MATERIAL SUPLEMENTAR

Lewis acid sites of Mg^{2+}-modified polystyrene sulfonic acid resin catalysys for synthesis of dibutyl succinate

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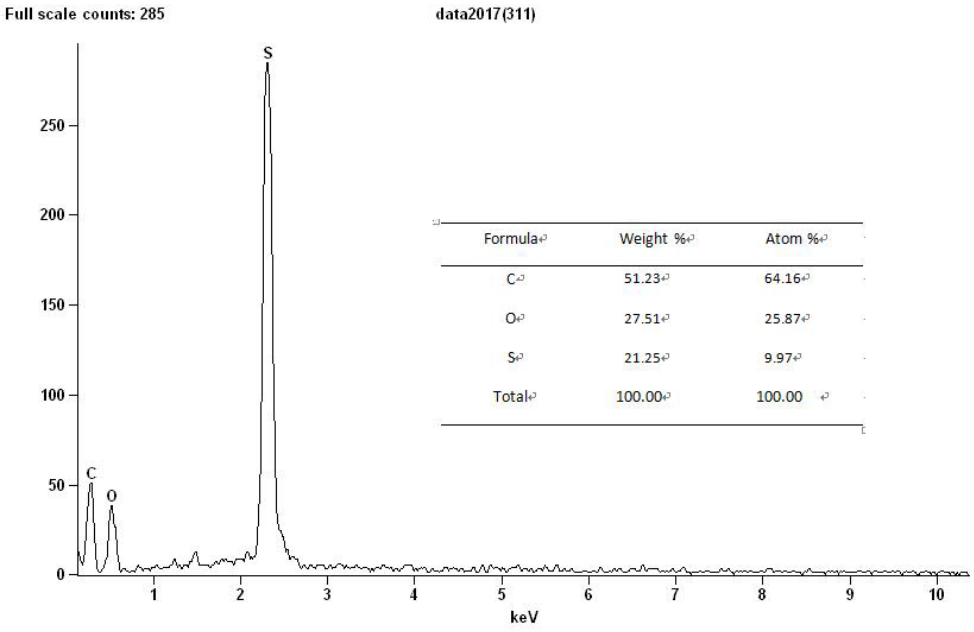
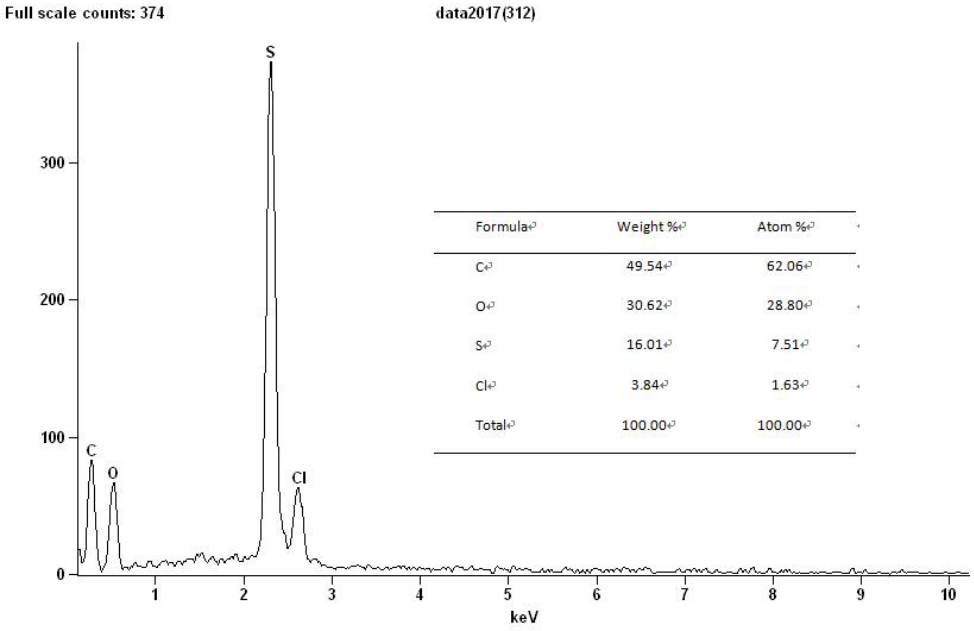
The D002, Cl-D002 and Mg-Cl-D002 were characterized by EDS to determine the elemental composition (Figure 1S). In the EDS spectrum, Mg, and Cl peaks were observed.

a)



Formula	Weight %	Atom %
C	51.23	64.16
O	27.51	25.87
S	21.25	9.97
Total	100.00	100.00

b)



Formula	Weight %	Atom %
C	49.54	62.06
O	30.62	28.80
S	16.01	7.51
Cl	3.84	1.63
Total	100.00	100.00

c)

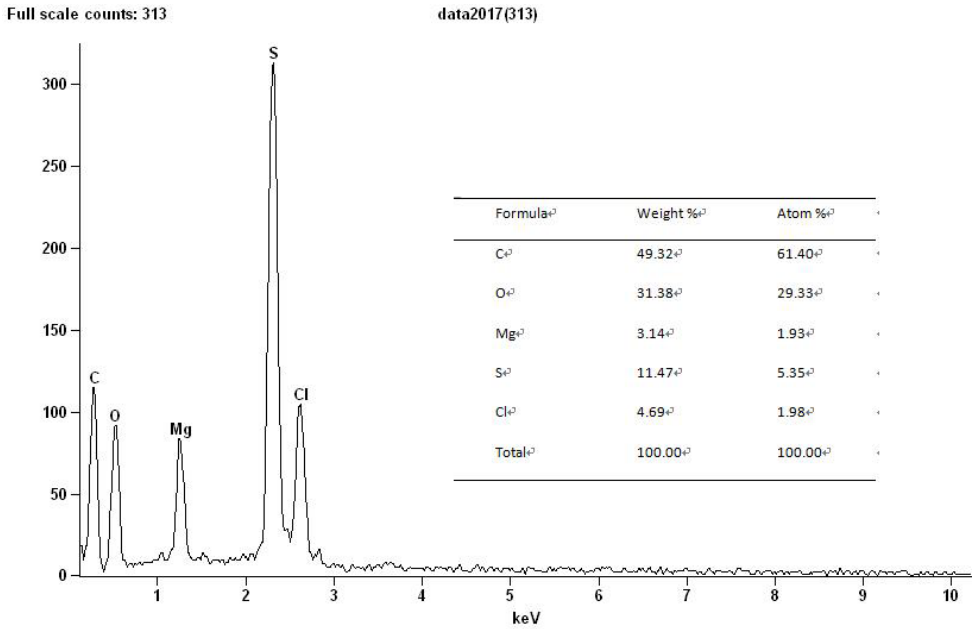
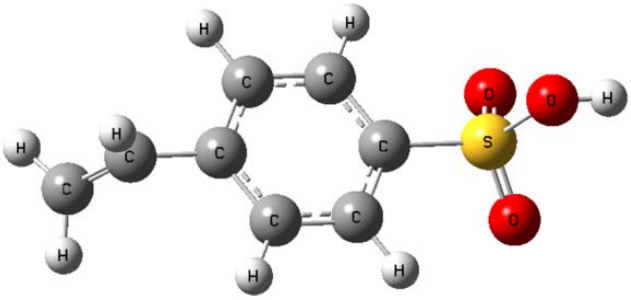


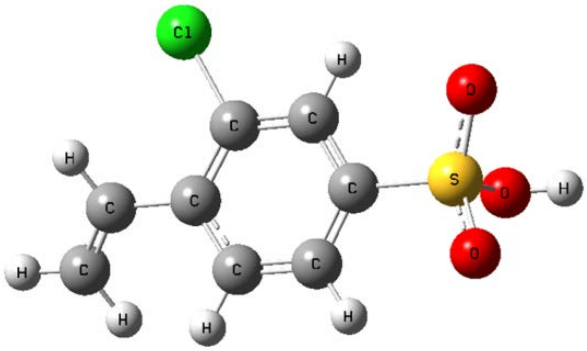
Figure 1S. a) *EDS image of the D002; b) EDS image of the Cl-D002; c) EDS image of the Mg-Cl-D002*

The optimum monomer structures (Figure 2S) of D002, Cl-D002 and $MgSO_4$-Cl-D002 have been studied using density functional theory methods at the B3LYP/6-311G(d,p) computational level (Table 1S), which agreein general with the structure reported in literature.[1,2] The total energy of the Cl-D002 and $MgSO_4$-Cl-D002 were lower than observed for the D002, so the optimum monomer structuresof Cl-D002 and $MgSO_4$-Cl-D002 may exist.[3]

a)



b)



c)

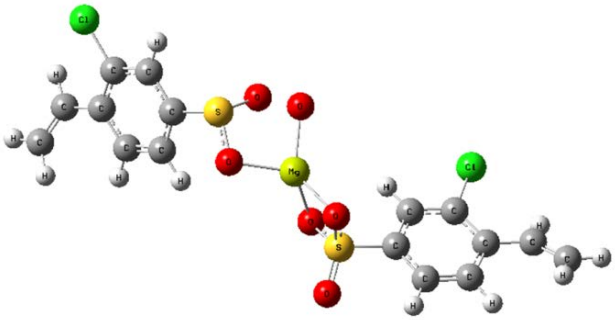


Figure 2S. *The optimum structure of: a) D002; b) Cl-D002; c) D002Mg-Cl-D002*

Table 1S. The total energies of resins

B3LYP/6-311G(d,p)	Total energies(a.u.)
D002	-933.61023
Cl-D002	-1393.22736
Mg-Cl-D002	-2985.43249

REFERENCES

1. Wang, B. H.; Dong, J. S.; Chen, S.; Wang, L. L.; Zhu, J.; *Chin. Chem. Lett.* **2014**, *25*, 1423.

2. Lang, X. W.; Jia, W. Z.;Wang, Y. A.; Zhu, Z. R.; *Catal. Commun.* **2015**, *70*, 58.

3. Arno, M.; Domingo, L. R.; *Theor. Chem. Acc.* **2002**, *108*, 232.