

2.NODIR VA NOYOB METALLAR KOMPLEKS BIRIKMALARI KOMPLEKS BIRIKMALARNING 3D AUGMENTAL MODELLARNI OPTIMIZATSIYALASH USULLARI

Suyunova Sarvinoz Normamat qizi,

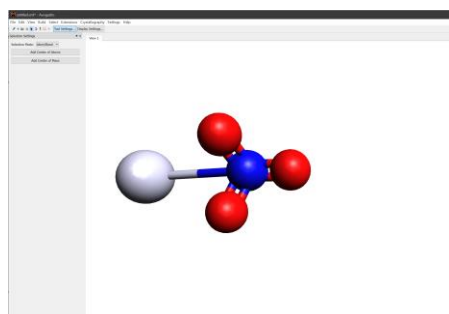
sarvinozsuyunova@gmail.com

Raximov Toxir Xakimovich,

tohir@mail.ru

Mirzo Ulug'bek nomidagi O'zbekiston Milliy Universiteti

Hech kimga sir emaski, koordinatsion birikmalar kimyosi sohasida tadqiqotchilar ham, talabalar ham komplekslarning ancha murakkab molekulalarining geometriyasi bilan bog'liq ma'lum qiyinchiliklarga duch kelishadi. Ushbu muammoni bartaraf etishning eng istiqbolli usullaridan biri bu kengaytirilgan haqiqat usulidir yani Augmental reallik. Umumiy mavjudligi va eng yuqori axborot



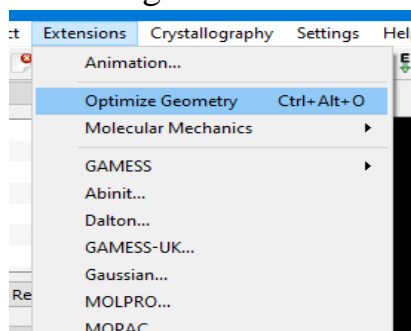
rasm № 1 AgNO₃ ning fazoviy 3D modeli AVOGADRO dasturida

modellarini yaratishimiz hamda

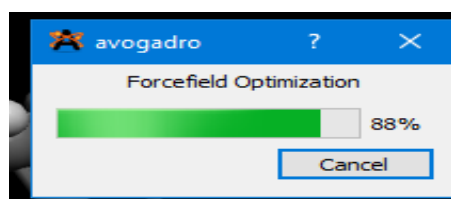
ularning modellarini optimizatsiyaga uchratishimiz zarur bo'ladi. Optimizatsiyaga

mazmuni tufayli u butun dunyoda tobora ommalashib bormoqda.

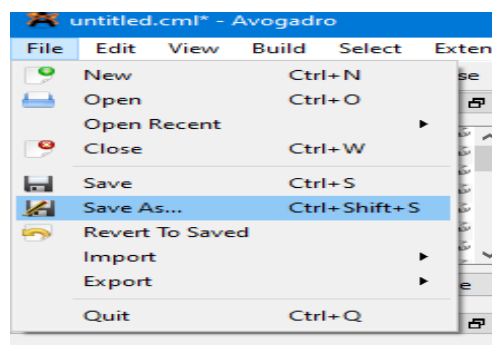
Buning uchun har bir molekulalarning 3D



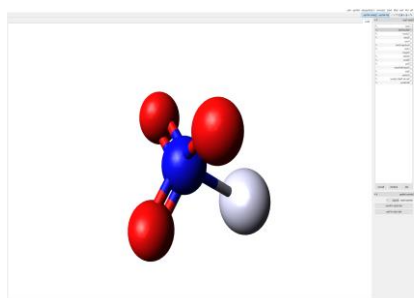
Rasm № 2 geometrik optimizatsiyalash



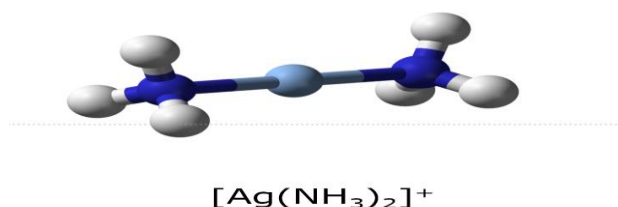
Rasm № 3 Geometrik optimizatsiyalash jarayoni va modellarni saqlash jarayoni.



ushratishimizdan asosiy maqsad molekulalarning 3D modellari orasidagi bog'lanish energiyalarini reallikka nisbatan yaqinlashtirish, ya'ni molekulalar orasidagi bog' energiyalari qanchalik kichik bo'lsa molekulalarning modellari shunchalik reallikka yaqin bo'ladi. 3D molekulalar modellarni yaratishimiz uchun biz kimyogarlardan uchun bizga eng qulay usullaridan biri bu AVOGADRO usuli. Ushbu dasturiy usul orqali molekulalarning fazoviy 3D modellarini yaratish ancha qulay. Bunda ushbu dasturdan foydalanish jarayonida molekulalarning energiyalarini ham hisoblash imkoniyatini beradi. Dastlab molekulani yaratib so'ngra uning energiyasini



rasm № 4 Optimizatsiya bo'lgan AgNO₃



rasm № 5 [Ag(NH₃)₂]⁺ kompleksining fazoviy modeli

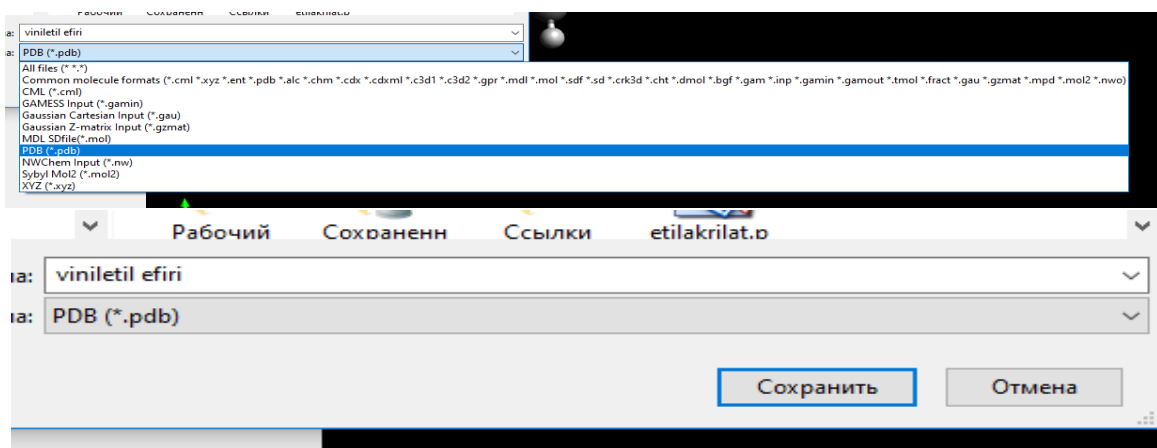
hisoblaymiz. Buning uchun masalan nodir metallardan kumush (Ag) metalining nitrat kislota (HNO₃) si bilan hosil qilgan birikmasi kumush nitrat AgNO₃ tuzining fazoviy 3D modelini AVOGADRO dasturida yaratish mumkin. ([rasm № 1 – 5](#)) yoki [Ag(NH₃)₂]⁺ kompleks birikmasini (rasm) Molekulalar uchun mo'ljallangan usullardan qulayini talab olganimizdan, so'ng molekulani geometrik optimizatsiya holatga keltirishimiz kerak bo'ladi (Rasm № 2). Buning uchun **Extensions** bo'limidan **Optimize Geometry ni tanlab olamiz** yoki kumyuter klaviaturasidan **ctrl+Alt+O** tugmalarini bosgan holatda amalga oshirishimiz mumkin bo'ladi. Optimizatsiyalanish 100% bo'lgan vaqtda molekulamiz to'liq geometrik optimizatsiyalangan bo'ladi. (Rasm № 3)

Modelimiz orasidagi bog'larni ham o'zgartirishimiz mumkin. (rasm №4)

Tayyor bo'lgan yangi manomerimizni PDB fayl shaklida saqlashimiz zarur bo'ladi. Buning uchun ishchi oynadan **File** bo'limini tanlaymiz **save** ni

yoki kompyuter klaviaturalari orqali **Ctrl + Shift + S** orqali saqlashimiz mumkin bo'ladi. Saqlash jarayonida PDB holatda saqlash bandini tanlab olishimiz kerak bo'ladi.

PDB fayl holatda saqlash imkoniyatini beradi. Saqlash tugamasini bosganimizdan so'ng yangi 3D ogmental reallik uchun yaratgan manomerlarimiz PDB fayl holatda



Rasm № 1 Modellarni PDB holatda saqlash.

saqlanadi. (Rasm №6)

1. Oliver Jones. Conclusions and Future Developments. 2020,, 71-74. https://doi.org/10.1007/978-981-15-6190-0_7
2. Irwansyah F. S. et al. Ogmented reality (AR) technology on the android operating system in chemistry learning //IOP conference series: Materials science and engineering. – IOP Publishing, 2018. – T. 288. – №. 1. – C. 012068.
3. Hay P. J. Gaussian basis sets for molecular calculations. The representation of 3 d orbitals in transition-metal atoms //The Journal of Chemical Physics. – 1977. – T. 66. – №. 10. – C. 4377-4384.
4. Felix Lederle, Eike G. Hübner. Organic chemistry lecture course and exercises based on true scale models. Chemistry Teacher International , Article ASAP.
5. 3D AUGMENTAL MOLEKULALAR MODELLASH UCHUN PDB FAYLLARNI YARATISH USULI T.X. Raximov, S.N. Suyunova O'zbekiston Milliy Universiteti respublika ilmiy amaliy konferensiya 2022.Namangan