

## Supporting Information

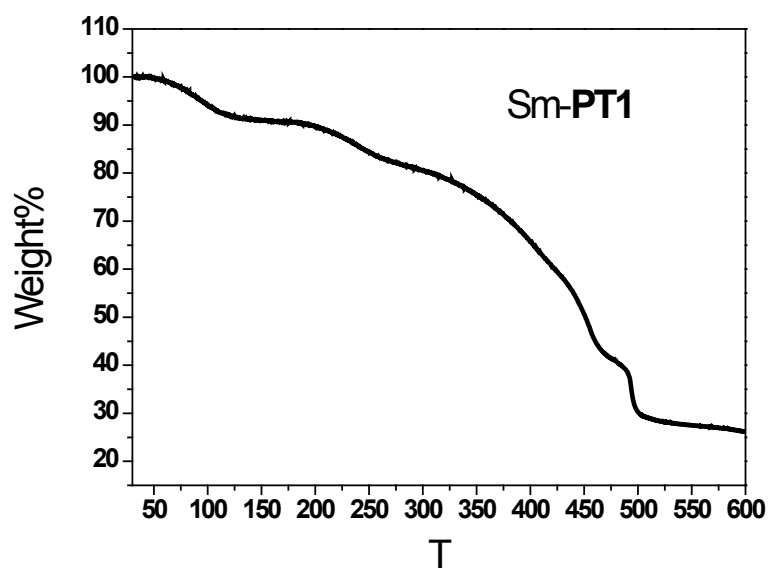
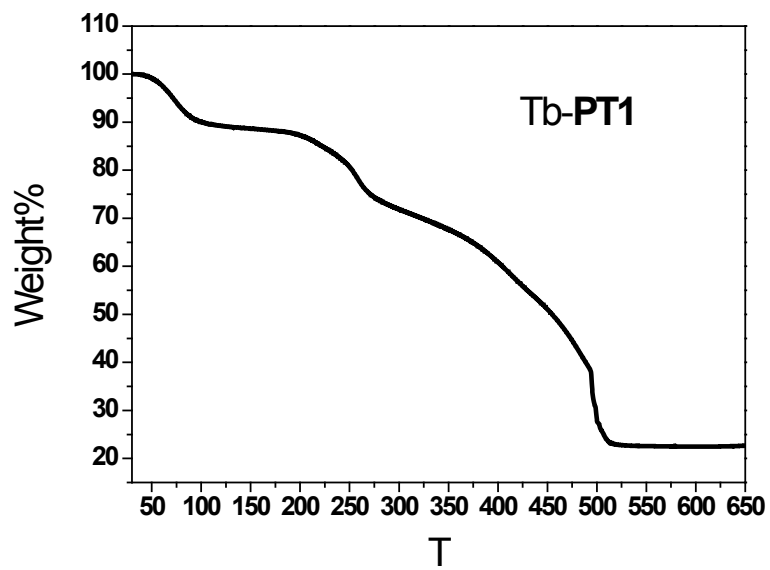
### Catalytic Performance of Lanthanide Molecular Solids Containing Well-modified Metal-organic Octahedra

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#### Contents:

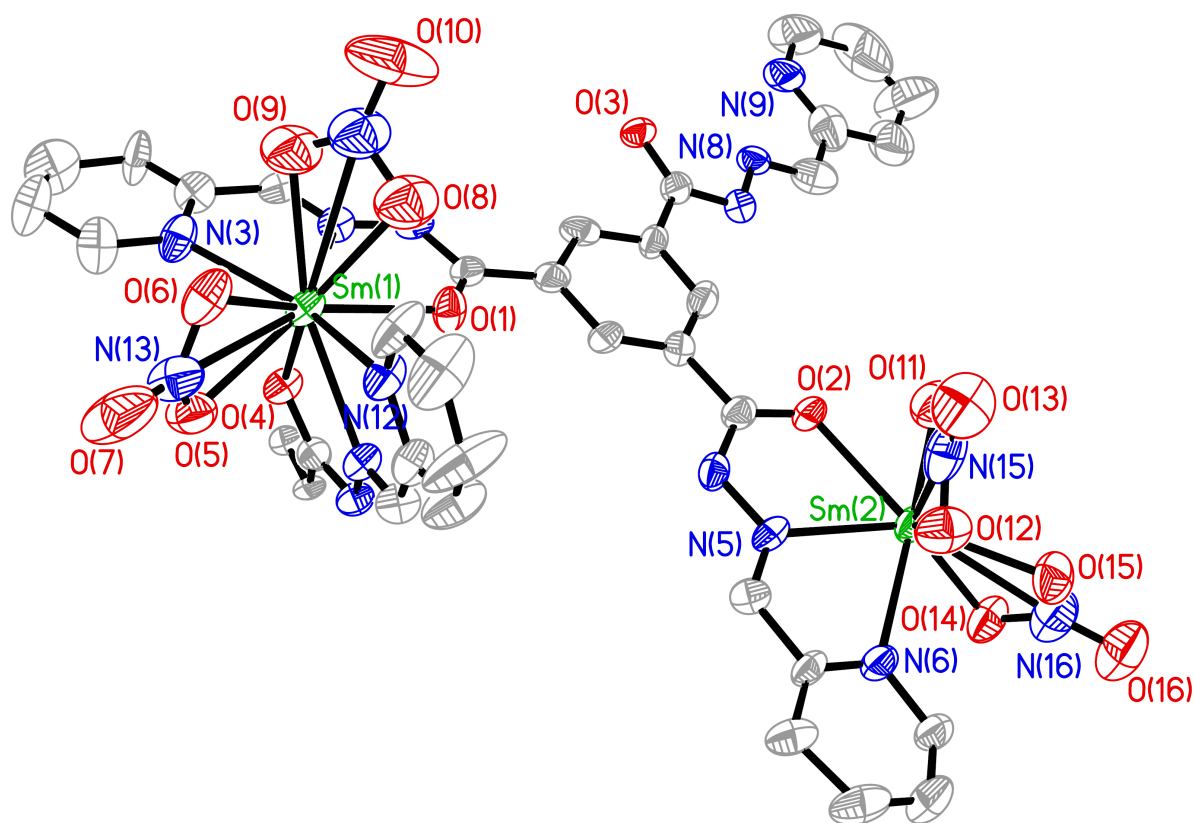
- 1 Thermogravimetric analysis (TGA) curve of the compound Tb-PT1 and Sm-PT1.
- 2 Crystal structure of Sm-PT1
3. Studying of cyanosilylation reactions catalyzed by Sm-PT1 and Tb-PT1
4. Studying of Aldol reactions catalyzed by Sm-PT1 and Tb-PT1

1 . **Figure S1** Thermogravimetric analysis (TGA) curve of the crystal Tb-PT1 and Sm-PT1.

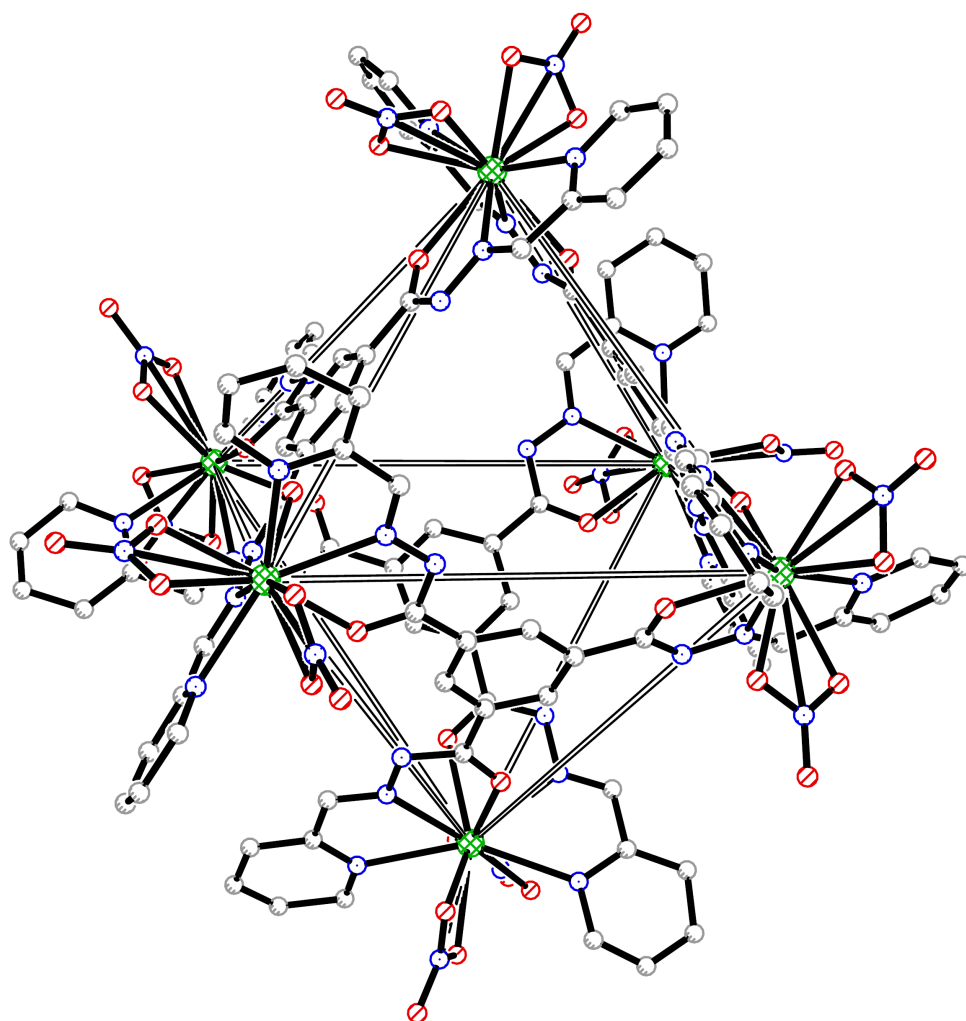


## 2 Crystal structure of Sm-PT1

**2.1 Figure S2** An ORTEP plot of the asymmetric unit in Sm-PT1, showing 30% probability displacement ellipsoids of non-hydrogen atoms. Hydrogen atoms, solvent molecule and the disordered part are omitted for clarity. Selective bond distances (Å): Sm(1)–O(6) 2.448(8), Sm(1)–O(1) 2.454(7), Sm(1)–O(4) 2.475(7), Sm(1)–O(5) 2.483(9), Sm(1)–N(2) 2.491(7), Sm(1)–O(8) 2.499(12), Sm(1)–O(9) 2.535(10), Sm(1)–N(11) 2.588(8), Sm(1)–N(12) 2.589(8), Sm(1)–N(3) 2.604(8), Sm(1)–N(13) 2.863(11), Sm(1)–N(14) 2.987(14), Sm(2)–O(14) 2.465(8), Sm(2)–O(15) 2.466(8), Sm(2)–O(3A) 2.482(6), Sm(2)–O(2) 2.495(6), Sm(2)–N(8A) 2.516(8), Sm(2)–O(12) 2.532(9), Sm(2)–O(11) 2.546(10), Sm(2)–N(5) 2.562(8), Sm(2)–N(6) 2.581(8), Sm(2)–N(9<sup>a</sup>), Sm(2)–N(16) 2.851(13), Sm(2)–N(15) 2.902(13). Symmetry Code: A 1-y, x-y, z.

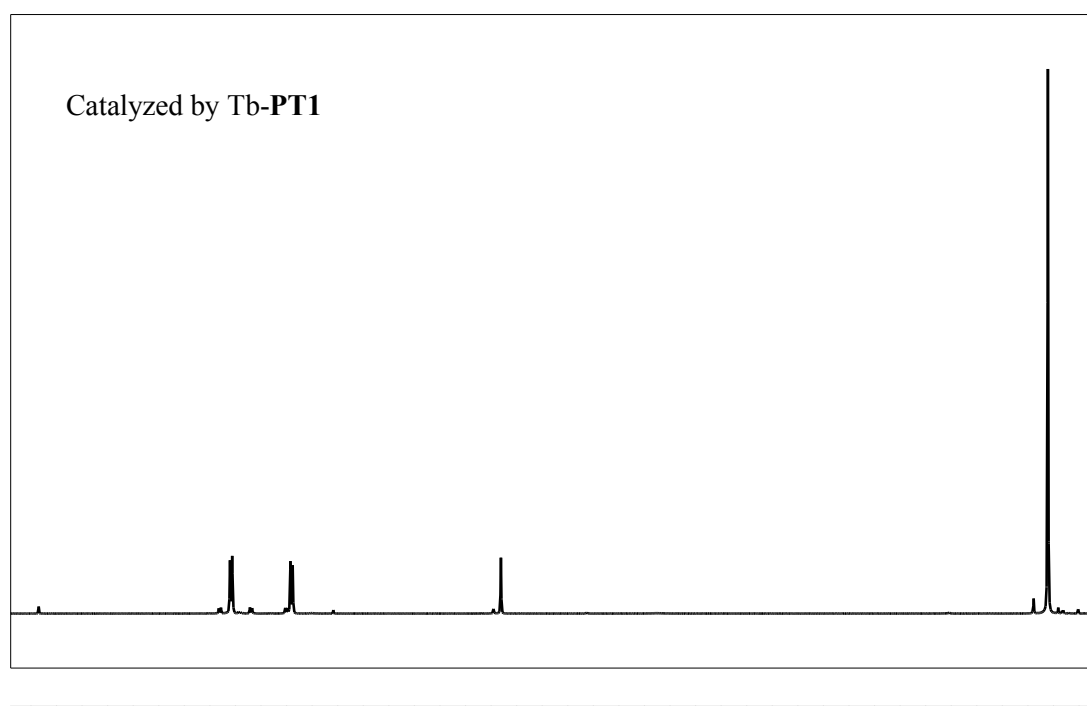
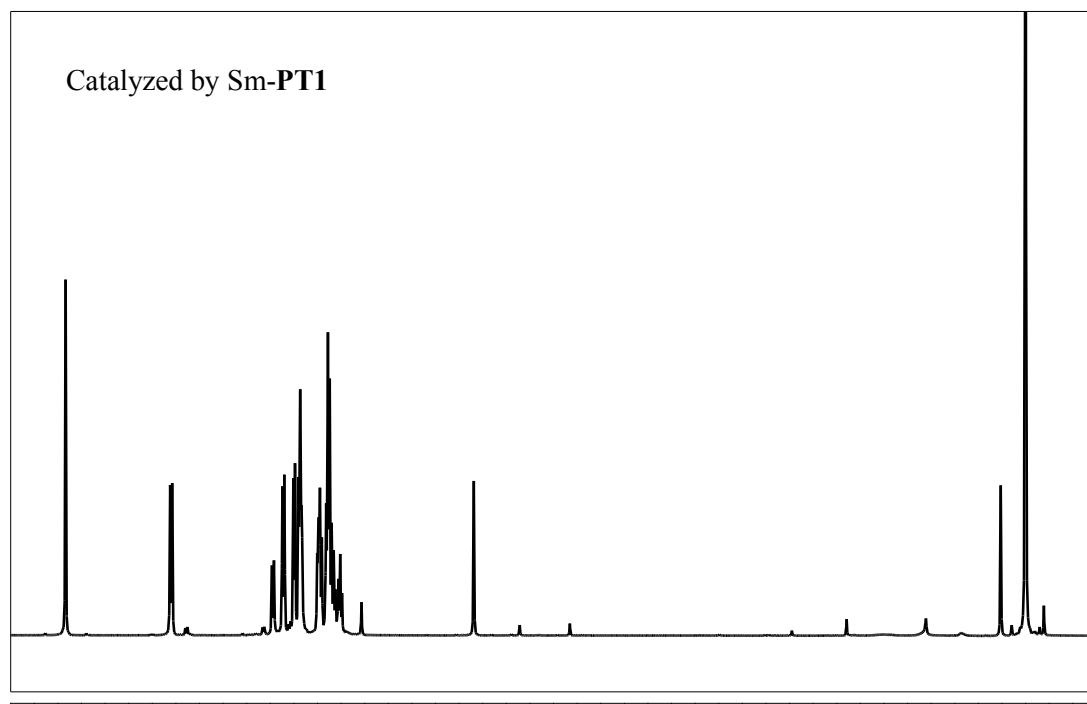


2.2 **Figure S3** Molecular structure of the octahedron in Sm-PT1, hydrogen atoms were omitted for clarity.

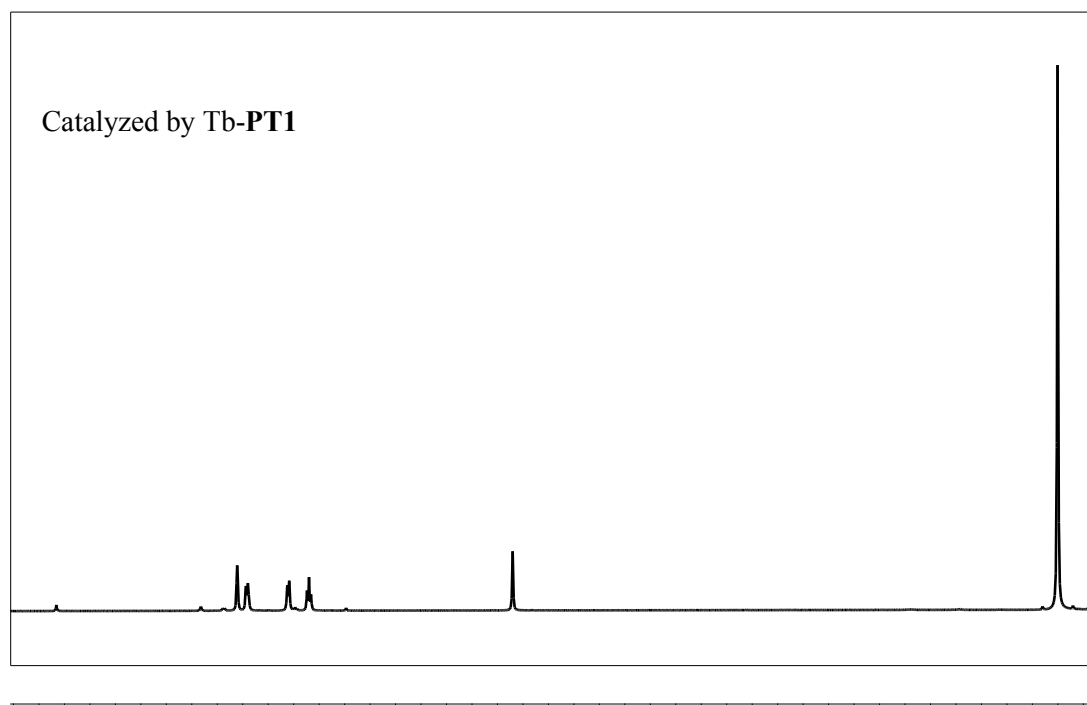
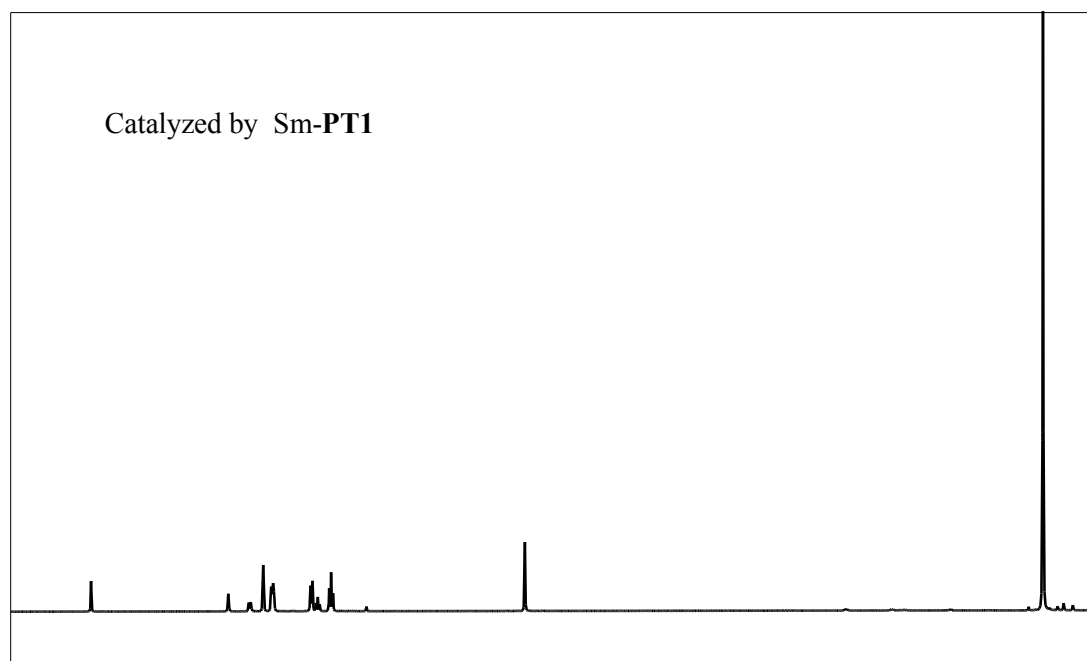


### 3 Studying of cyanosilylation reactions catalyzed by Sm-PT1 and Tb-PT1

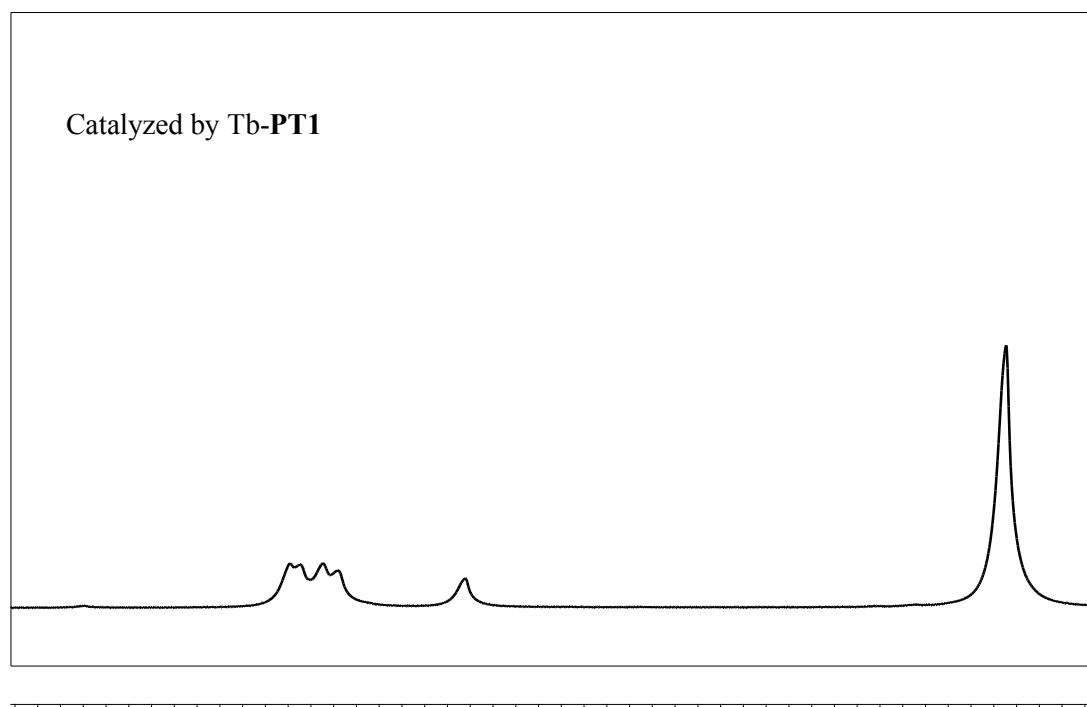
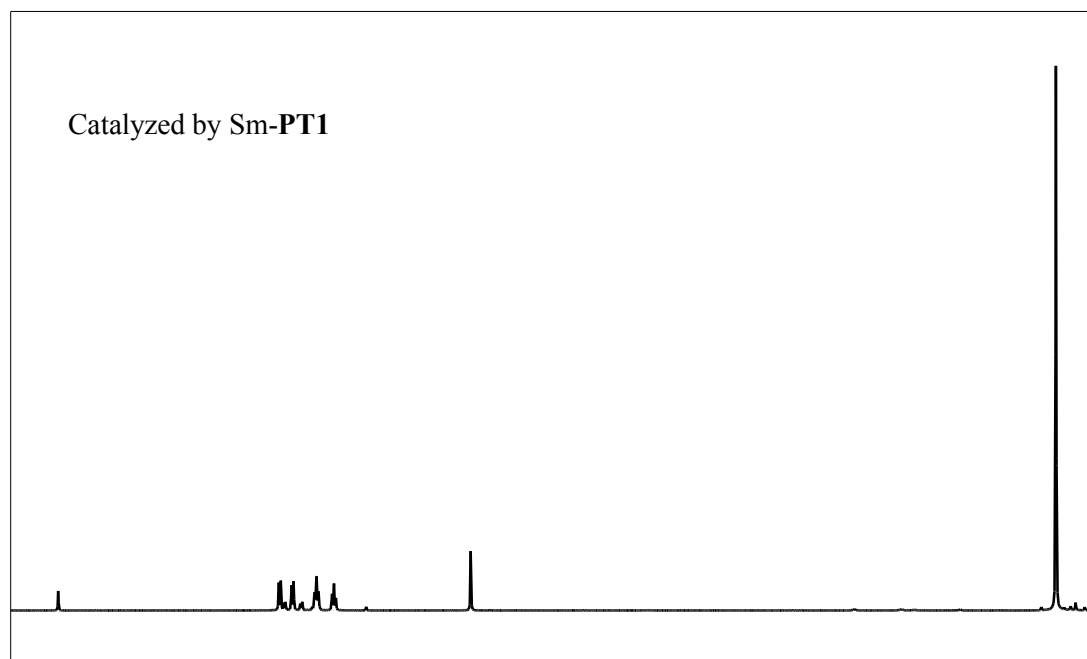
#### 3.1 Figure S3 The crude product of (4-Nitrophenyl)-2-(trimethylsilyloxy) acetonitrile (entry 1)



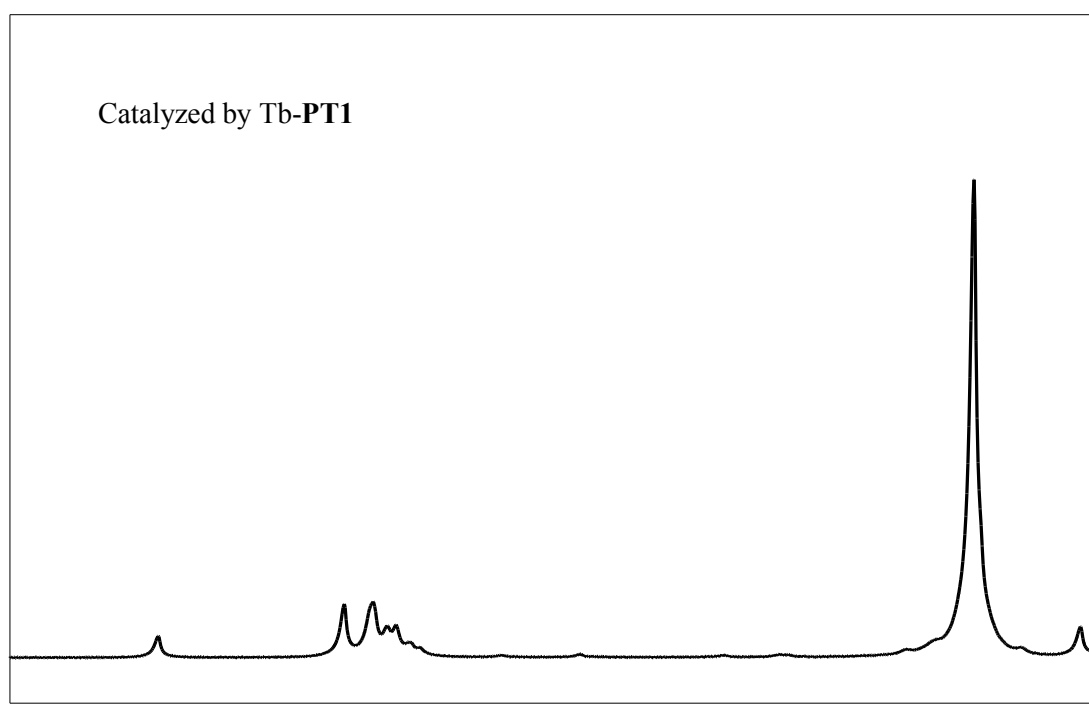
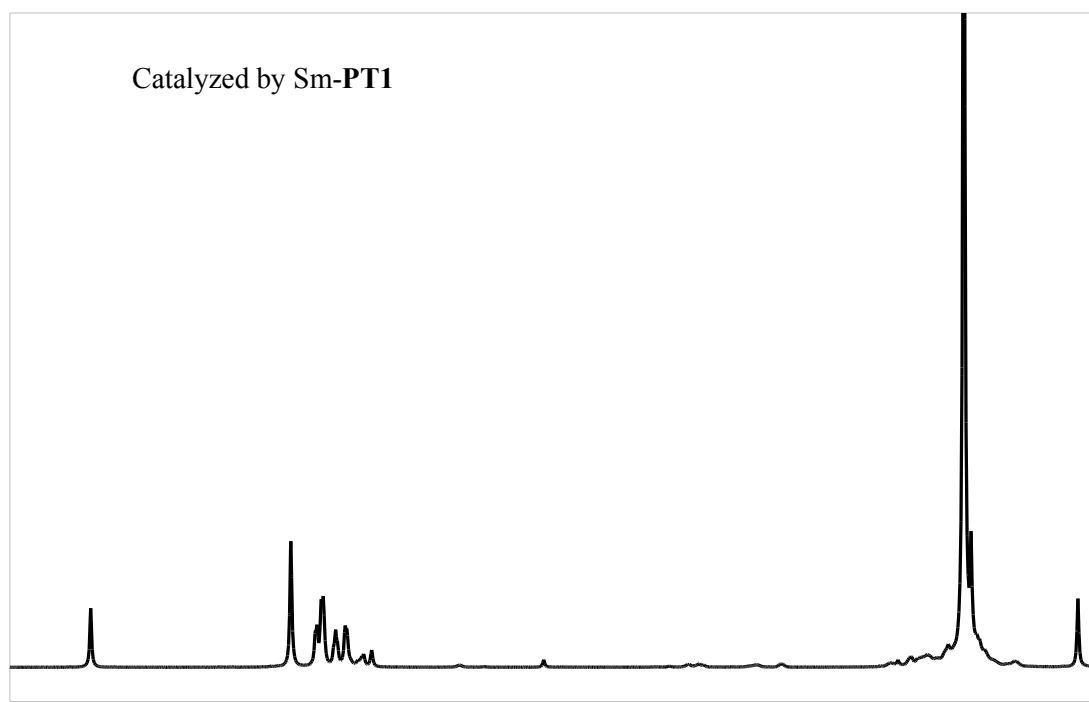
**3.2 Figure S4** The crude product of (3-Nitrophenyl)-2-(trimethylsilyloxy) acetonitrile (entry 2)



**3.3 Figure S5** The crude product of (2-Nitrophenyl)-2-(trimethylsilyloxy) acetonitrile (entry 3)



**3.4 Figure S6** The crude product of (3-phenylene-3, 5-di-tert-butylbenzoyl-2-(trimethylsilyloxy) acetonitrile (entry 4)



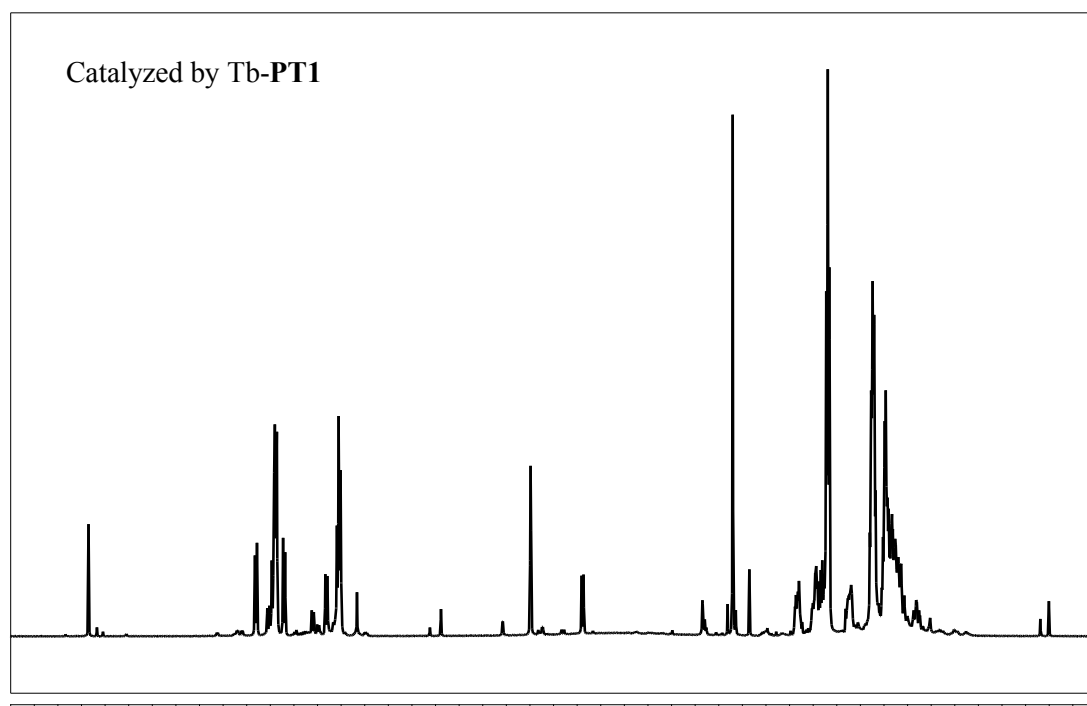
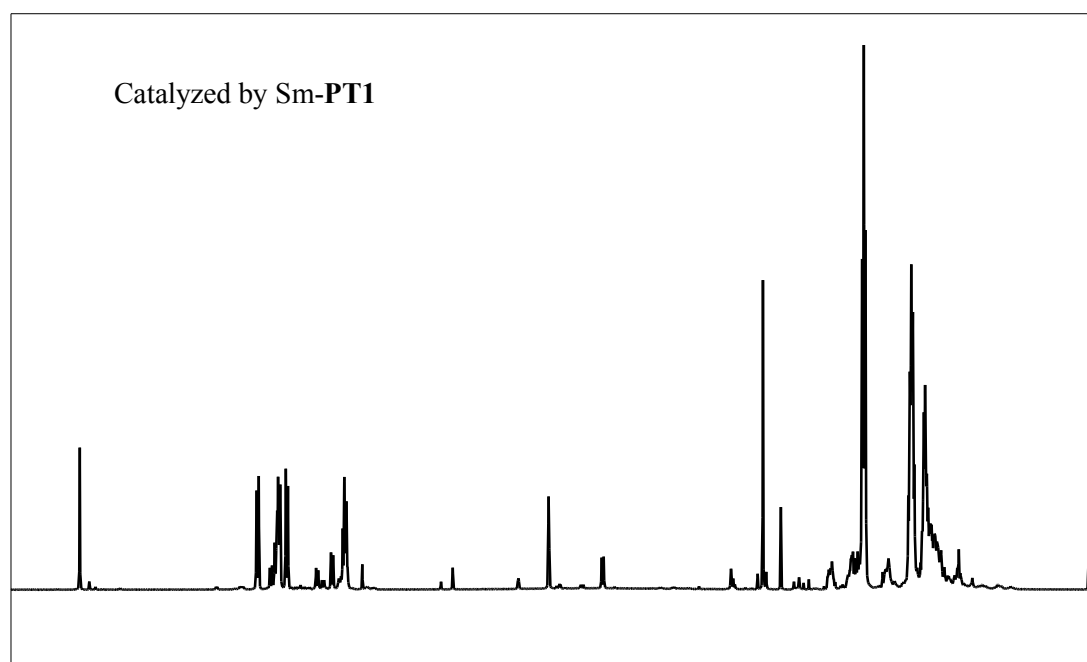


**3.5 Table S1** Study on Recycling of Tb-PT1 and Sm-PT1 for entry 1.

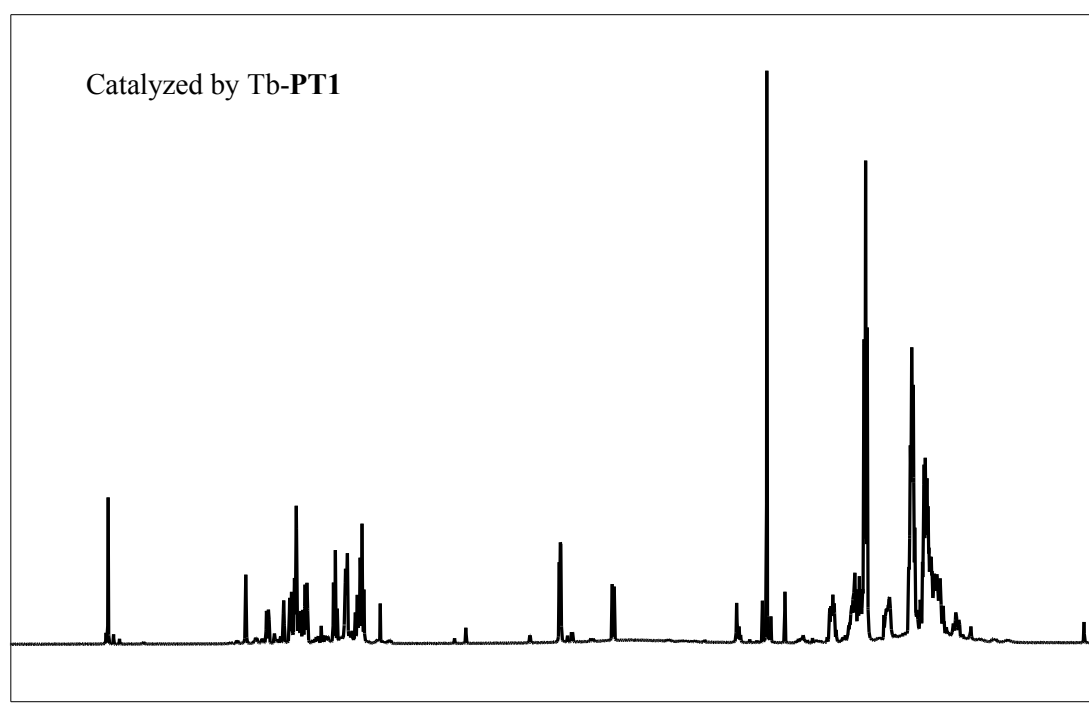
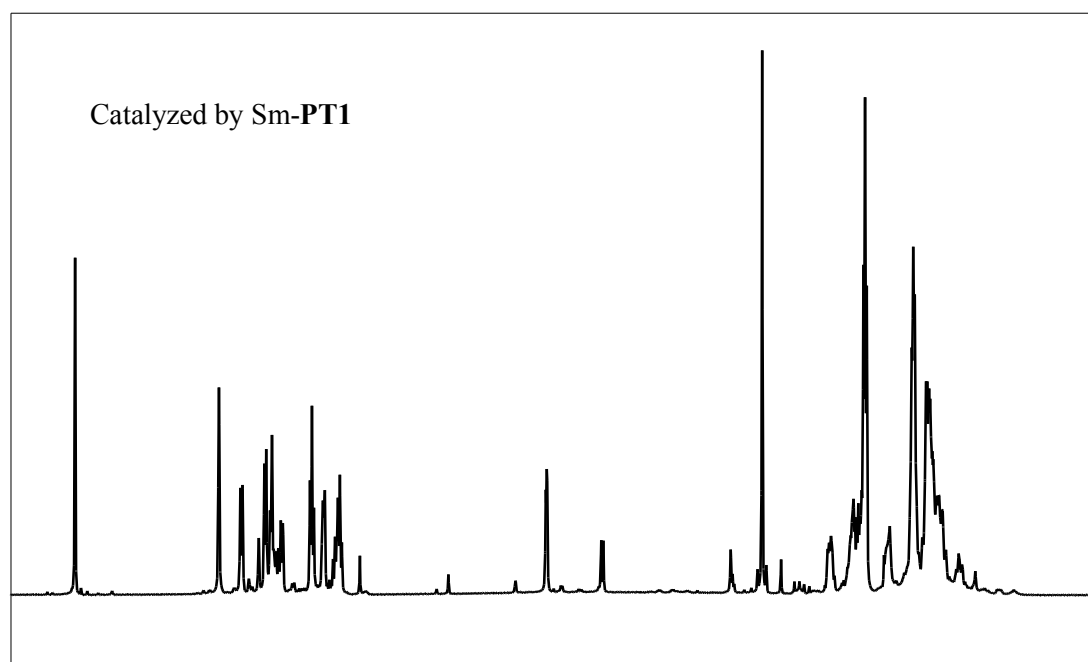
	Tb-PT1 Con.(%)	Sm-PT1 Con.(%)
Freshly	90.5	79.3
Recycle once	90.2	78.3
Recycle twice	89.0	77.6

#### 4. Studying of Aldol reactions catalyzed by Sm-PT1 and Tb-PT1

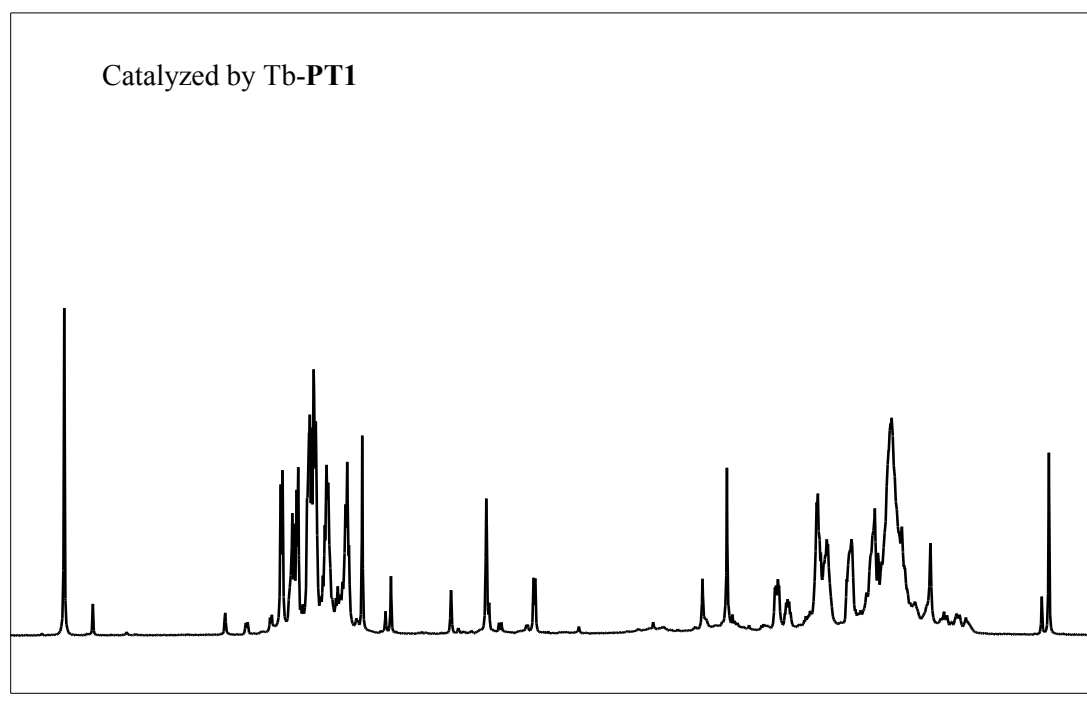
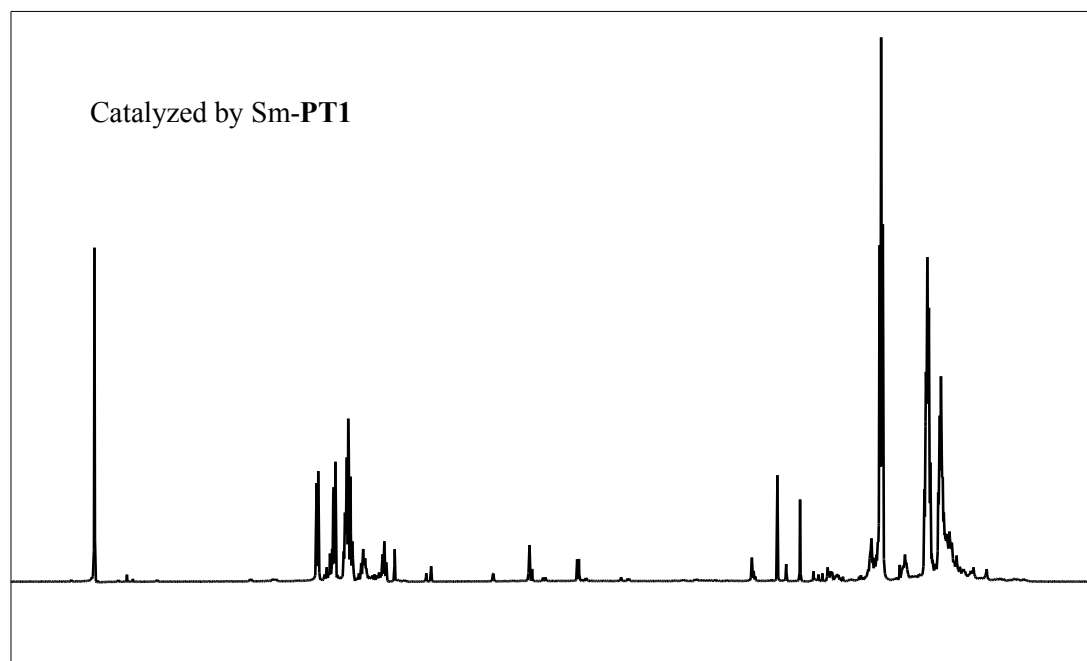
##### 4.1 Figure S7 The crude product of 2-(Hydroxy-(4-nitrophenyl)methyl)cyclohexan-1-one (entry 5)



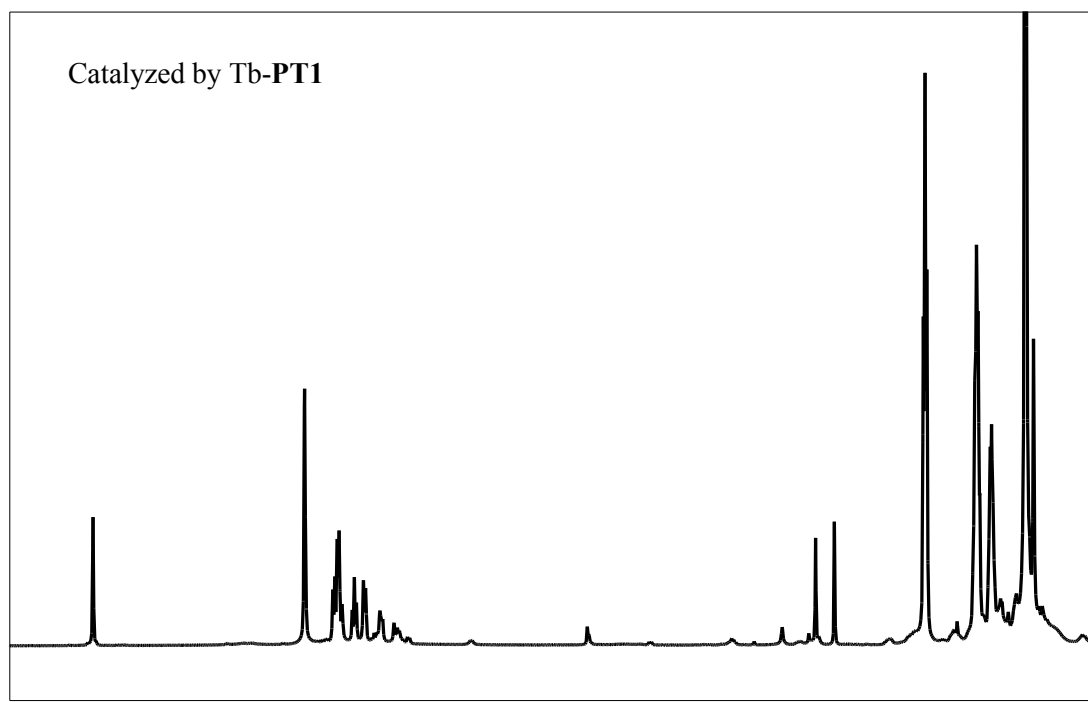
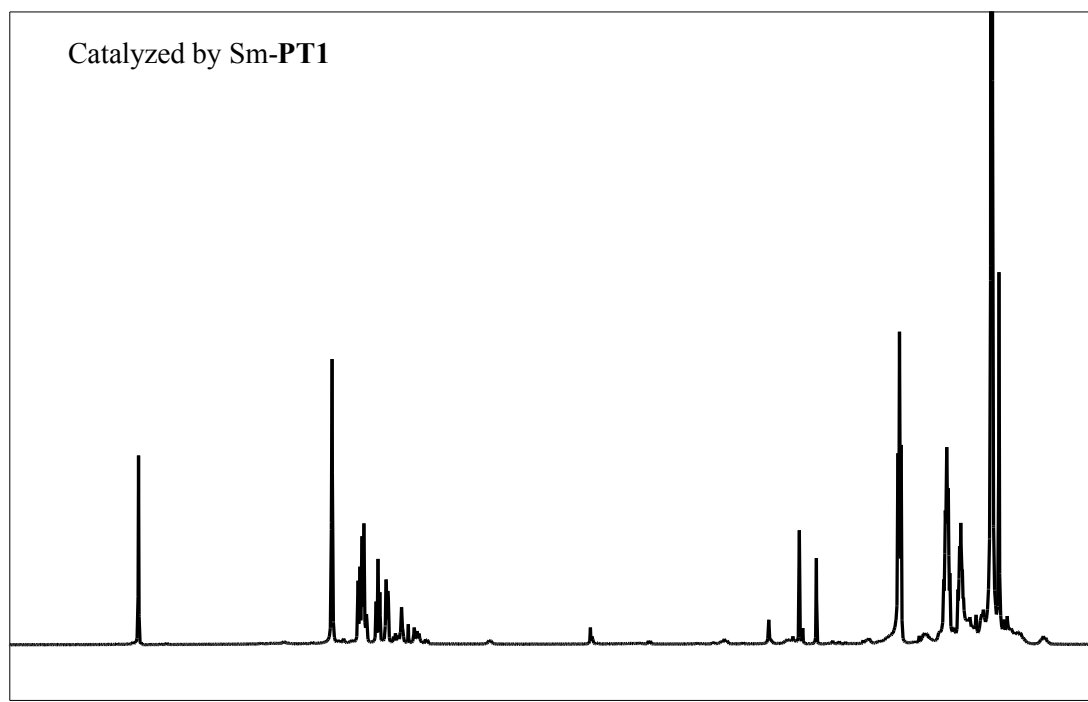
**4.2 Figure S8** The crude product of 2-(Hydroxy-(3-nitrophenyl)methyl)cyclohexan-1-one (entry 6)



**4.3 Figure S9** The crude product of 2-(Hydroxy-(2-nitrophenyl)methyl)cyclohexan-1-one (entry 7)



**4.4 Figure S10** The product of 2-(Hydroxy-(3-phenylene-(3, 5-di-tert-butylbenzoyl))methyl) cyclohexan-1-one (entry 8).



#### 4.5 Table S2 Study on Recycling of Tb-PT1 for entry 5

	Tb-PT1		Sm-PT1	
	Con.%	Dr(s/a)	Con.%	Dr(s/a)
freshly	80.5	2.0:1	64.9	2.1:1
Recycle once	80.2	2.0:1	63.1	2.1:1
Recycle twice	78.5	2.0:1	62.3	2.1:1