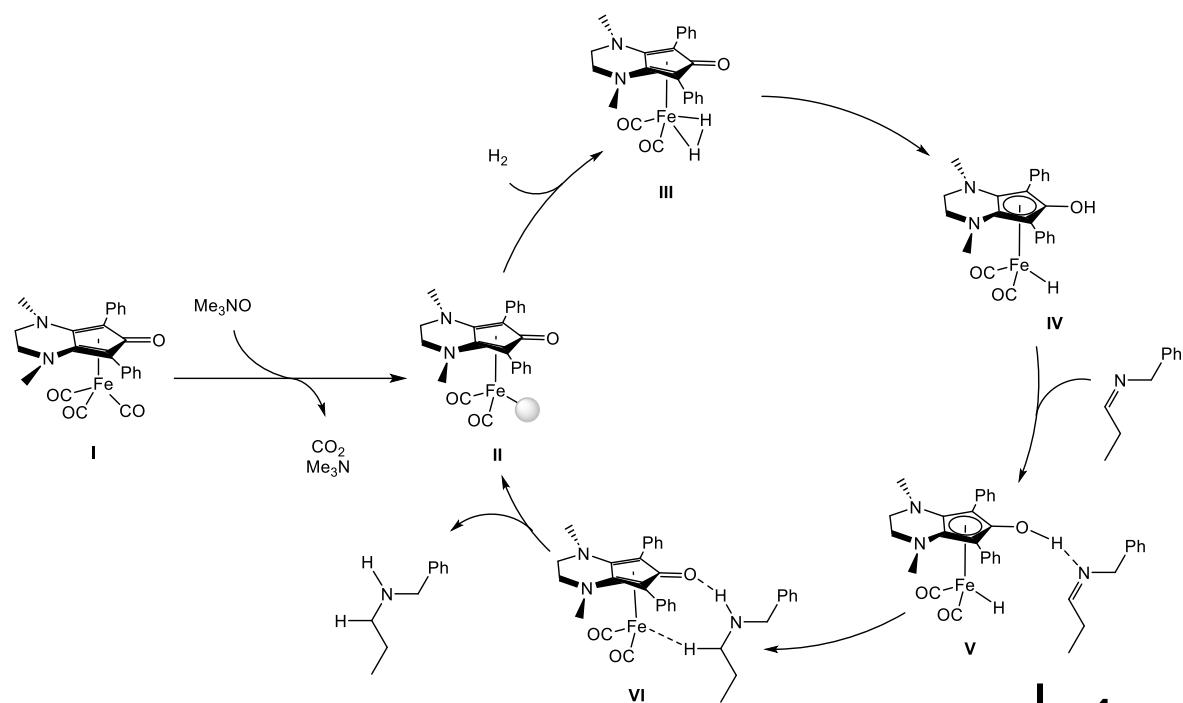
Catalytic cycle



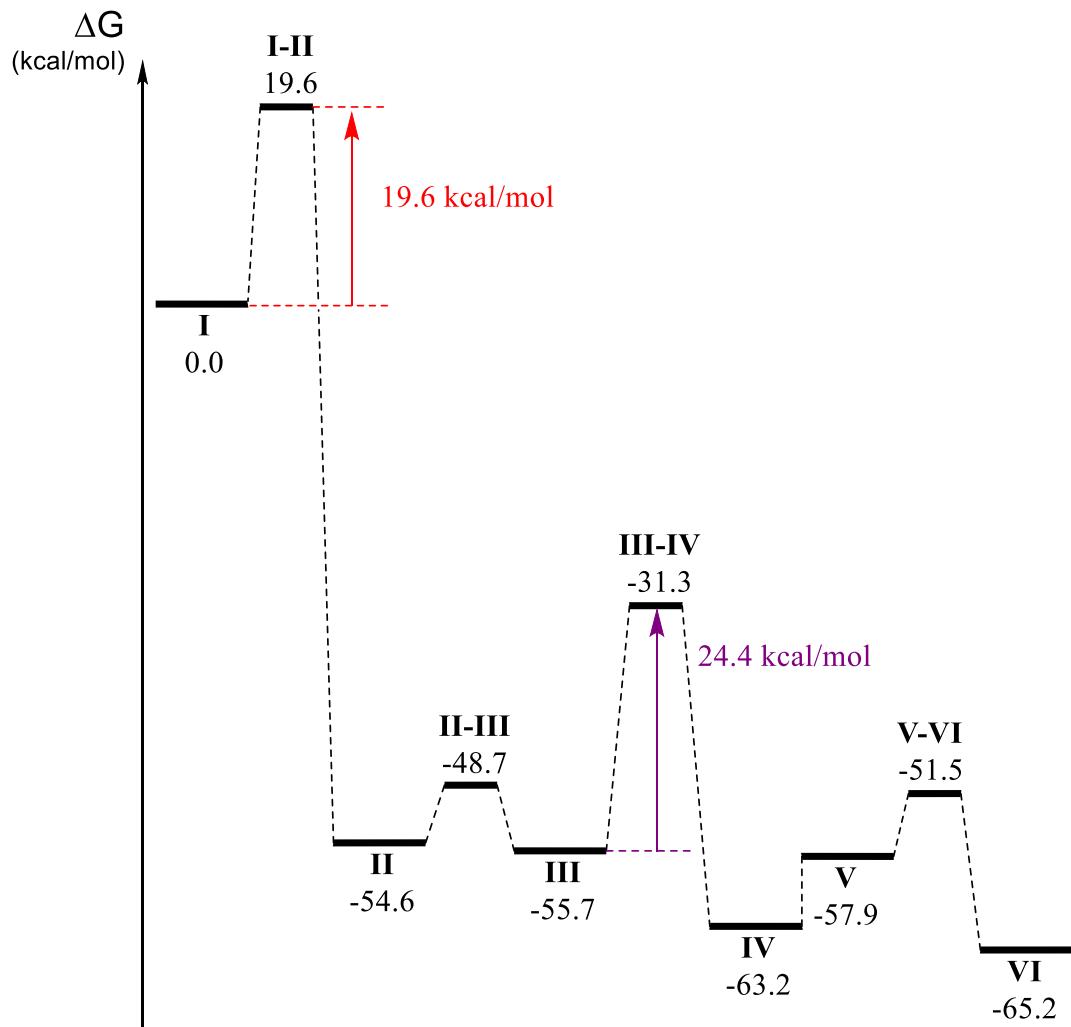
INTRODUCTION



Rate determining step (rds)

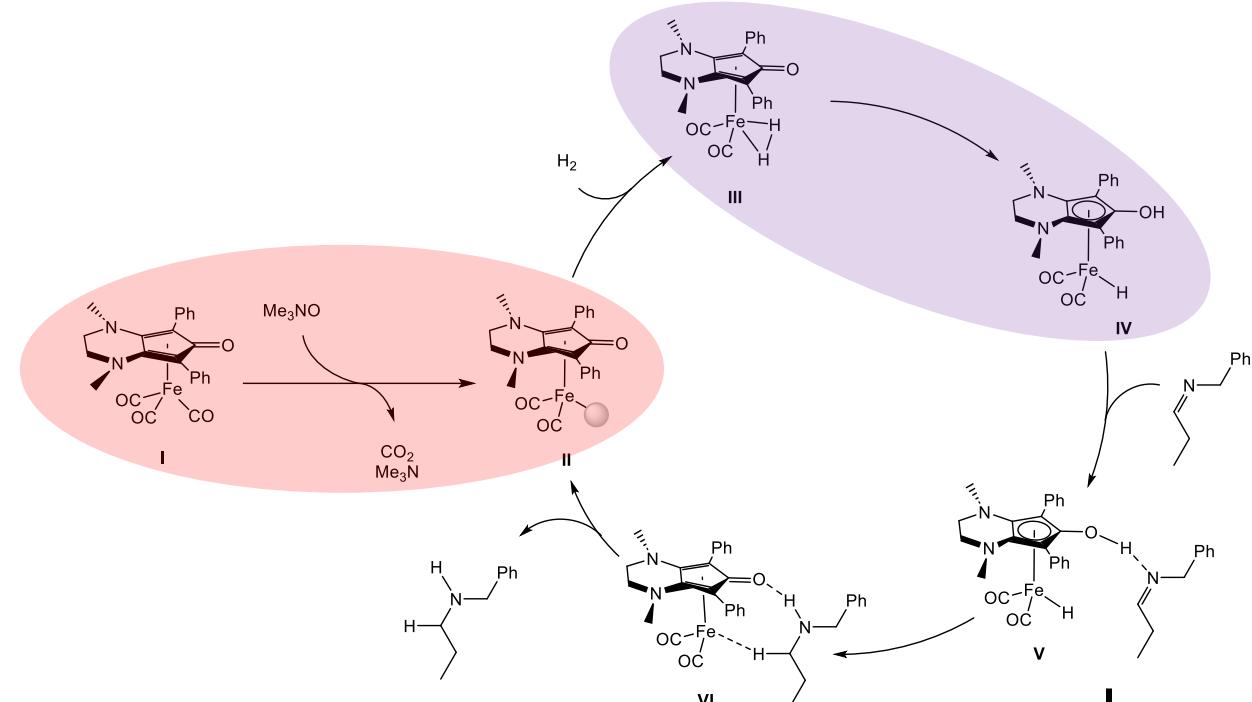


INTRODUCTION

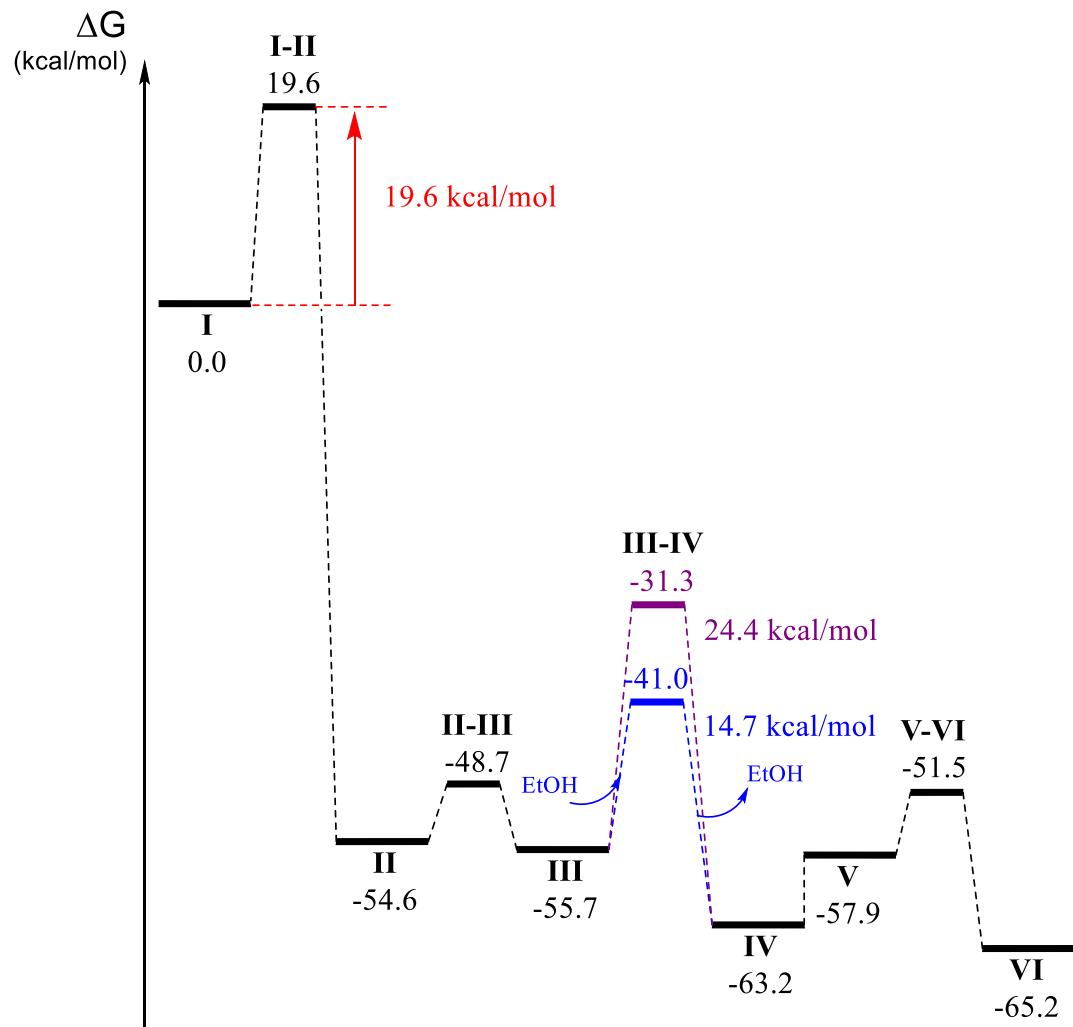


Rate determining step (rds)

- Activation of the catalyst: 19,6 kcal/mol
- Hydrogen transfer: 24,4 kcal/mol

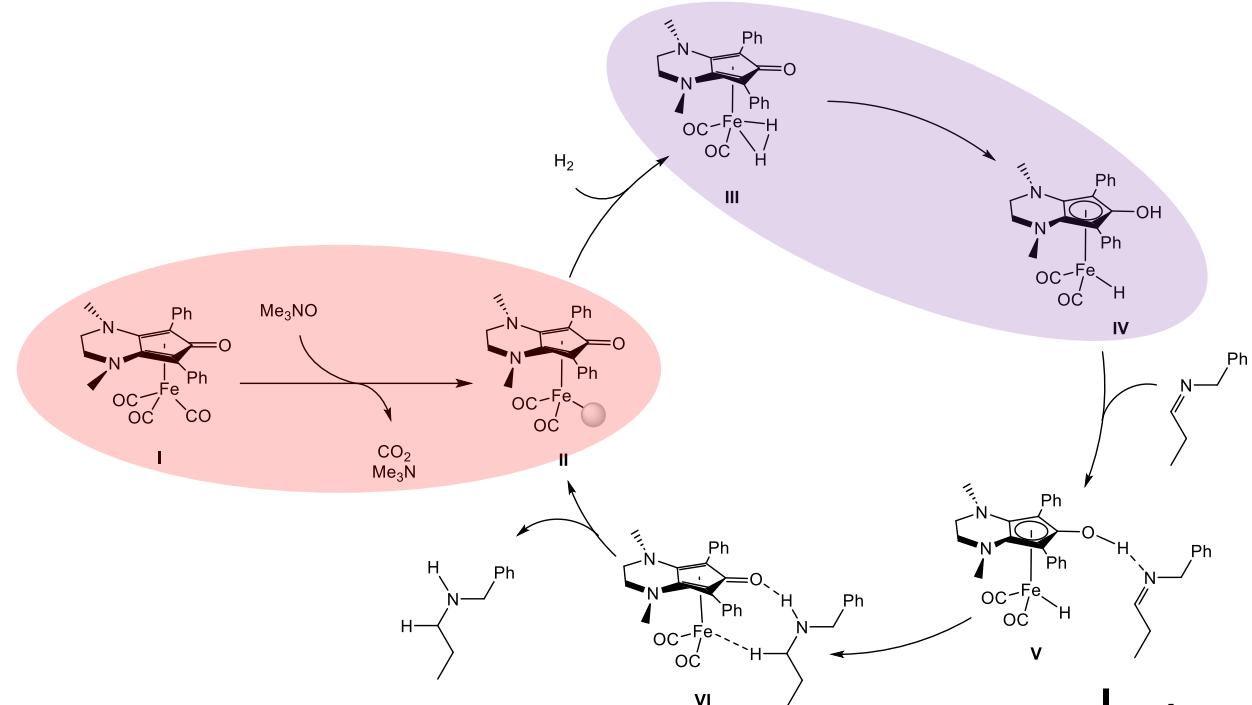


INTRODUCTION

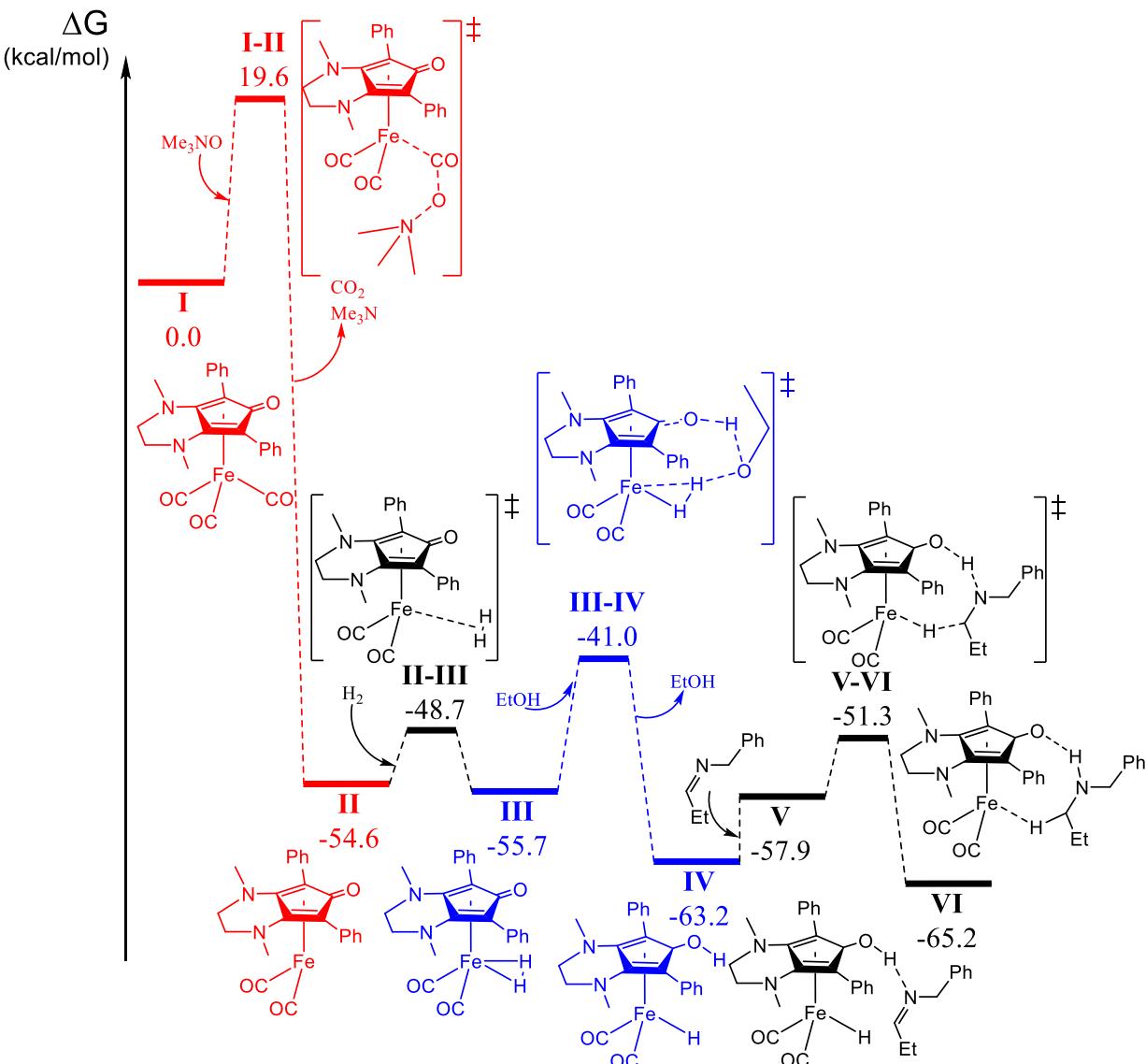


Rate determining step (rds)

- Activation of the catalyst: 19,6 kcal/mol
- ~~Hydrogen transfer: 24,4 kcal/mol~~
- Hydrogen transfer: 14,7 kcal/mol

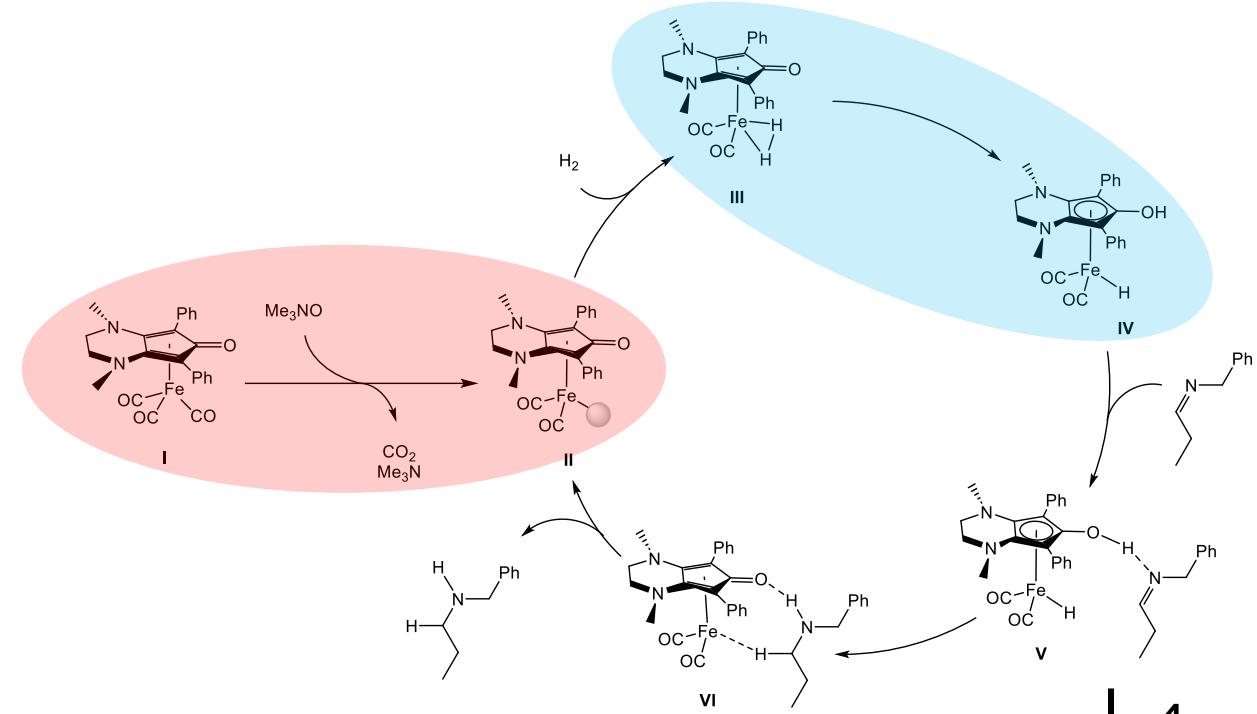


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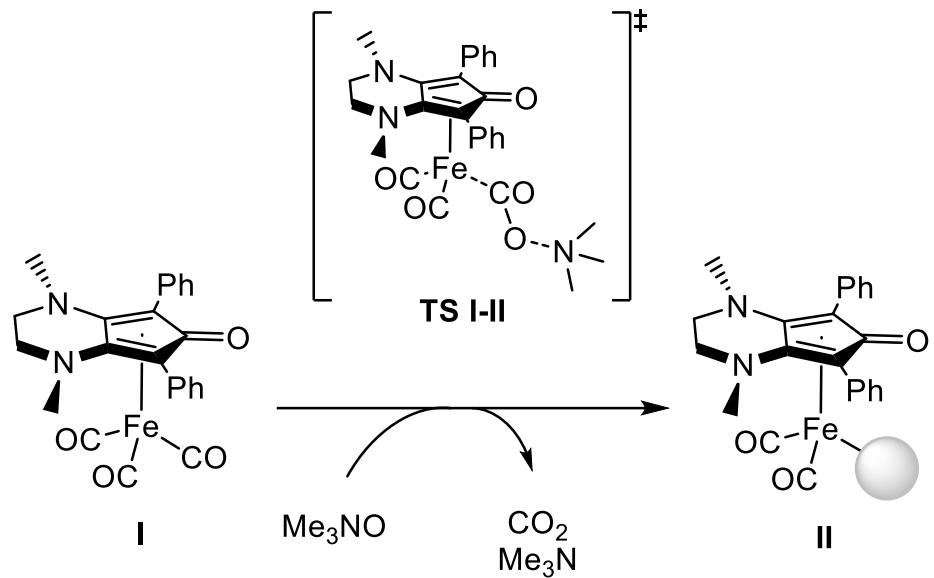
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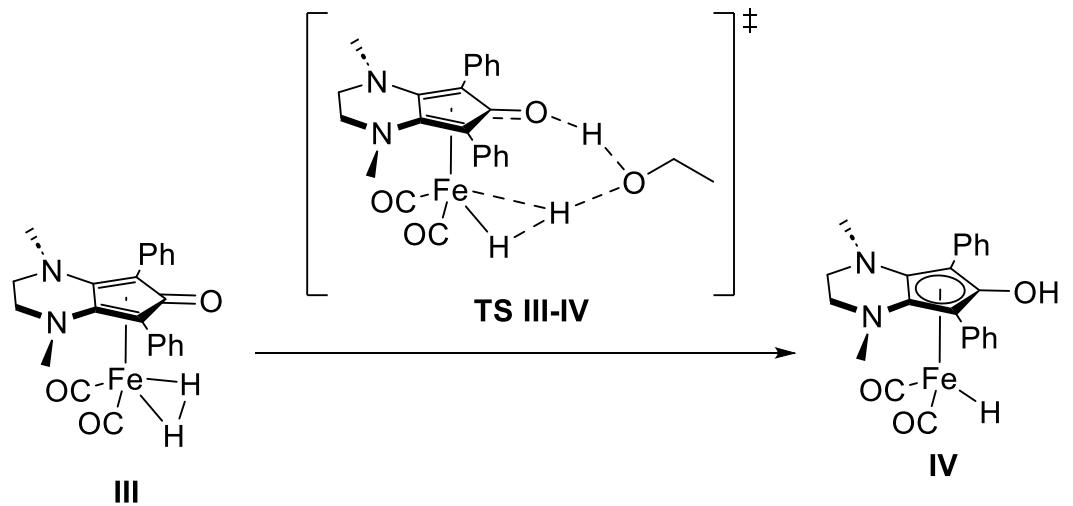


INTRODUCTION

Activation of the catalysts



Hydrogenation of the keto group



OBJECTIVES

Main objectives:

- Investigate the behavior of **different catalyst structures** to identify strategies to **lower activation barriers**, enabling operation under milder conditions that reduce undesired parallel reactions.
- Analyze the results obtained from the modifications made to the catalyst to **understand their impact on catalytic performance**.
- Conduct various tests to **provide a plausible explanation** for the observed results, ensuring a thorough understanding of the catalytic processes involved.

METHODOLOGY

Calculations

- Gaussian 09
 - BP86
 - H, C, O, N, F and Si → SVP
 - Fe → SDD
 - M06 + PCM
 - H, C, O, N, F and Si → cc-pVTZ
 - Fe → SDD
- }
- Optimization of the geometries
- Solvation energy

METHODOLOGY

Complementary studies

- Electronic and geometrical indicators
 - Atomic charges (Natural Population Analysis)
 - Mayer Bond Order (MBO)
 - Fukui function
 - Bond lengths
- Steric maps (SambVca)
- Aromaticity (ESI-3D)

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Atomic charges:
distribution of the electron density in each atom.

Mayer Bond Order (MBO):
average number of electrons shared between two atoms.

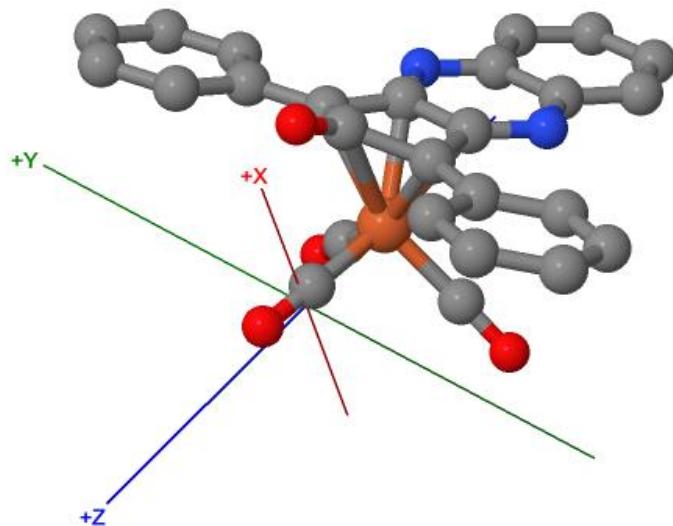
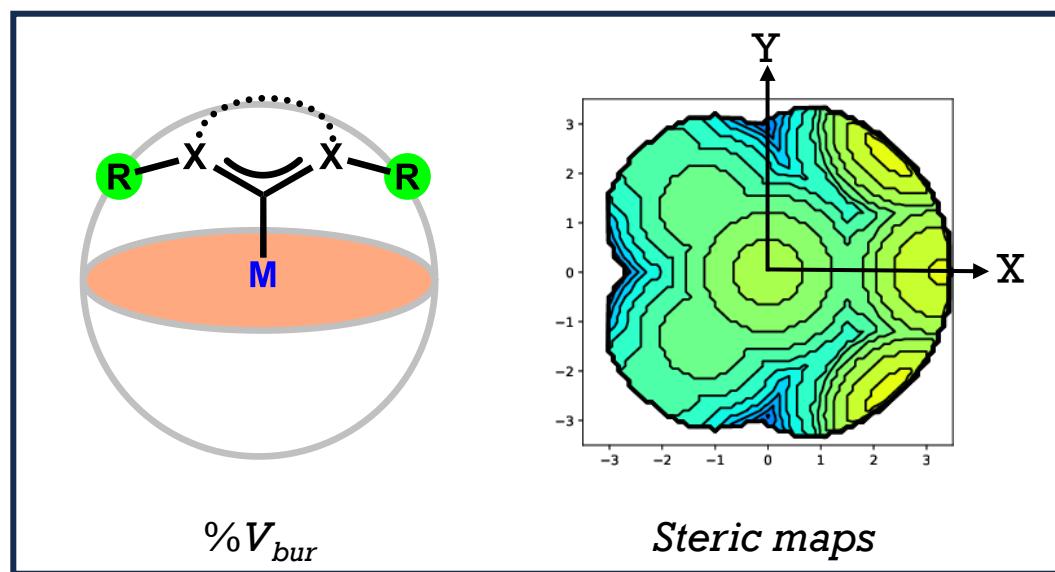
Fukui function:
describes the capacity of an atom to deal with an electrophilic attack.

$$f_k = - \left(\frac{\partial q_k}{\partial N} \right)_{\nu(r)} \implies f_k = q_k^{N-1} - q_k^N$$

METHODOLOGY

Complementary studies

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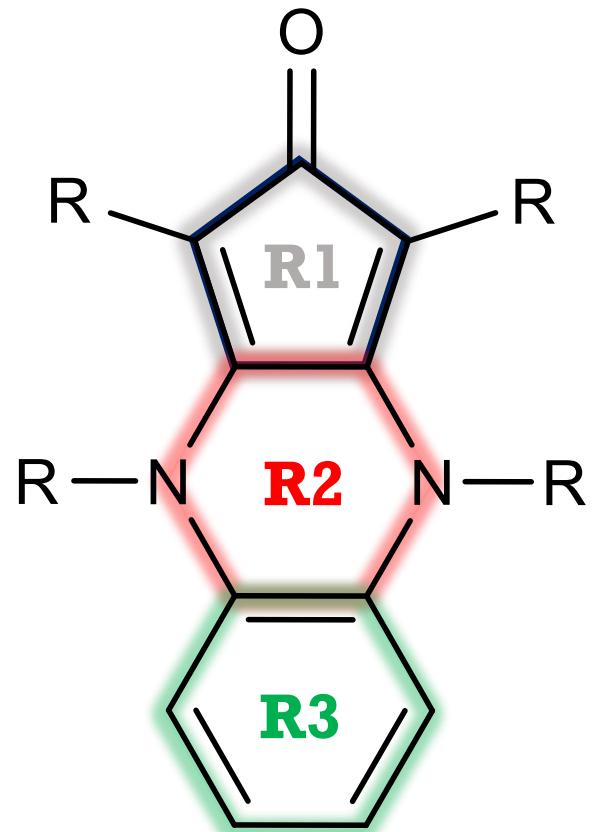
METHODOLOGY

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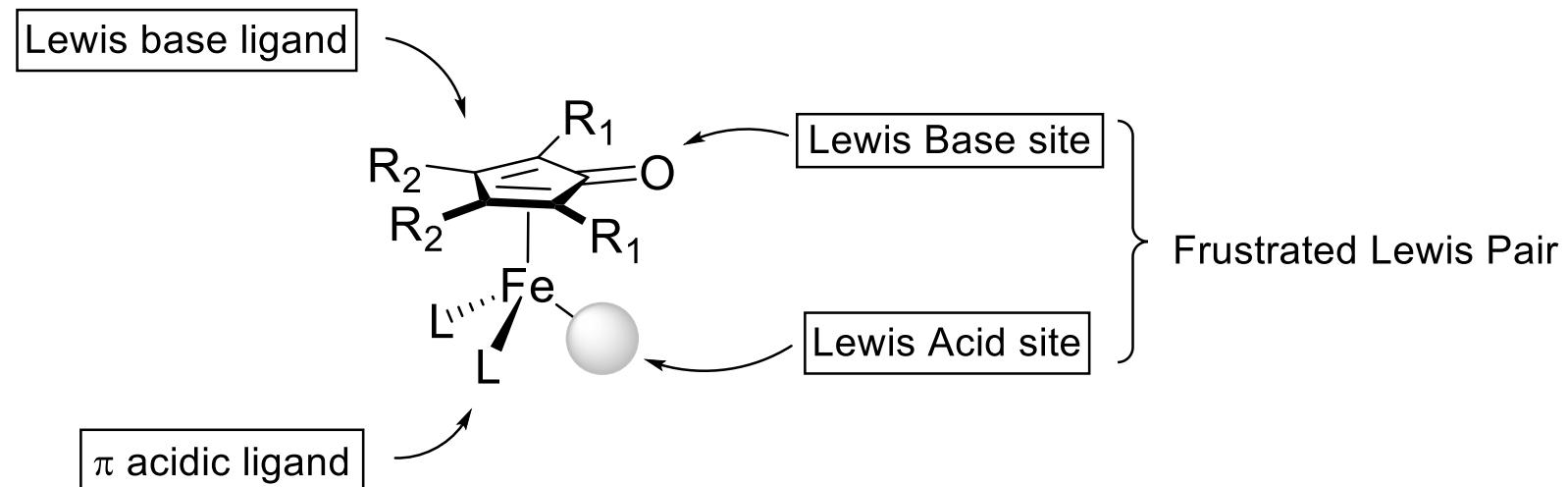
Used indices:

- HOMA
- $I_{ring} - I_{NG}$
- MCI - I_{NB}
- FLU
- BOA
- BLA
- PDI



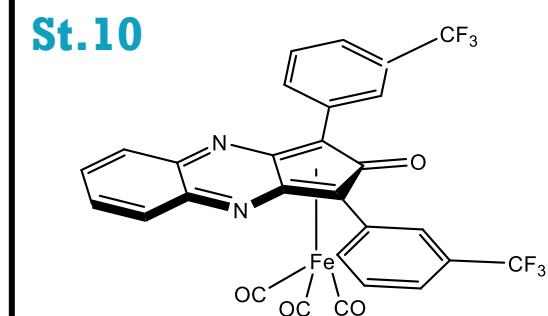
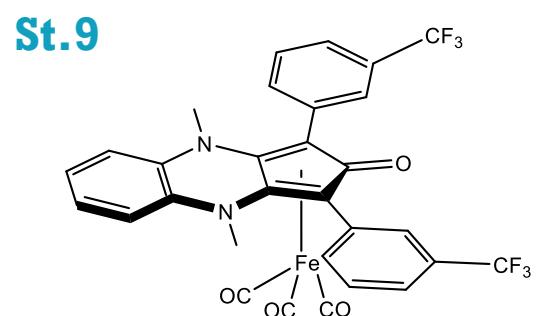
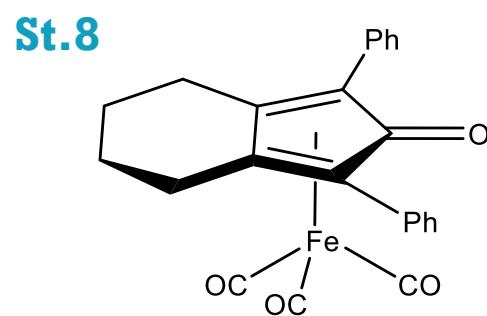
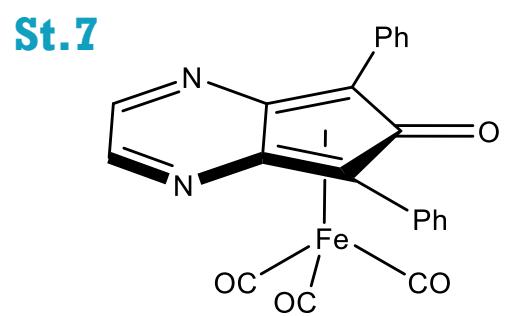
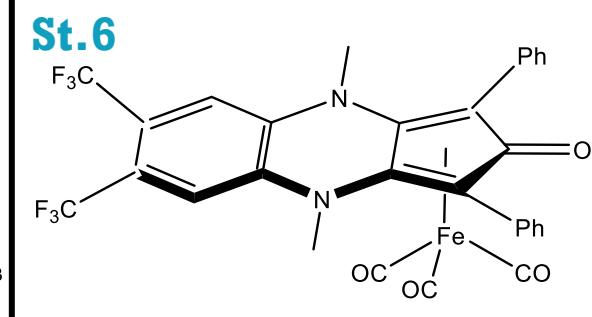
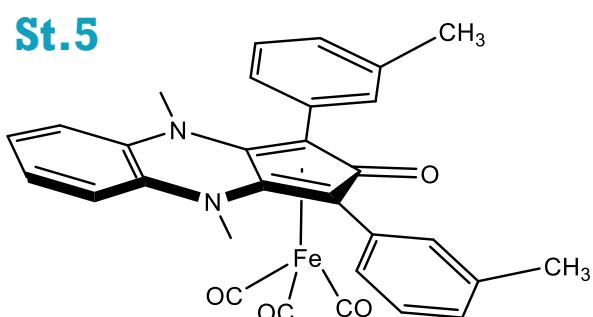
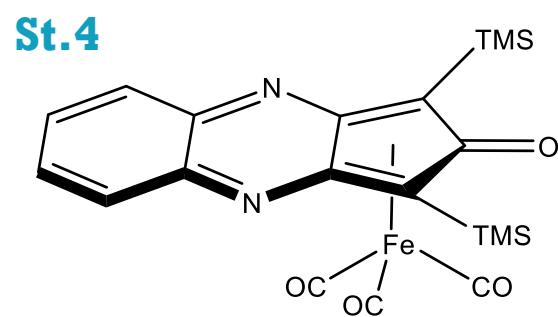
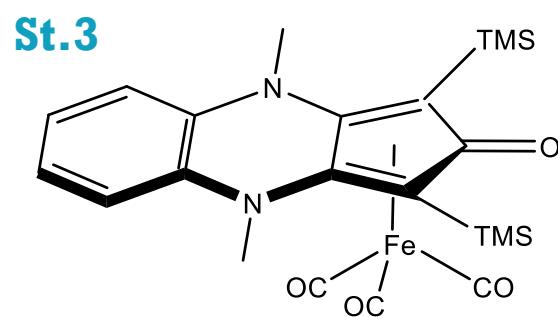
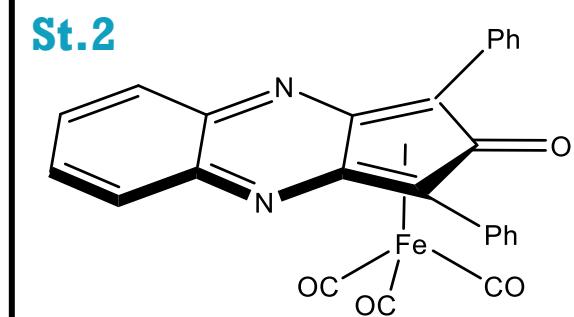
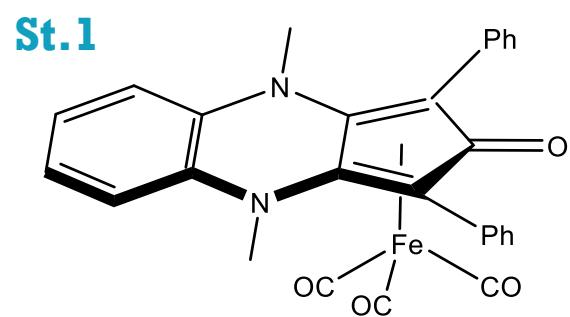
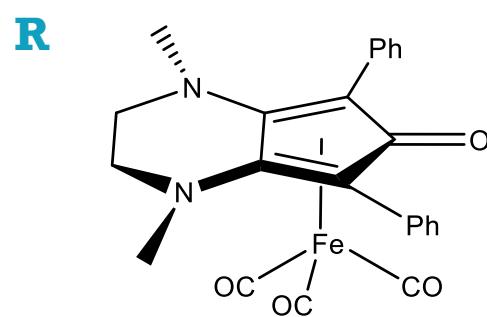
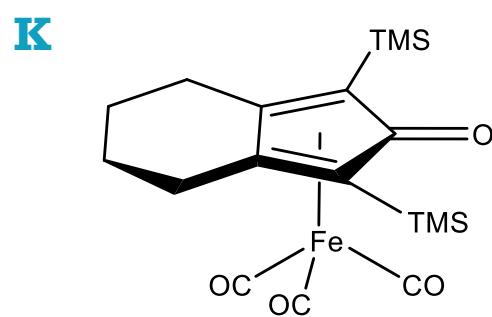
RESULTS AND DISCUSSION

- Examine how the presence of various electron-withdrawing (EWG) and electron-donating (EDG) substituents affects the reactivity and stability of ligands.
- Introduction of a third annulated ring, aromatic, next to the 6-membered ring also annulated to the 5-membered ring of the cyclopentadienone.



RESULTS AND DISCUSSION

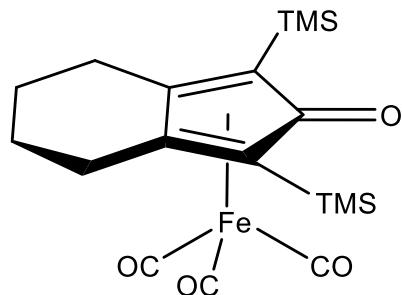
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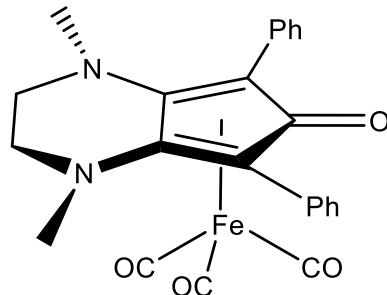
RESULTS AND DISCUSSION

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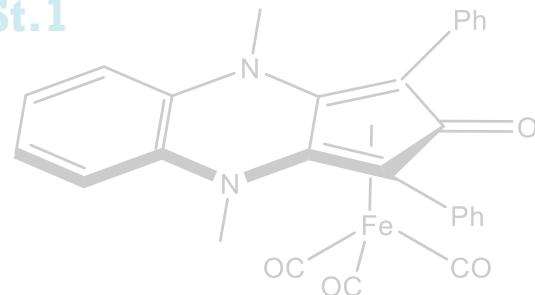
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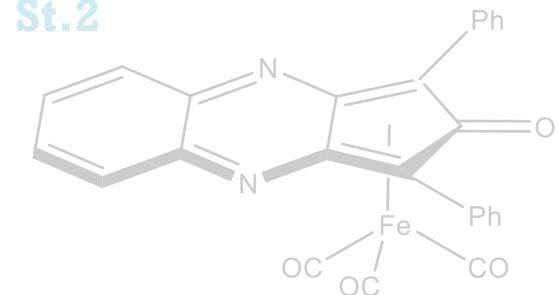
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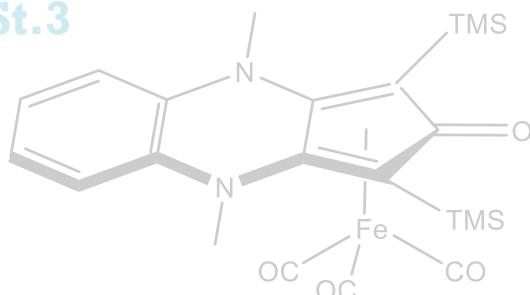
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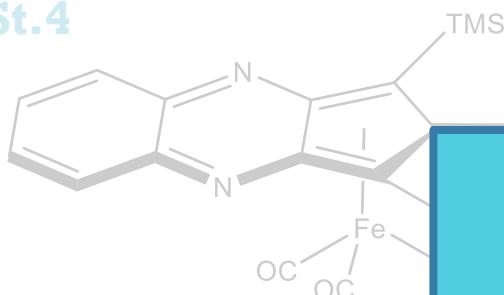
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St.3



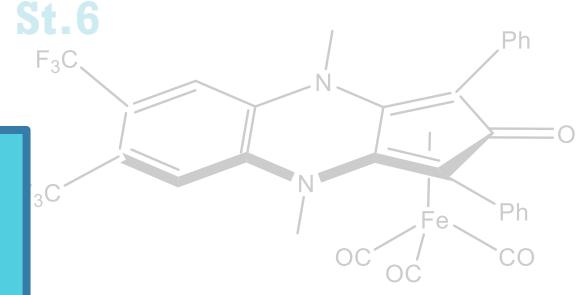
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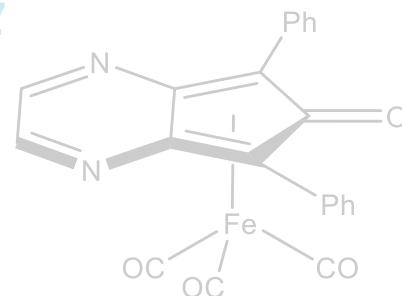
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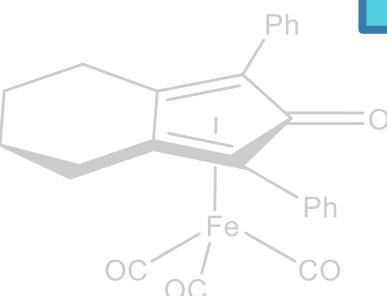
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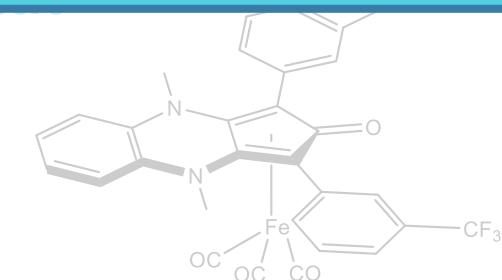
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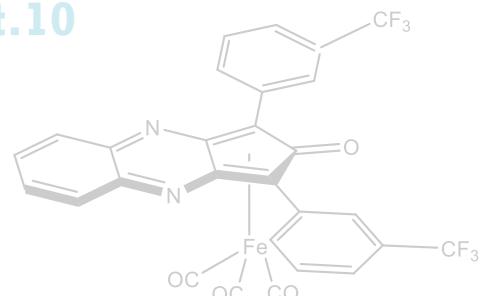
St.8



ORIGINAL
CATALYSTS



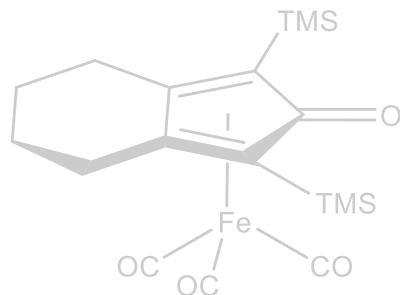
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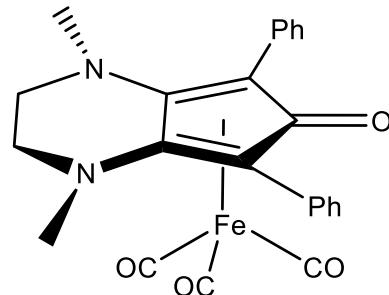
RESULTS AND DISCUSSION

[STRUCTURES]

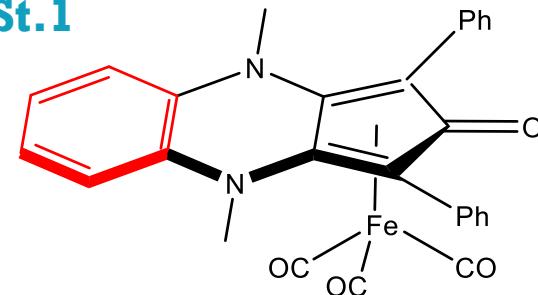
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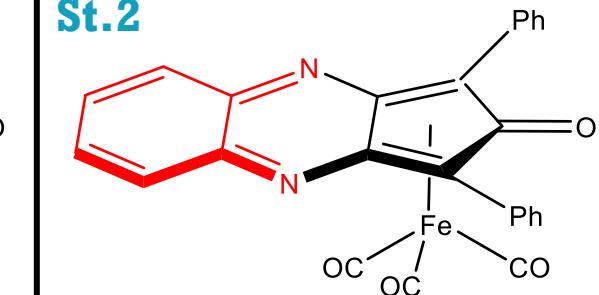
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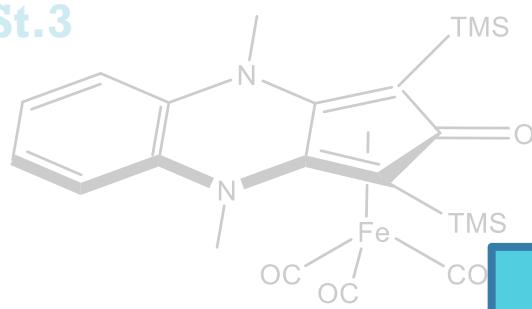
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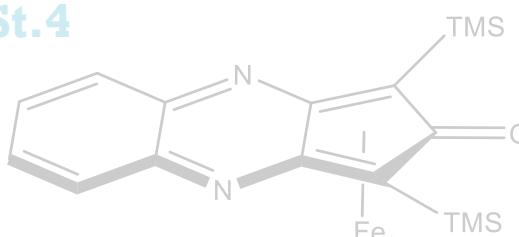
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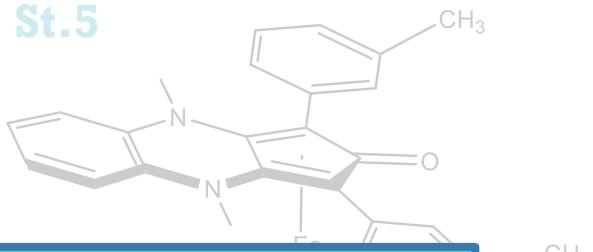
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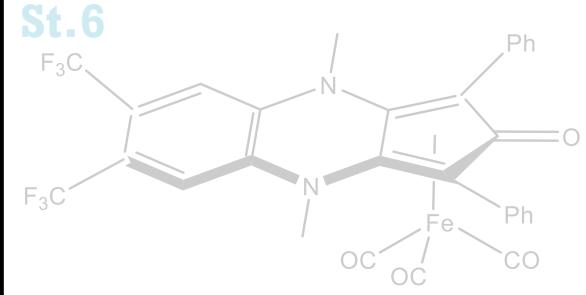
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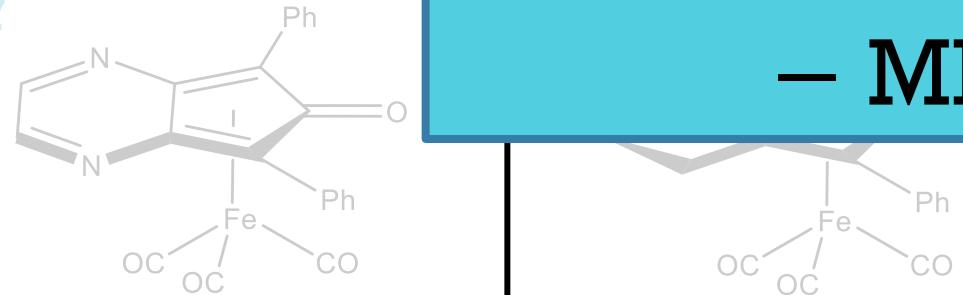
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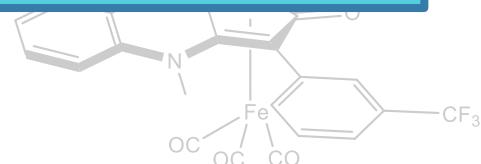
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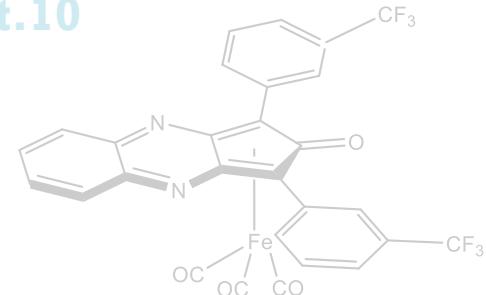
St.7



+ ANNULATED RING
- METHYL

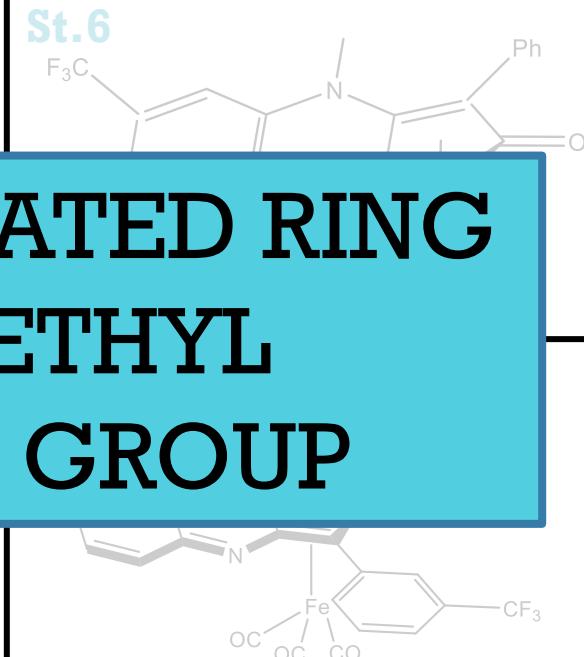
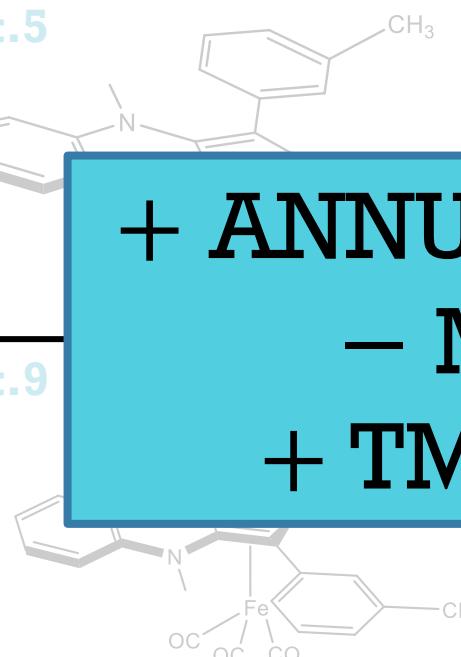
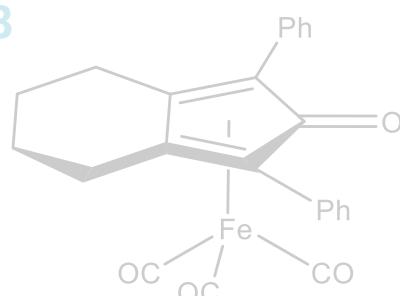
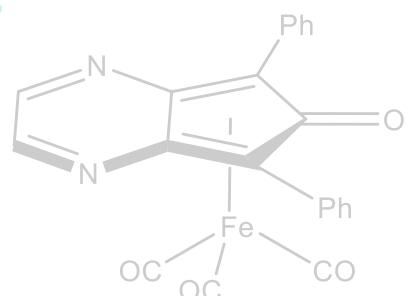
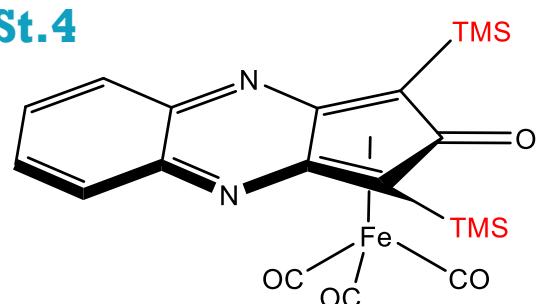
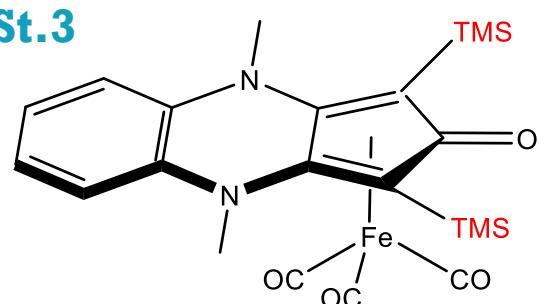
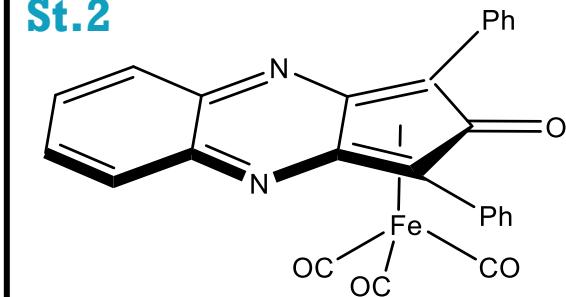
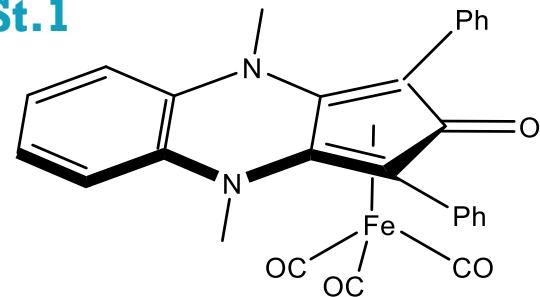
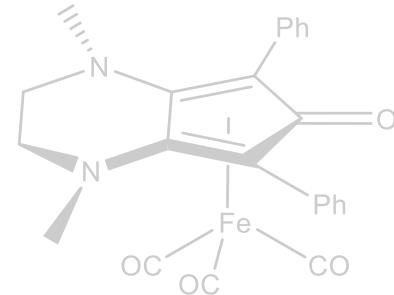
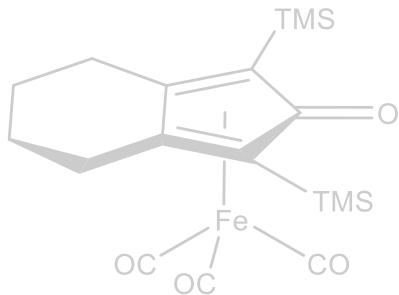


St.10



RESULTS AND DISCUSSION

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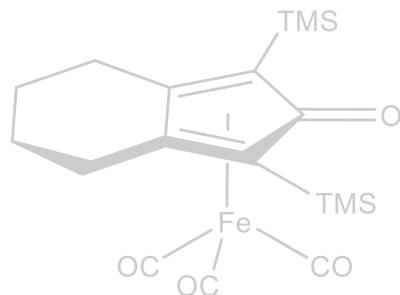


+ ANNULATED RING
– METHYL
+ TMS GROUP

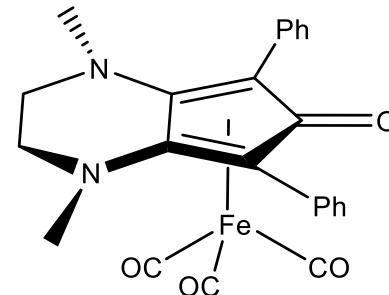
RESULTS AND DISCUSSION

[STRUCTURES]

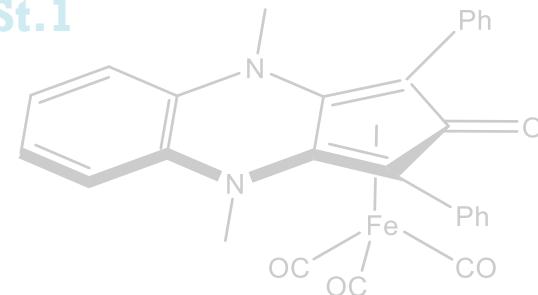
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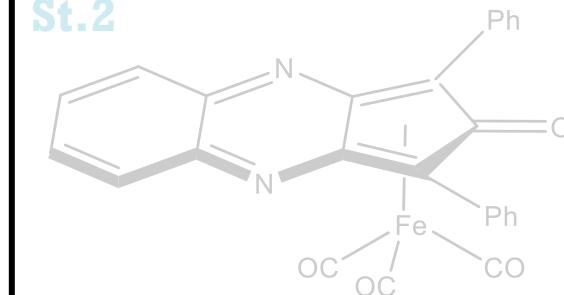
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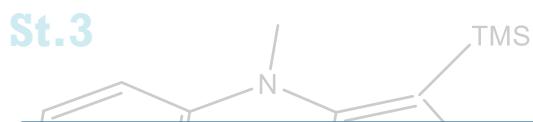
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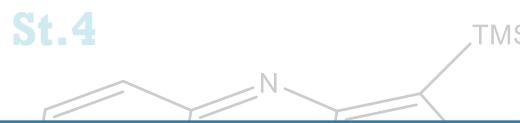
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St.3

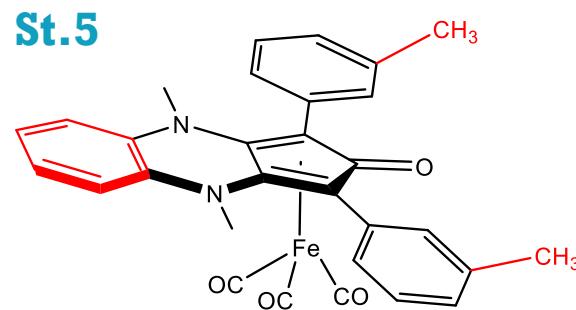


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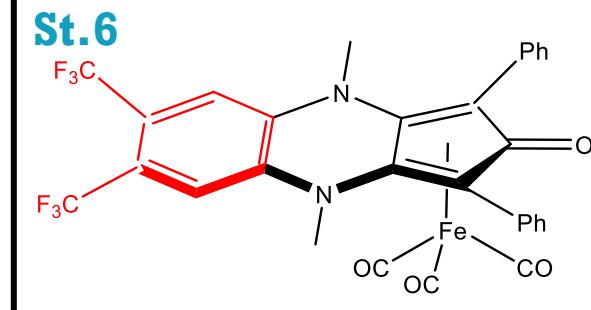


+ ANNULATED RING
+ Ph(*m*-X) GROUP
+ CF₃ TERMINAL GROUP

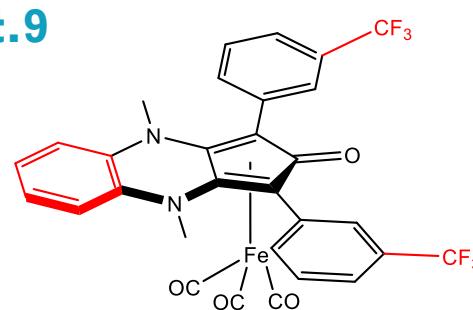
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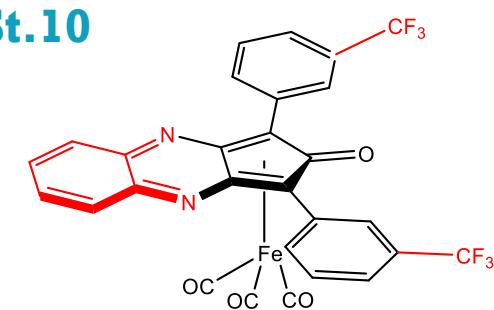
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St.9



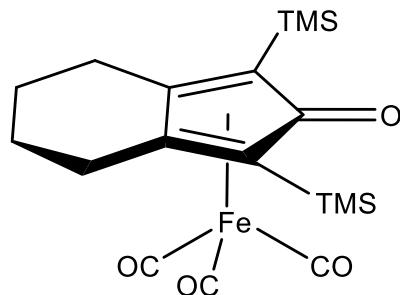
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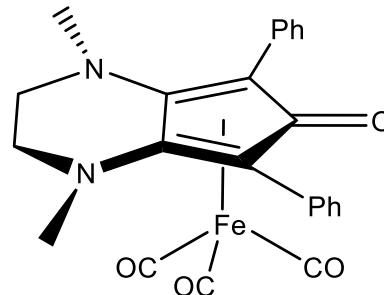
RESULTS AND DISCUSSION

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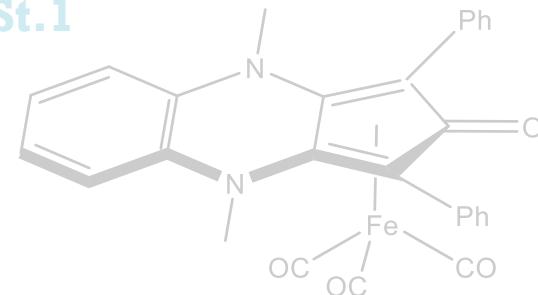
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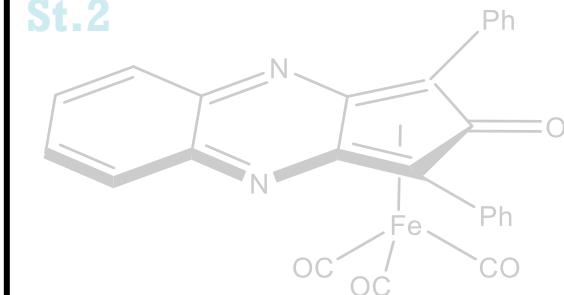
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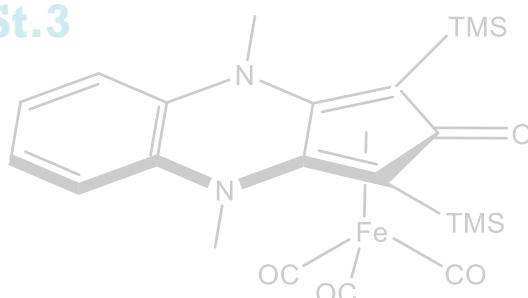
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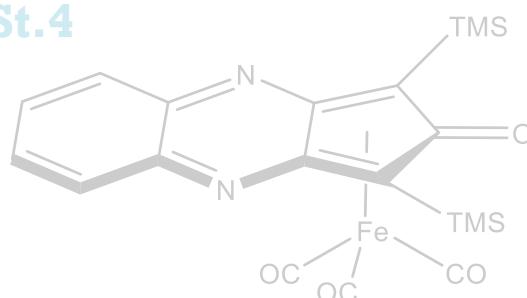
St.2



St.3



St.4

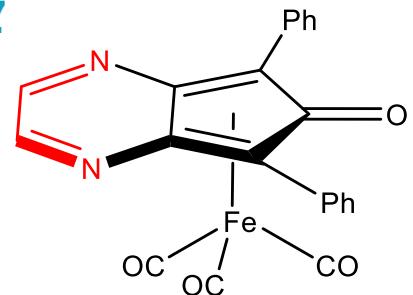


St.

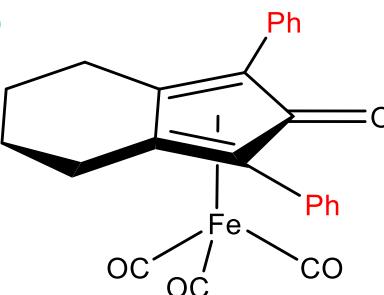
– METHYL
– TMS GROUP



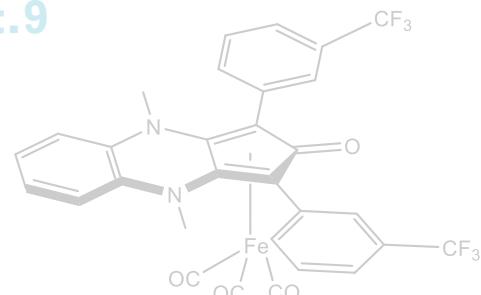
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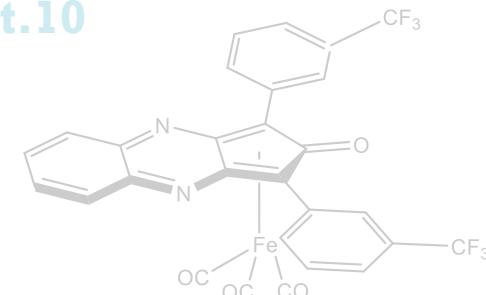
St.8



St.9

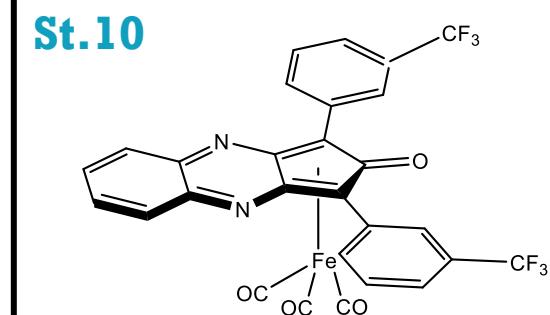
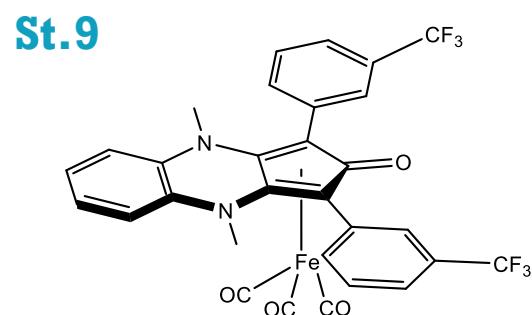
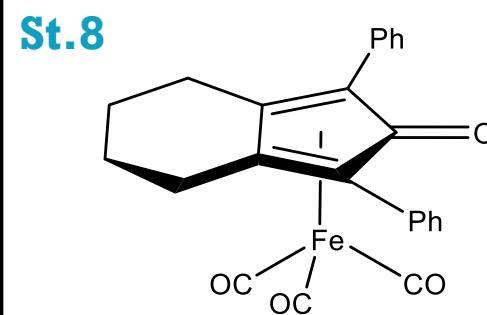
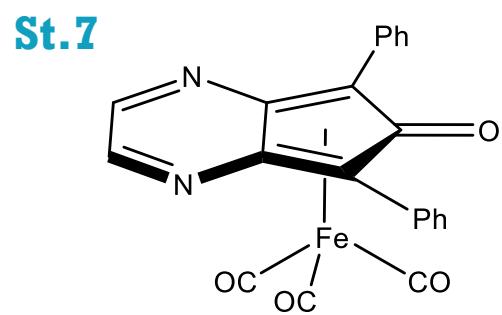
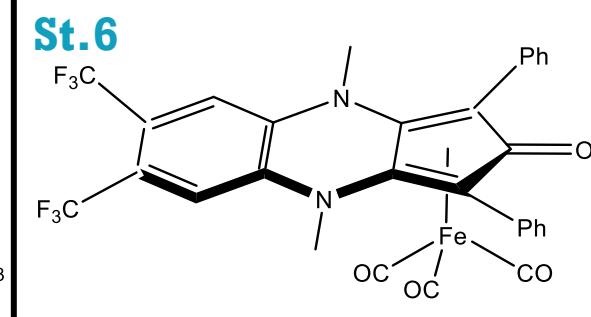
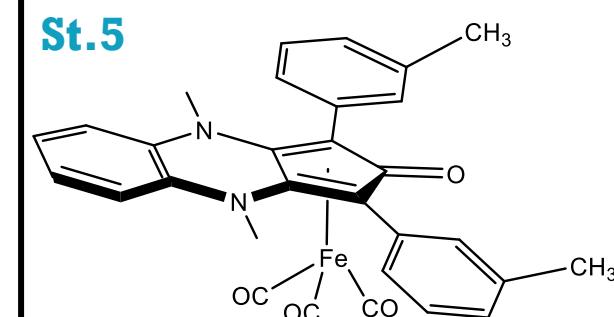
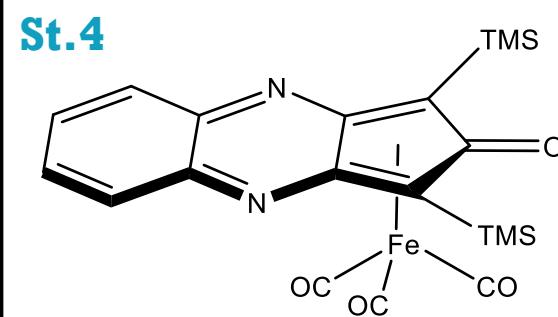
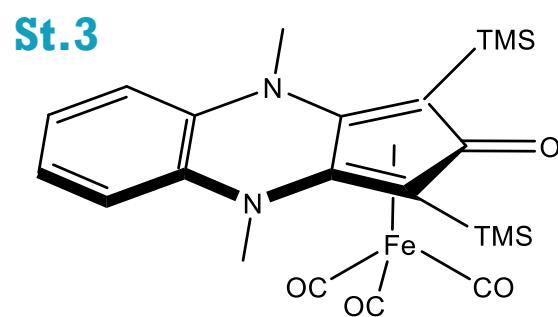
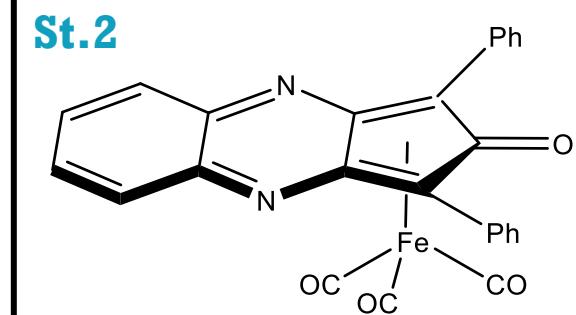
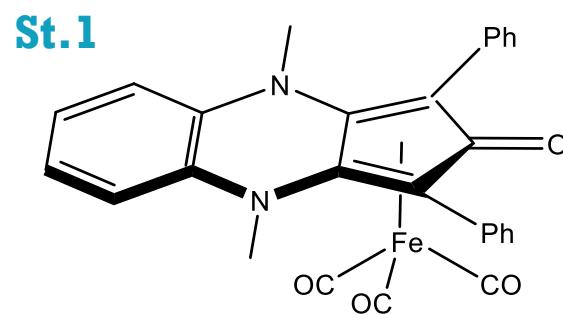
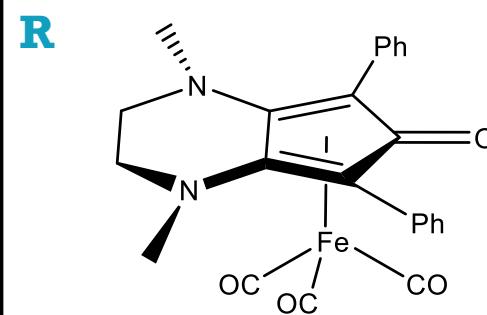
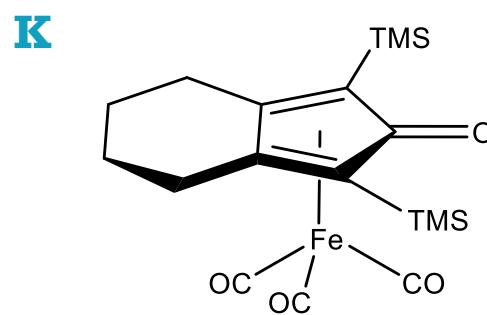


St.10



RESULTS AND DISCUSSION

[STRUCTURES]



RESULTS AND DISCUSSION

[KINETIC COST]

Gibbs energy for studied catalysts (kcal/mol).

	K	R	St.1	St.2	St.3	St.4	St.5	St.6	St.7	St.8	St.9	St.10
I → I-II	18.4	20.6	17.4	9.3	24.2	14.9	18.8	17.8	10.2	15.5	17.2	10.2
III → III-IV	12.5	16.0	13.1	9.8	20.7	11.4	16.2	15.0	11.0	13.9	15.6	10.3

RESULTS AND DISCUSSION

[KINETIC COST]

Gibbs energy for studied catalysts (kcal/mol).

	K	R	St.1	St.2	St.3	St.4	St.5	St.6	St.7	St.8	St.9	St.10
I → I-II	18.4	20.6	17.4	9.3	24.2	14.9	18.8	17.8	10.2	15.5	17.2	10.2
III → III-IV	12.5	16.0	13.1	9.8	20.7	11.4	16.2	15.0	11.0	13.9	15.6	10.3



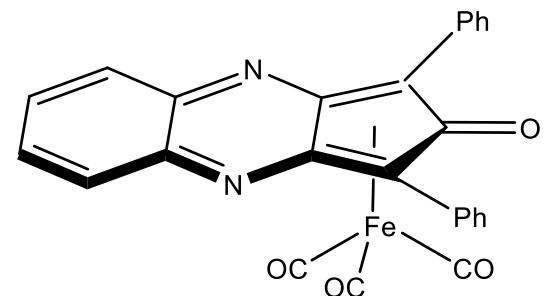
→ values below Renaud's catalyst, more than 3 kcal/mol



→ values below Renaud's catalyst, up to 3 kcal/mol



→ values over Renaud's catalyst



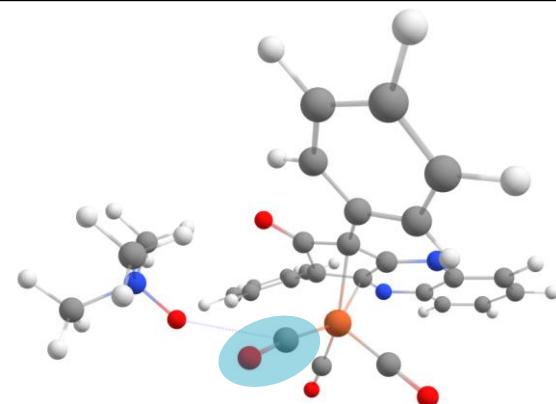
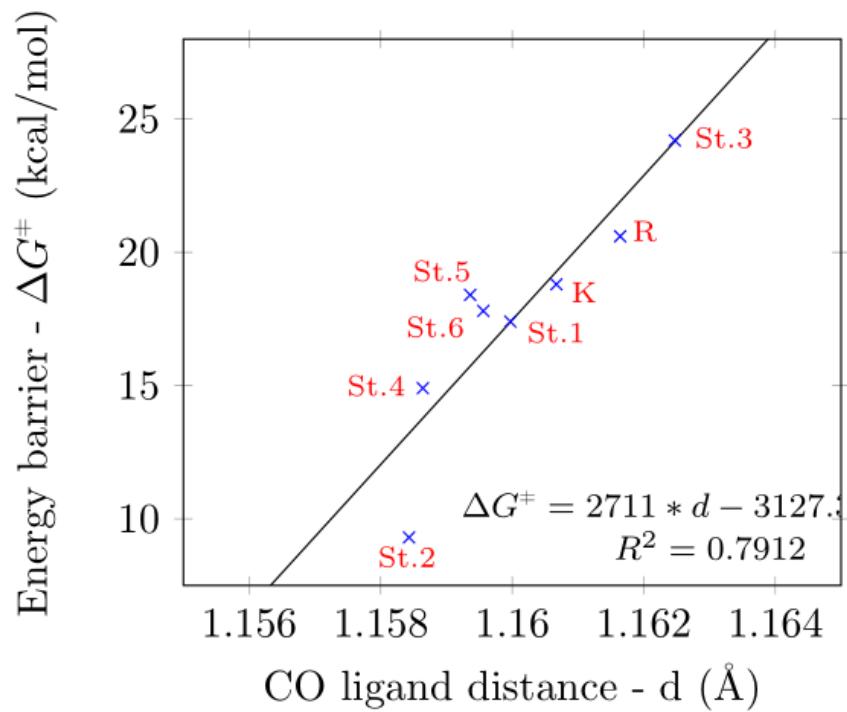
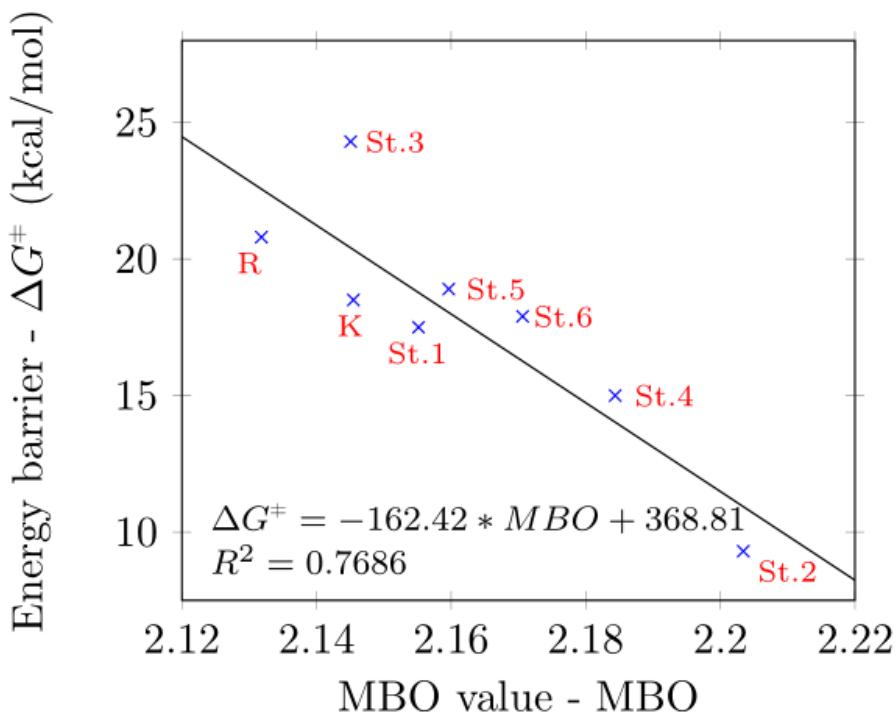
St.2 catalyst

RESULTS AND DISCUSSION

[STRUC. CHAR.]

Activation of the catalyst

	K	R	St.1	St.2	St.3	St.4	St.5	St.6
I → I-II	18.4	20.6	17.4	9.3	24.2	14.9	18.8	17.8
III → III-IV	12.5	16.0	13.1	9.8	20.7	11.4	16.2	15.0

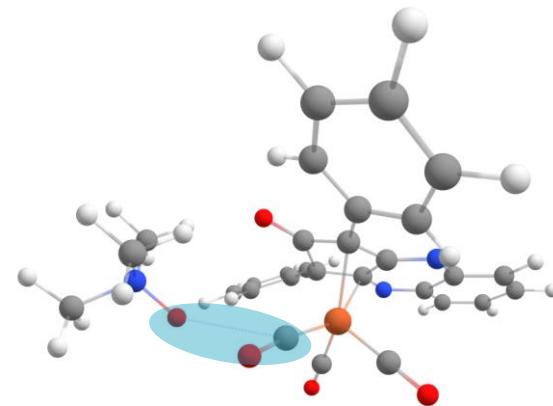


RESULTS AND DISCUSSION

[STRUC. CHAR.]

Activation of the catalyst

(e)	K	R	St.1	St.2	St.3	St.4	St.5	St.6
<i>q</i> Fe	-1.509	-1.528	-1.492	-1.350	-1.502	-1.393	-1.507	-1.510
<i>q</i> C	0.928	0.905	0.903	0.938	0.897	0.946	0.9013	0.905



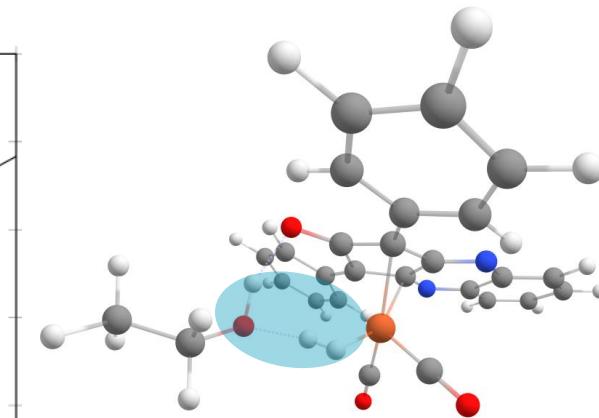
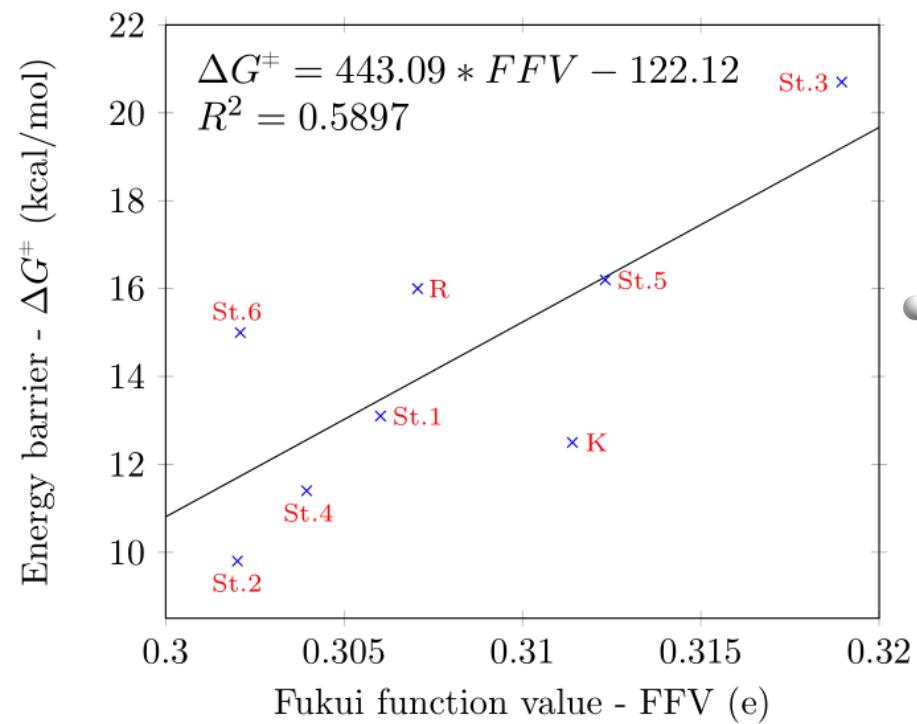
		K	R	St.1	St.2	St.3	St.4	St.5	St.6
I	d(Fe–C)		1.795	1.797	1.804	1.775	1.798	1.776	1.806
	d(C–O) (ligand)		1.159	1.162	1.160	1.158	1.163	1.159	1.161
I-II	d(Fe–C)		1.879	1.892	1.885	1.787	1.906	1.845	1.888
	d(C–O) (ligand)		1.185	1.188	1.179	1.158	1.194	1.181	1.179
	d(C–O) (ligand-Me ₃ NO)		1.188	1.820	1.954	3.151	1.742	1.947	1.981

RESULTS AND DISCUSSION

[STRUC. CHAR.]

Hydrogen transfer

	K	R	St.1	St.2	St.3	St.4	St.5	St.6
I → I-II	18.4	20.6	17.4	9.3	24.2	14.9	18.8	17.8
III → III-IV	12.5	16.0	13.1	9.8	20.7	11.4	16.2	15.0

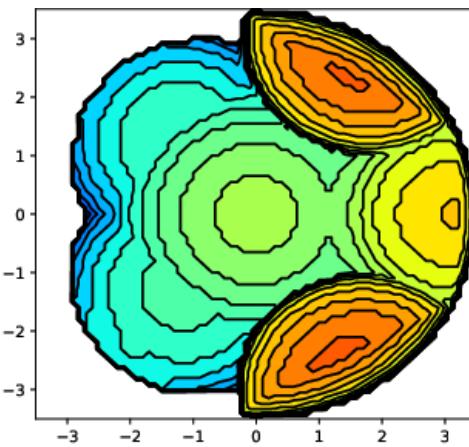


	(Å)	K	R	St.1	St.2	St.3	St.4	St.5	St.6
III	d(Fe–H)	1.636	1.654	1.663	1.613	1.689	1.613	1.669	1.667
	d(Fe–H)	1.588	1.592	1.620	1.561	1.603	1.563	1.616	1.612
III-IV	d(H–O) (H - EtOH)	1.397	1.350	1.341	1.539	1.328	1.536	1.332	1.348
	d(H–O) (EtOH - keto)	1.494	1.401	1.412	1.610	1.374	1.569	1.432	1.441

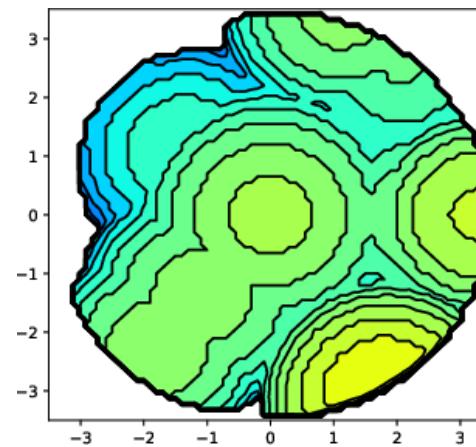
RESULTS AND DISCUSSION

[STERIC MAPS]

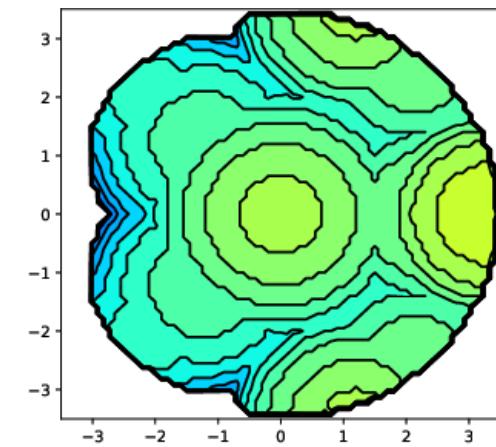
Steric maps of the intermediate I.



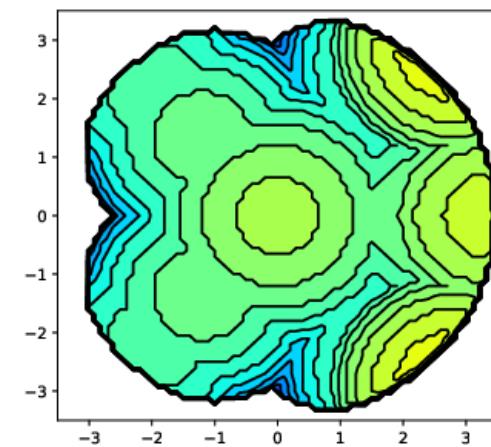
K



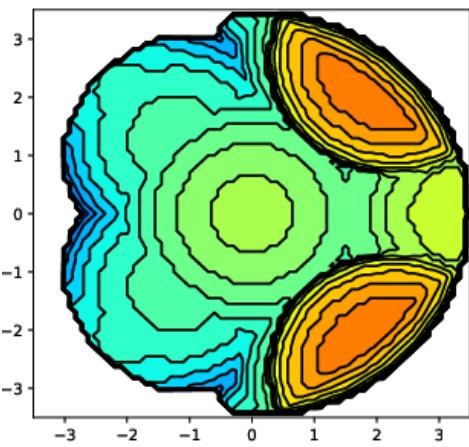
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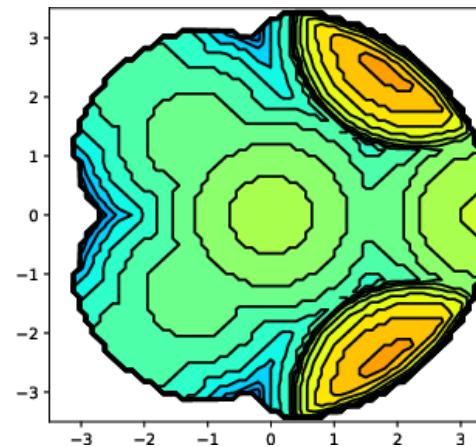
St.1



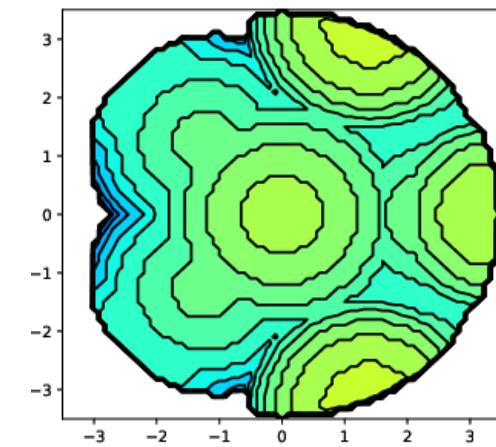
St.2



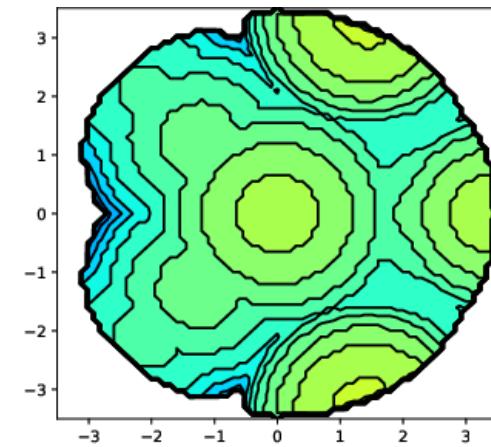
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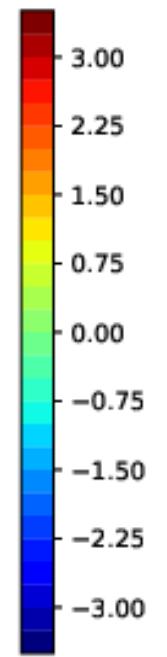
St.4



St.5



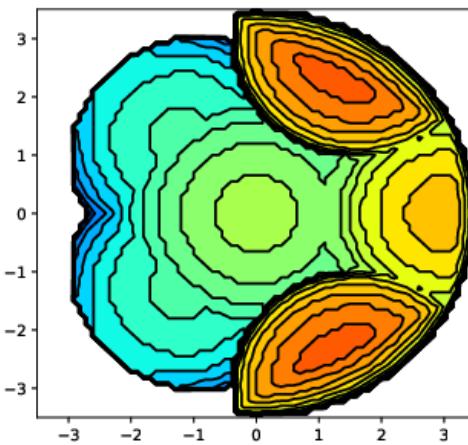
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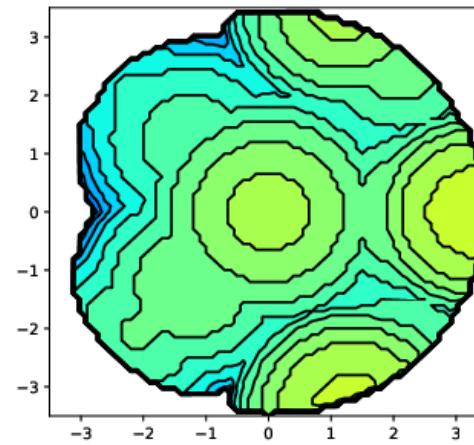
RESULTS AND DISCUSSION

[STERIC MAPS]

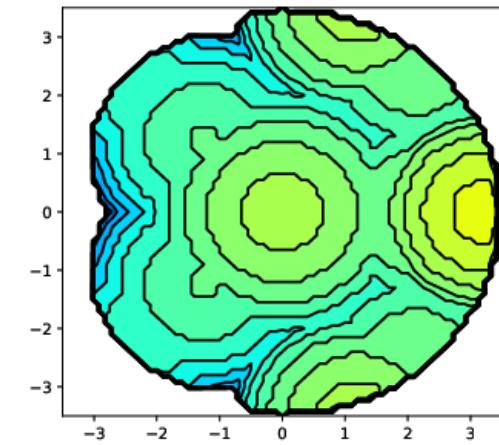
Steric maps of the intermediate **III**.



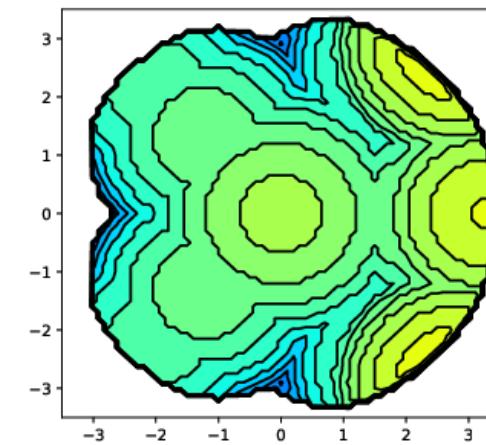
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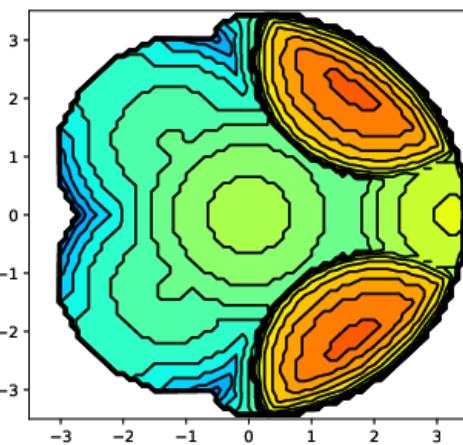
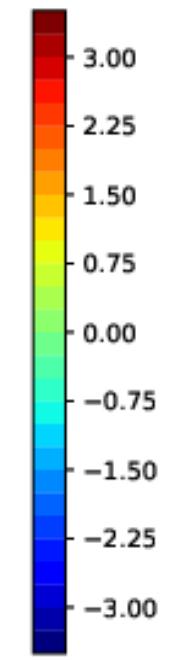
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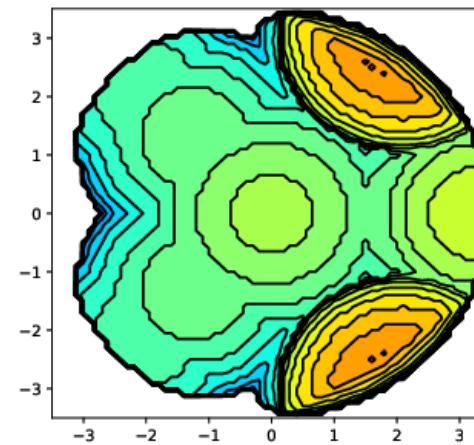
St.1



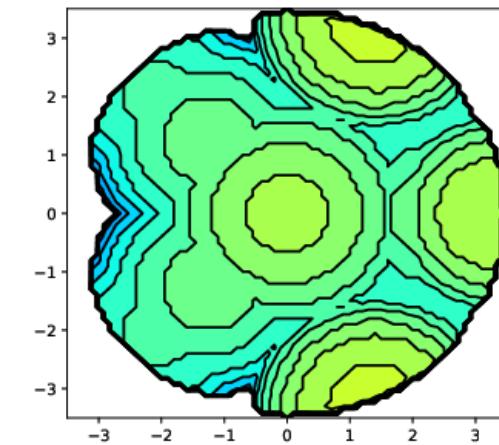
St.2



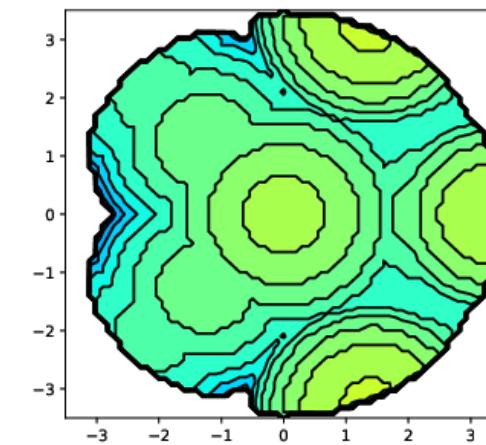
St.3



St.4



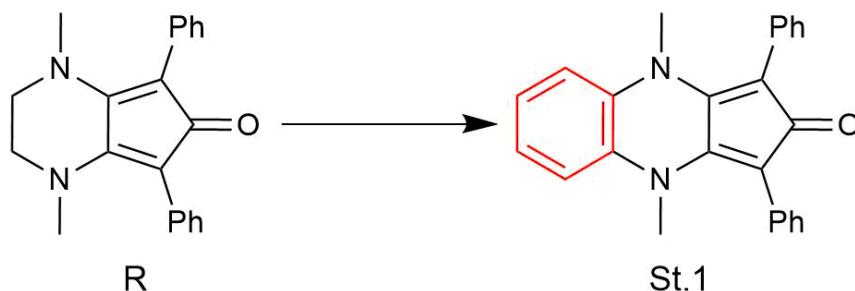
St.5



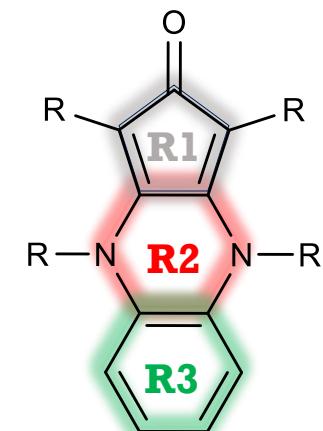
St.6

RESULTS AND DISCUSSION

[AROMATICITY]

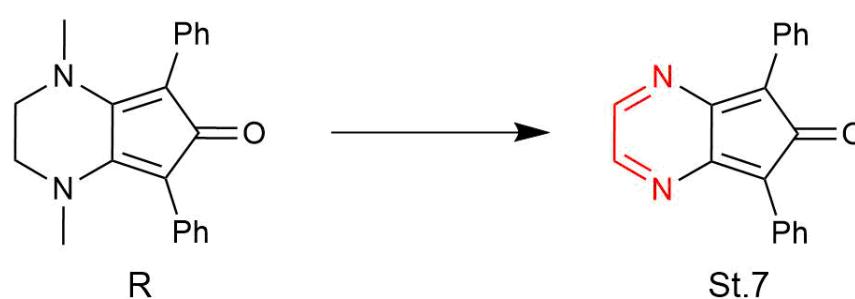


				Gibbs energy for studied catalysts (kcal/mol).									
	K	R	St.1	St.2	St.3	St.4	St.5	St.6	St.7	St.8	St.9	St.10	
I → I-II	18.4	20.6	17.4	9.3	24.2	14.9	18.8	17.8	10.2	15.5	17.2	10.2	
III → III-IV	12.5	16.0	13.1	9.8	20.7	11.4	16.2	15.0	11.0	13.9	15.6	10.3	



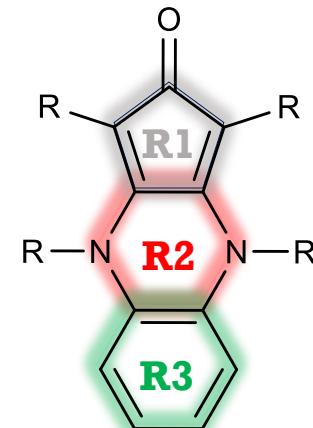
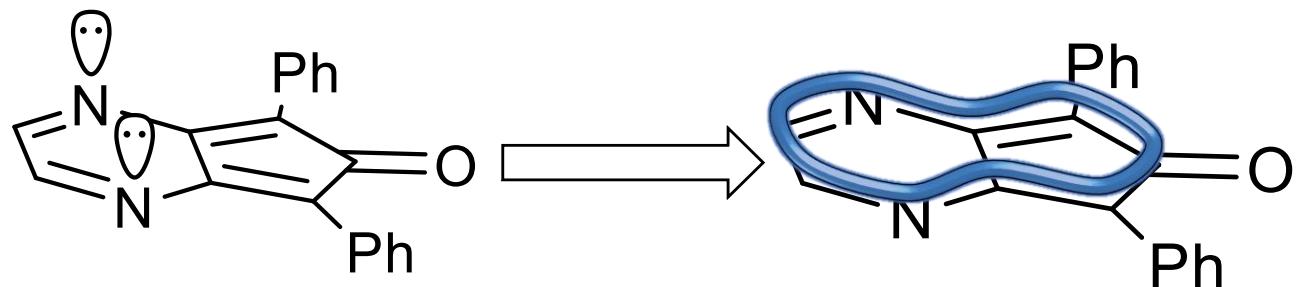
RESULTS AND DISCUSSION

[AROMATICITY]



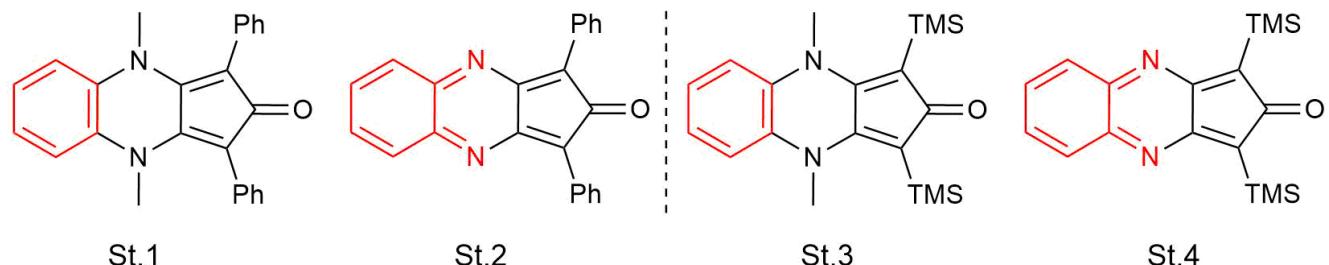
Gibbs energy for studied catalysts (kcal/mol).												
	K	R	St.1	St.2	St.3	St.4	St.5	St.6	St.7	St.8	St.9	St.10
I → I-II	18.4	20.6	17.4	9.3	24.2	14.9	18.8	17.8	10.2	15.5	17.2	10.2
III → III-IV	12.5	16.0	13.1	9.8	20.7	11.4	16.2	15.0	11.0	13.9	15.6	10.3

Catalyst	Ring	MCI	I _{ring}	I _{NG}	I _{NB}	FLU	BOA	BLA	PDI	HOMA
R	1	0.0062	0.0076	0.0310	0.0290	0.0770	0.0176	0.0122	—	-1.2788
	2	0.0004	0.0004	0.0184	0.0171	0.0488	0.0893	0.0367	0.0119	-0.6781
St.7	1	0.0059	0.0071	0.0306	0.0287	0.0752	0.0524	0.0156	—	-1.4825
	2	0.0208	0.0159	0.0344	0.0334	0.0374	0.1774	0.0297	0.0642	0.5772



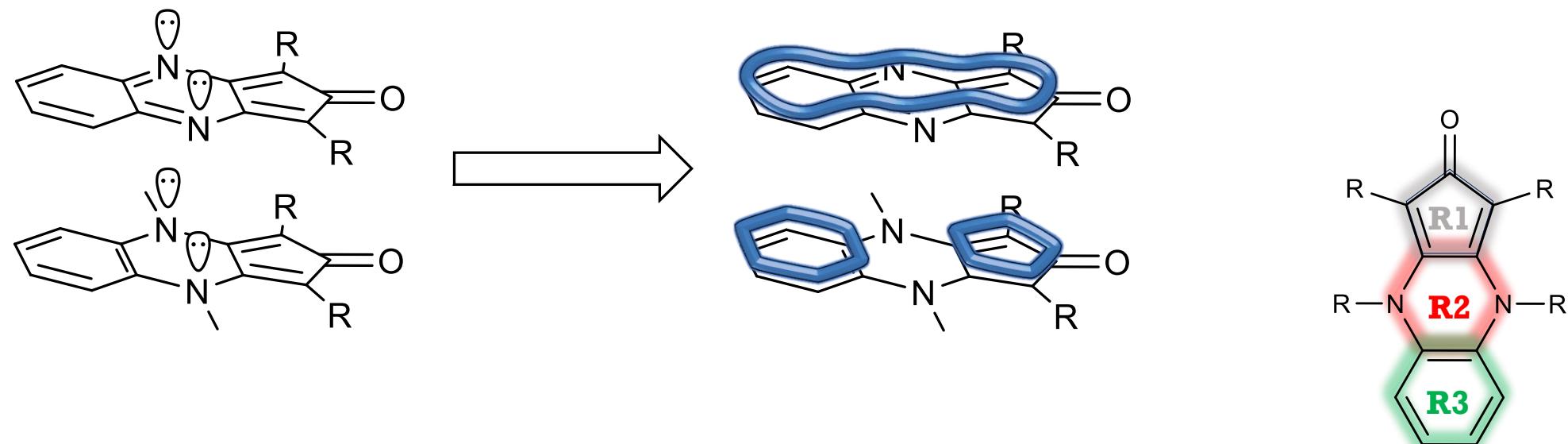
RESULTS AND DISCUSSION

[AROMATICITY]



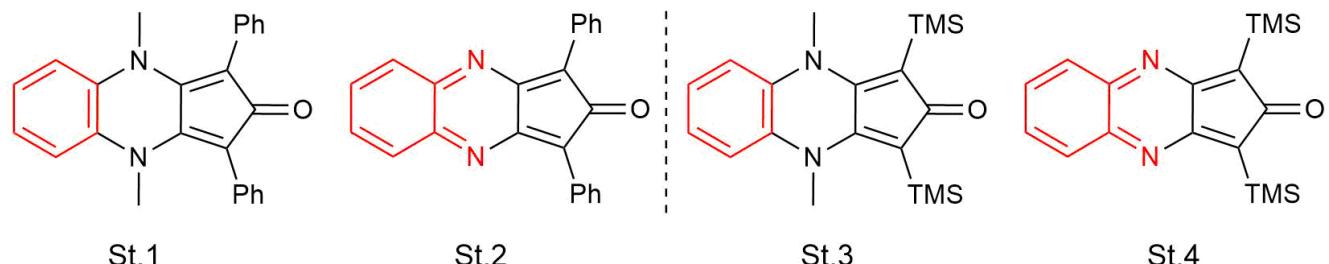
Gibbs energy for studied catalysts (kcal/mol).

	K	R	St.1	St.2	St.3	St.4
I → I-II	18.4	20.6	17.4	9.3	24.2	14.9
III → III-IV	12.5	16.0	13.1	9.8	20.7	11.4



RESULTS AND DISCUSSION

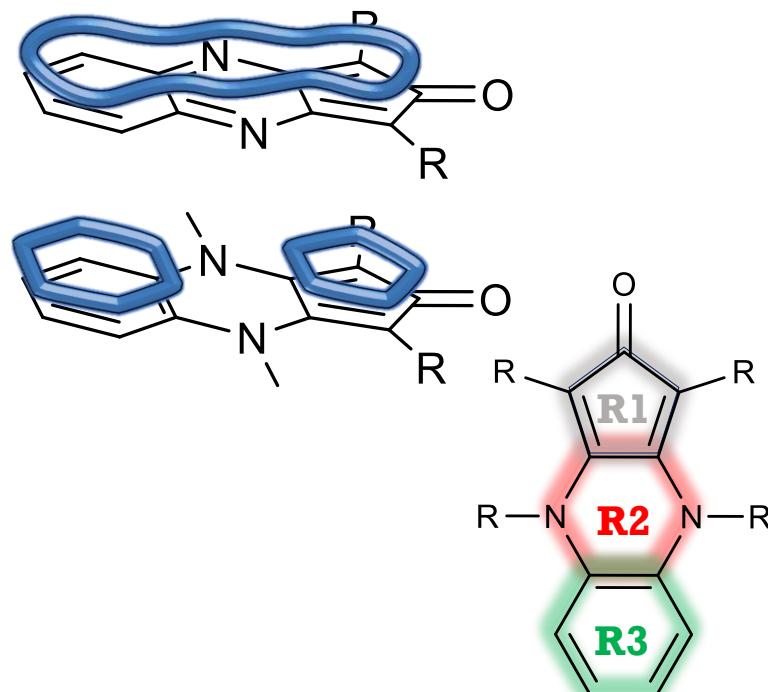
[AROMATICITY]



Gibbs energy for studied catalysts (kcal/mol).

	K	R	St.1	St.2	St.3	St.4
I → I-II	18.4	20.6	17.4	9.3	24.2	14.9
III → III-IV	12.5	16.0	13.1	9.8	20.7	11.4

Catalyst	Ring	MCI	I _{ring}	I _{NG}	I _{NB}	FLU	BOA	BLA	PDI	HOMA
St.1	1	0.0066	0.0083	0.0315	0.0294	0.0732	0.0055	0.0097	—	-1.1220
	2	0.0024	0.0020	0.0244	0.0233	0.0272	0.0953	0.0263	0.0164	0.4440
	3	0.0524	0.0358	0.0394	0.0390	0.0036	0.0477	0.0100	0.0864	0.8477
St.2	1	0.0054	0.0065	0.0300	0.0282	0.0794	0.0050	0.0038	—	-1.1220
	2	0.0165	0.0124	0.0330	0.0321	0.0256	0.0477	0.0046	0.0594	0.4440
	3	0.0208	0.0166	0.0346	0.0334	0.0258	0.1991	0.0250	0.0568	0.8477
St.3	1	0.0069	0.0090	0.0321	0.0296	0.0558	0.0097	0.0086	—	-1.1802
	2	0.0024	0.0020	0.0243	0.0233	0.0285	0.0890	0.0253	0.0169	0.4325
	3	0.0523	0.0358	0.0393	0.0390	0.0036	0.0481	0.0097	0.0864	0.8534
St.4	1	0.0056	0.0072	0.0307	0.0284	0.0638	0.0205	0.0008	—	-1.5009
	2	0.0166	0.0125	0.0330	0.0322	0.0272	0.0551	0.0046	0.0595	0.2862
	3	0.0207	0.0165	0.0346	0.0334	0.0261	0.2006	0.0243	0.0567	0.3614



RESULTS AND DISCUSSION

[AROMATICITY]

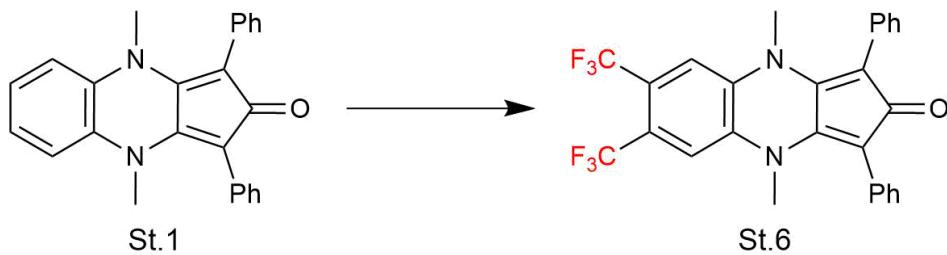
Gibbs energy for studied catalysts (kcal/mol).

	K	R	St.1	St.2	St.3	St.4	St.5	St.6	St.7	St.8	St.9	St.10
I → I-II	18.4	20.6	17.4	9.3	24.2	14.9	18.8	17.8	10.2	15.5	17.2	10.2
III → III-IV	12.5	16.0	13.1	9.8	20.7	11.4	16.2	15.0	11.0	13.9	15.6	10.3

Catalyst	Ring	MCI	I _{ring}	I _{NG}	I _{NB}	FLU	BOA	BLA	PDI	HOMA
St.1	1	0.0066	0.0083	0.0315	0.0294	0.0732	0.0055	0.0097	—	-1.1220
	2	0.0024	0.0020	0.0244	0.0233	0.0272	0.0953	0.0263	0.0164	0.4440
	3	0.0524	0.0358	0.0394	0.0390	0.0036	0.0477	0.0100	0.0864	0.8477
St.9	1	0.0066	0.0082	0.0315	0.0293	0.0735	0.0599	0.0076	—	-1.1087
	2	0.0024	0.0020	0.0244	0.0234	0.0272	0.1003	0.0282	0.0165	0.4419
	3	0.0526	0.0360	0.0394	0.0390	0.0036	0.0465	0.0098	0.0867	0.8504
St.5	1	0.0066	0.0083	0.0315	0.0293	0.0741	0.0093	0.0089	—	-1.0785
	2	0.0024	0.0021	0.0245	0.0234	0.0264	0.0923	0.0275	0.0138	0.4380
	3	0.0521	0.0357	0.0393	0.0389	0.0036	0.0460	0.0098	0.0860	0.8413

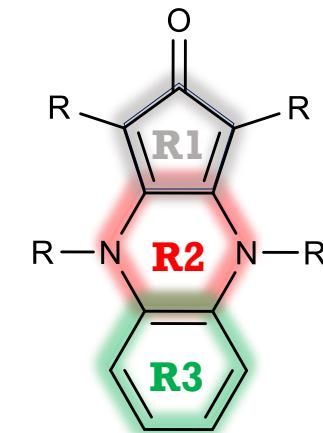
RESULTS AND DISCUSSION

[AROMATICITY]



Gibbs energy for studied catalysts (kcal/mol).												
	K	R	St.1	St.2	St.3	St.4	St.5	St.6	St.7	St.8	St.9	St.10
I → I-II	18.4	20.6	17.4	9.3	24.2	14.9	18.8	17.8	10.2	15.5	17.2	10.2
III → III-IV	12.5	16.0	13.1	9.8	20.7	11.4	16.2	15.0	11.0	13.9	15.6	10.3

Catalyst	Ring	MCI	I _{ring}	I _{NG}	I _{NB}	FLU	BOA	BLA	PDI	HOMA
St.1	1	0.0066	0.0083	0.0315	0.0294	0.0732	0.0055	0.0097	–	-1.1220
	2	0.0024	0.0020	0.0244	0.0233	0.0272	0.0953	0.0263	0.0164	0.4440
	3	0.0524	0.0358	0.0394	0.0390	0.0036	0.0477	0.0100	0.0864	0.8477
St.6	1	0.0066	0.0083	0.0315	0.0293	0.0749	0.0121	0.0099	–	-1.1371
	2	0.0026	0.0022	0.0248	0.0236	0.0255	0.0588	0.0186	0.0137	0.4855
	3	0.0444	0.0310	0.0384	0.0379	0.0050	0.0332	0.0077	0.0766	0.8312



CONCLUSIONS

1. Explored the potential of modified Knölker-type iron complexes as catalysts for catalytic hydrogenation.
2. Computational analyses revealed that altering the substituents on the cyclopentadienone structure significantly reduces energy barriers, enhancing reactivity.
3. Advanced computational techniques provided a detailed understanding of the electronic and geometric properties of the catalysts.
4. Demonstrated that careful structural modifications can lead to the development of more efficient and sustainable catalysts.

Modifying catalytic sustainability: aromaticity, conceptual DFT and steric mapping

Carles Alcaide i Blaya

Supervisors:

Dr. Albert Poater Teixidor

Dra. Sílvia Simon Rabaseda

Modifying catalytic sustainability: aromaticity, conceptual DFT and steric mapping

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Correlacions del índexs d'aromaticitat pels intermedis I i III (St.1 a St.6)

	<i>MCI</i>	<i>Iring</i>	<i>I_NG</i>	<i>I_NB</i>	<i>FLU</i>	<i>BOA</i>	<i>BLA</i>	<i>PDI</i>	<i>HOMA</i>
MCI	1								
Iring	0,99092	1							
<i>I_NG</i>	0,813111	0,875709	1						
<i>I_NB</i>	0,861008	0,910597	0,99423	1					
FLU	-0,719329	-0,657272	-0,441387	-0,522308	1				
BOA	0,042001	0,007665	-0,050811	-0,01131	-0,435547	1			
BLA	-0,250379	-0,315462	-0,505525	-0,464894	-0,250509	0,70784	1		
PDI	0,949827	0,961322	0,972424	0,973618	-0,730348	-0,122839	-0,626943	1	
HOMA	0,574338	0,533514	0,452668	0,515381	-0,896696	0,408549	0,311603	0,488149	1

Correlacions del índexs d'aromaticitat pels estats de transició I-II i III-IV (St.1 a St.6)

	<i>MCI</i>	<i>Iring</i>	<i>I_NG</i>	<i>I_NB</i>	<i>FLU</i>	<i>BOA</i>	<i>BLA</i>	<i>PDI</i>	<i>HOMA</i>
MCI	1								
Iring	0,986202	1							
<i>I_NG</i>	0,784385	0,865403	1						
<i>I_NB</i>	0,829496	0,896371	0,995162	1					
FLU	-0,732986	-0,669458	-0,471439	-0,539769	1				
BOA	0,113556	0,088357	0,057337	0,080886	-0,240826	1			
BLA	-0,099673	-0,171047	-0,380705	-0,352452	-0,10996	0,668696	1		
PDI	0,952797	0,963255	0,96971	0,968167	-0,734278	0,069282	-0,432981	1	
HOMA	0,556871	0,516436	0,47015	0,521191	-0,891266	0,222036	0,106725	0,494006	1

Índex d'aromaticitat pels estats de transició I-II i III-IV

Catalyst	Ring	MCI	I _{ring}	I _{NG}	I _{NB}	FLU	BOA	BLA	PDI	HOMA
K I-II	1	0,009747	0,011851	0,033874	0,03171	0,042374	0,02546	0,013623	—	-0,942953
	2	0,000338	0,000348	0,018174	0,016811	0,08011	0,05388	0,01389	0,011426	-3,503055
K III-IV	1	0,011739	0,013929	0,034987	0,032912	0,033566	0,02424	0,001689	—	-0,505022
	2	0,000336	0,000347	0,018172	0,016792	0,079761	0,053996	0,013483	0,011583	-3,476028
R I-II	1	0,007244	0,008892	0,031983	0,029882	0,065658	0,024784	0,004108	—	-0,909326
	2	0,000273	0,000367	0,018343	0,016225	0,04771	0,043717	0,02234	0,012746	-0,730832
R III-IV	1	0,008893	0,01061	0,033133	0,031134	0,054225	0,032758	0,004649	—	-0,542367
	2	0,000299	0,000376	0,018411	0,016469	0,047723	0,053427	0,025807	0,012679	-0,737181
Catalyst	Ring	MCI	I _{ring}	I _{NG}	I _{NB}	FLU	BOA	BLA	PDI	HOMA
St.1 I-II	1	0,007536	0,009316	0,032283	0,03012	0,064853	0,02978	0,004779	—	-0,806461
	2	0,002249	0,001868	0,024052	0,023055	0,027398	0,067395	0,017033	0,016307	0,456618
	3	0,051495	0,035315	0,039258	0,038851	0,003801	0,053582	0,011073	0,085634	0,838039
St.1 III-IV	1	0,009348	0,011157	0,033468	0,031447	0,053268	0,041494	0,008406	—	-0,419831
	2	0,002297	0,001946	0,024217	0,023137	0,026544	0,06894	0,019668	0,01374	0,492405
	3	0,051589	0,035385	0,039271	0,038863	0,003699	0,046348	0,010247	0,085513	0,832797

Índex d'aromaticitat pels estats de transició I-II i III-IV

Catalyst	Ring	MCI	I _{ring}	I _{NG}	I _{NB}	FLU	BOA	BLA	PDI	HOMA
St.2 I-II	1	0,005898	0,00698	0,030471	0,028679	0,077076	0,047335	0,012809	—	-1,392426
	2	0,016326	0,012335	0,032945	0,032081	0,025692	0,048622	0,004052	0,058865	0,382203
	3	0,020998	0,016717	0,034657	0,033456	0,025497	0,196298	0,023379	0,056902	0,398493
St.2 III-IV	1	0,006965	0,008275	0,031526	0,029649	0,064283	0,024724	0,001122	—	-0,984515
	2	0,016978	0,012752	0,033128	0,032291	0,024869	0,035412	0,001564	0,059832	0,385355
	3	0,022009	0,017317	0,034862	0,033719	0,024671	0,194025	0,023945	0,057937	0,418035

Catalyst	Ring	MCI	I _{ring}	I _{NG}	I _{NB}	FLU	BOA	BLA	PDI	HOMA
St.3 I-II	1	0,008443	0,010590	0,033120	0,030812	0,047764	0,026237	0,003400	—	-1,001857
	2	0,002105	0,001780	0,023860	0,022802	0,028223	0,049285	0,014471	0,014038	0,459270
	3	0,051162	0,035114	0,039221	0,038809	0,003755	0,047702	0,009447	0,085133	0,840830
St.3 III-IV	1	0,009921	0,012227	0,034086	0,031822	0,038790	0,040573	0,000855	—	-0,525112
	2	0,002310	0,001968	0,024264	0,023158	0,027330	0,065152	0,018512	0,013948	0,461141
	3	0,051313	0,035226	0,039242	0,038828	0,003729	0,044115	0,009051	0,085332	0,839934

Índex d'aromaticitat pels estats de transició I-II i III-IV

Catalyst	Ring	MCI	I _{ring}	I _{NG}	I _{NB}	FLU	BOA	BLA	PDI	HOMA
St.4 I-II	1	0,006293	0,007971	0,031291	0,029053	0,059421	0,034395	0,001776	–	-1,359512
	2	0,017067	0,012734	0,033121	0,032320	0,024932	0,024826	0,000839	0,059395	0,337254
	3	0,023741	0,018320	0,035190	0,034147	0,023074	0,185957	0,022433	0,059619	0,424610
St.4 III-IV	1	0,007583	0,009397	0,032338	0,030157	0,050539	0,043357	0,004181	–	-0,921155
	2	0,017162	0,012846	0,033169	0,032350	0,025704	0,038864	0,001455	0,059960	0,340818
	3	0,022267	0,017445	0,034905	0,033784	0,024517	0,193205	0,023228	0,058220	0,398764

Catalyst	Ring	MCI	I _{ring}	I _{NG}	I _{NB}	FLU	BOA	BLA	PDI	HOMA
St.5 I-II	1	0,007471	0,009245	0,032233	0,030067	0,065685	0,012375	0,001685	–	-0,777744
	2	0,002238	0,001895	0,024110	0,023036	0,026889	0,064262	0,018236	0,013438	0,472640
	3	0,051116	0,035105	0,039219	0,038803	0,003774	0,049831	0,010608	0,085092	0,830616
St.5 III-IV	1	0,009043	0,010879	0,033299	0,031238	0,054179	0,004143	0,005819	–	-0,418301
	2	0,002297	0,001943	0,024212	0,023137	0,026454	0,067917	0,019549	0,013405	0,476666
	3	0,051391	0,035271	0,039250	0,038838	0,003721	0,047114	0,010268	0,085333	0,831365

Índex d'aromaticitat pels estats de transició I-II i III-IV

Catalyst	Ring	MCI	I _{ring}	I _{NG}	I _{NB}	FLU	BOA	BLA	PDI	HOMA
St.6 I-II	1	0,007647	0,009407	0,032345	0,030208	0,065448	0,046147	0,021952	–	-0,814199
	2	0,002319	0,001993	0,024313	0,023174	0,026426	0,030672	0,009056	0,013603	0,505645
	3	0,042939	0,030058	0,038218	0,037692	0,005337	0,035370	0,008136	0,074833	0,818369
St.6 III-IV	1	0,009414	0,011215	0,033503	0,031490	0,053684	0,020758	0,011606	–	-0,437773
	2	0,002396	0,002056	0,024440	0,023300	0,025975	0,035604	0,010827	0,013845	0,525521
	3	0,043578	0,030445	0,038299	0,037785	0,005202	0,033168	0,007922	0,075586	0,820731



Regressió multilineal tenint en compte la càrrega del C del lligand, el MBO del Fe-C i l'energia del LUMO.

Resumen

qC-MBO Fe/C-LUMO

Estadísticas de la regresión

Coeficiente de correlación múl 0,94104786

Coeficiente de determinación I 0,88557108

R^2 ajustado 0,79974939

Error típico 1,93493687

Observaciones 8

ANÁLISIS DE VARIANZA

	Grados de libert	Suma de cuadrados	Promedio de los cuadrados	F	Valor crítico de F
Regresión	3	115,8994089	38,63313631	10,31873282	0,023593681
Residuos	4	14,97592271	3,743980677		
Total	7	130,8753316			

	Coeficientes	Error típico	Estadístico t	Probabilidad	Inferior 95%	Superior 95%	Inferior 95,0%	Superior 95,0%
Intercepción	-210,39314	121,5500412	-1,730917884	0,158512303	-547,8701573	127,0838769	-547,8701573	127,0838769
Variable X 1	21,1949265	77,85191835	0,272246682	0,798907723	-194,9566512	237,3465041	-194,9566512	237,3465041
Variable X 2	155,721308	60,05619599	2,592926599	0,060497049	-11,02142337	322,4640394	-11,02142337	322,4640394
Variable X 3	66,7258726	42,23688983	1,579800806	0,189302022	-50,54253344	183,9942786	-50,54253344	183,9942786