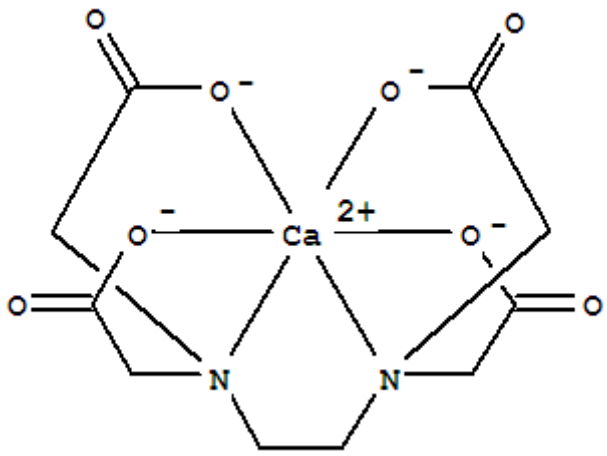
KIM309-01,02 KUANTUM KİMYASI

UYGULAMA ÖDEVİ



$(Ca^{2+}$-EDTA$)^{2-}$ Kompleksi

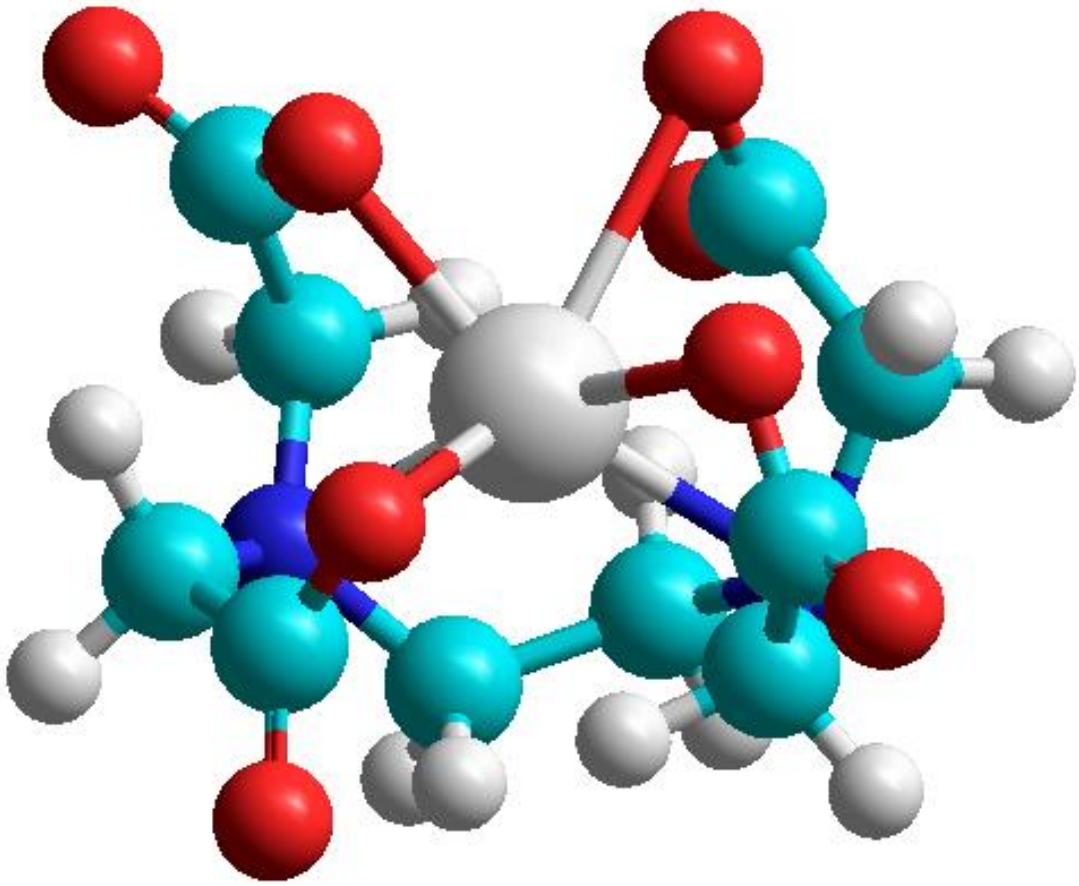
Adı-Soyadı: Kuantum Kimyası

No: 12345678

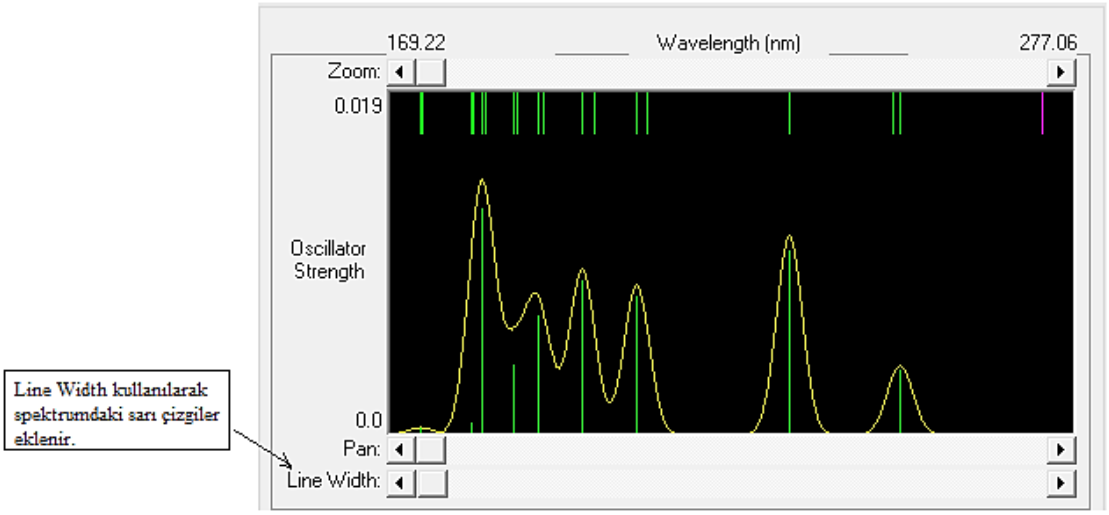
Şube: 01

Optimizasyona başlamadan önce kompleksin yükü ve spin multiplicy belirlenir molekül çizilir ve Moleküler Mekanik sonra Semi Empirical/PM3 seviyesinde optimize edilir. Optimizasyon sonrasında kompleksin UV ve IR spektrumları oluşturulur.

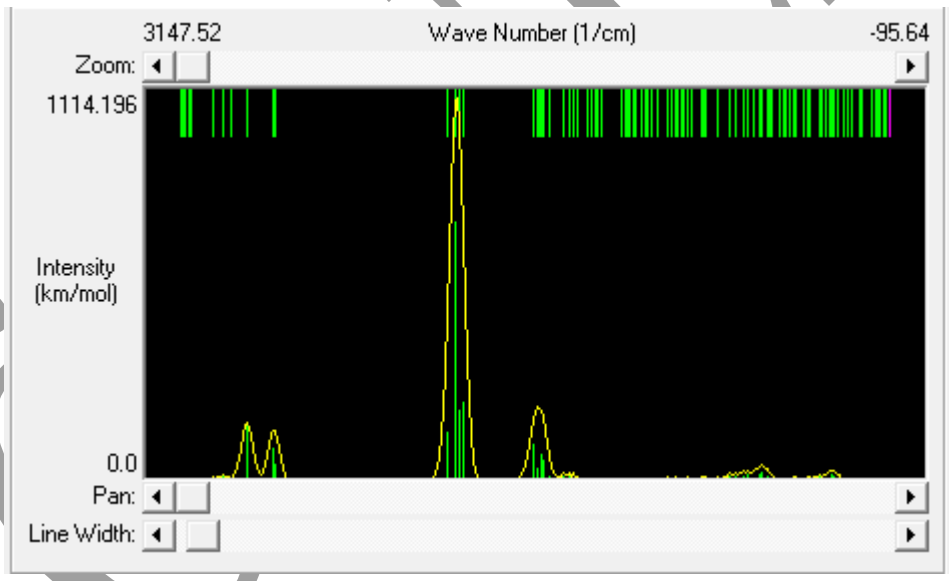
Molekülün 3D Yapısı:



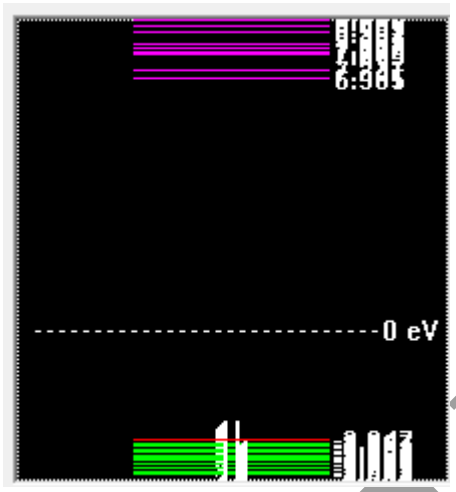
Kompleksin UV-Görünür Bölge Spektrumu

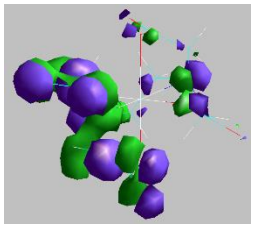
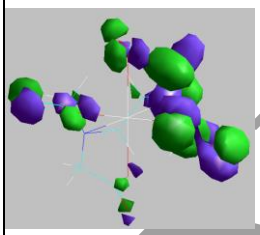
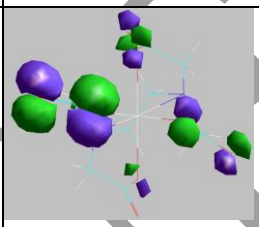
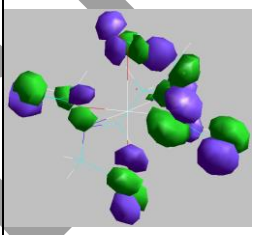
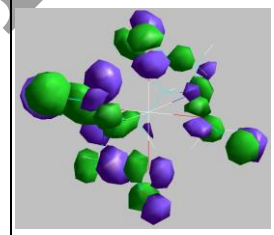
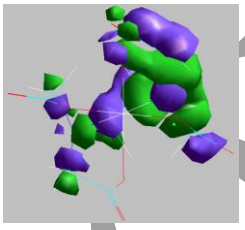
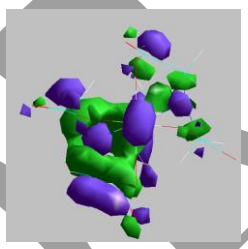
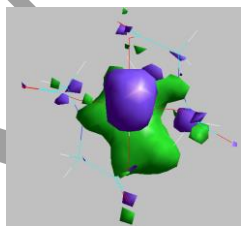
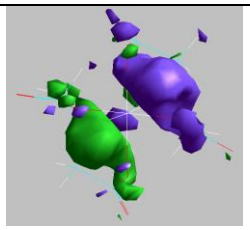
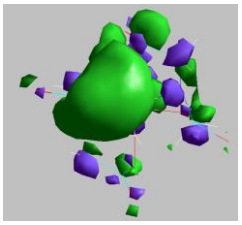


Kompleksin IR Spektrumu:



Kompleksin Moleküler Enerji Diyagramı:

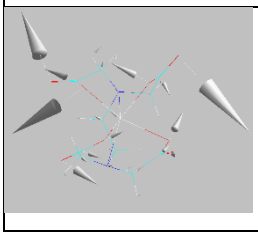
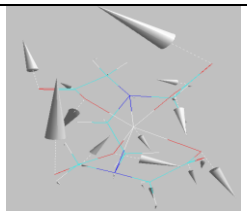
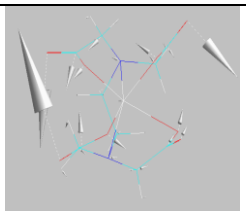
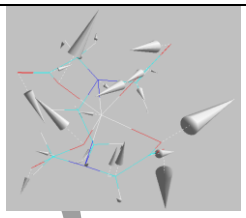
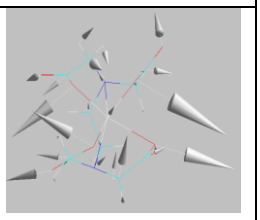


HOMO orbitali	HOMO -1 orbitali	HOMO -2 orbitali	HOMO -3 orbitali	HOMO -4 orbitali
				
LUMO orbitali	**LUMO+1 orbitali**	**LUMO+2 orbitali**	**LUMO+3 orbitali**	**LUMO+4 orbitali**
				

Elektronik Geçişler:

Geçiş	Oscillator Strength	Geçiş Dalgaboyu, nm
HOMO→LUMO	0.0000	272.2
1→3	0.0037	249.7
1→4	0.0000	248.6
1→5	0.0104	232.3
1→6	0.0000	209.9

IR Spektrumundan 5 Normal Mod ve Frekansları:

1.Normal Mod Frekans: 51.78	2.Normal Mod Frekans: 66.93	3.Normal Mod Frekans: 71.91	4.Normal Mod Frekans: 90.28	5.Normla Mod Frekans: 102.06
				

Karşılaştırma:

Literatürden araştırılarak deneysel λ_{max} değeriyle hesaplanan değer karşılaştırılarak yorumlanır.