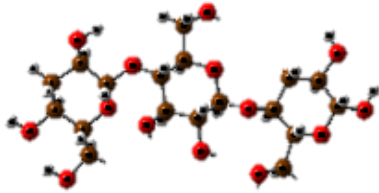
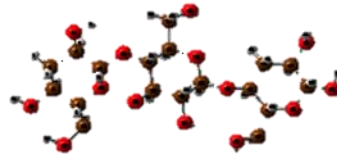




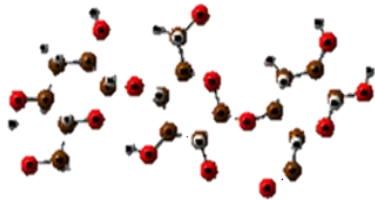
شکل S1. پیکر بندی های مختلف بهینه سازی شده از سل تری اوز



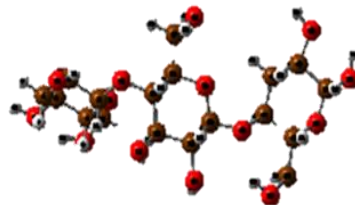
Cel-1



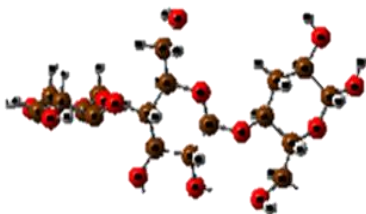
Cel-2



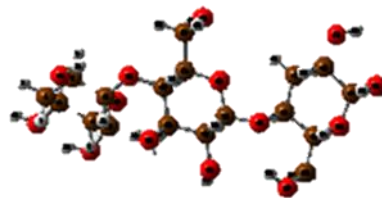
Cel-3



Cel-4

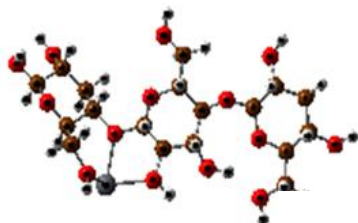


Cel-5

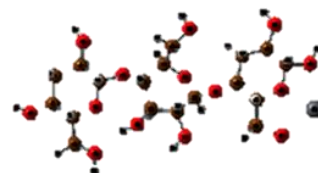


Cel-6

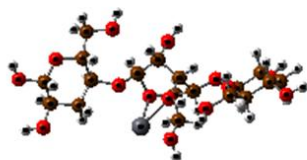
شکل S2. شکل هندسی و پیکربندی های بهینه شده و اختلاف انرژی آنها به پایدار ترین پیکربندی



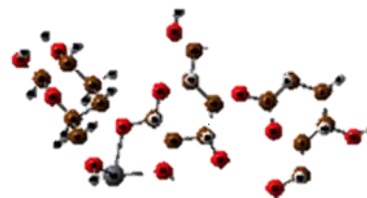
cel-pb1=0.0464



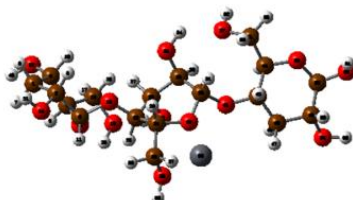
cel-pb2=0.1227



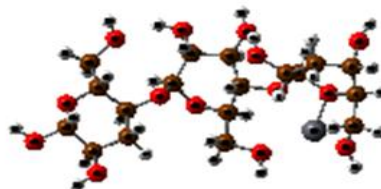
cel-Pb3= 0.1214



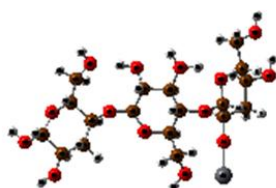
cel-Pb4= 0.0297



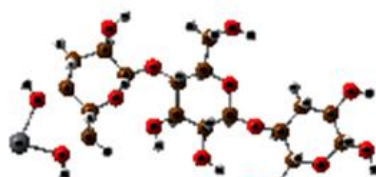
cel-Pb5=0



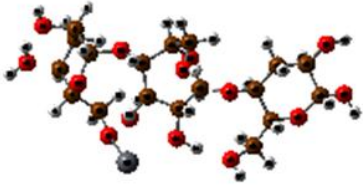
cel-Pb6=0.0970



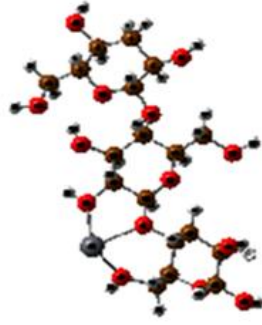
cel-Pb7= 0.0102



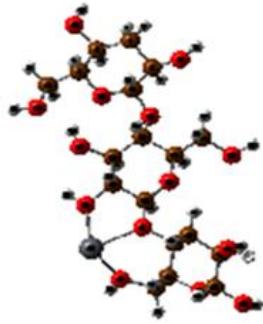
cel-Pb8= 0.0463



cel-Pb9=0.0970



cel-Pb10= 0.0110



cel-Pb11=0.0029