

Calculating the Number of Modes of Vibrations in Linear BeCl_2 Molecule using Jmol and Stimulated FTIR Spectra

VISINIGIRI KAVYA SRI

Department of Freshman Engineering, Kalasalingam Academy of Research and Education, Krishnakoil, Tamil Nadu, India – 626126

1.Introduction:

Vibrational spectroscopy provides critical insight into the molecular structure and dynamics of chemical compounds. One fundamental aspect of this analysis is determining the number of vibrational modes, which directly relates to the molecular geometry and atomic composition. In this study, we investigate the linear beryllium chloride (BeCl_2) molecule, a simple triatomic system, to calculate its normal modes of vibration. Using molecular visualization software Jmol, we model the geometry and symmetry of BeCl_2 , and simulate its infrared (FTIR) spectra to identify vibrational frequencies. The correlation between molecular structure, symmetry, and vibrational modes is explored to deepen our understanding of the physical behavior of such linear molecules

2.Molecular Vibrations:

Molecular Vibrations in BeCl_2 :

Beryllium chloride (BeCl_2) is a linear triatomic molecule with symmetry in its gaseous phase. Molecular vibrations in such systems arise from the periodic motion of atoms around their equilibrium positions.

- For a non-linear molecule with N atoms, there are $3N - 6$ normal vibrational modes
- For a linear molecule with N atoms, there are $3N - 5$ modes.

Since BeCl_2 contains three atoms (Be and two Cl atoms), it has 4 normal modes of motion, including translations and rotations, and 3 fundamental vibrational modes.

The three vibrational modes in BeCl_2 are:

1. Symmetric Stretch (IR inactive due to lack of dipole moment change),
2. Asymmetric Stretch (IR active),
3. Bending Mode (IR active).

The symmetric stretch does not change the dipole moment in a centrosymmetric molecule like linear BeCl_2 , making it inactive in the infrared spectrum. However, the asymmetric stretch and bending vibration involve a net change in dipole moment and are thus observable in FTIR spectroscopy. Simulating these vibrations helps in understanding molecular symmetry and the selection rules that govern infrared activity.

★ *The following steps to calculate the number of vibrational modes:*

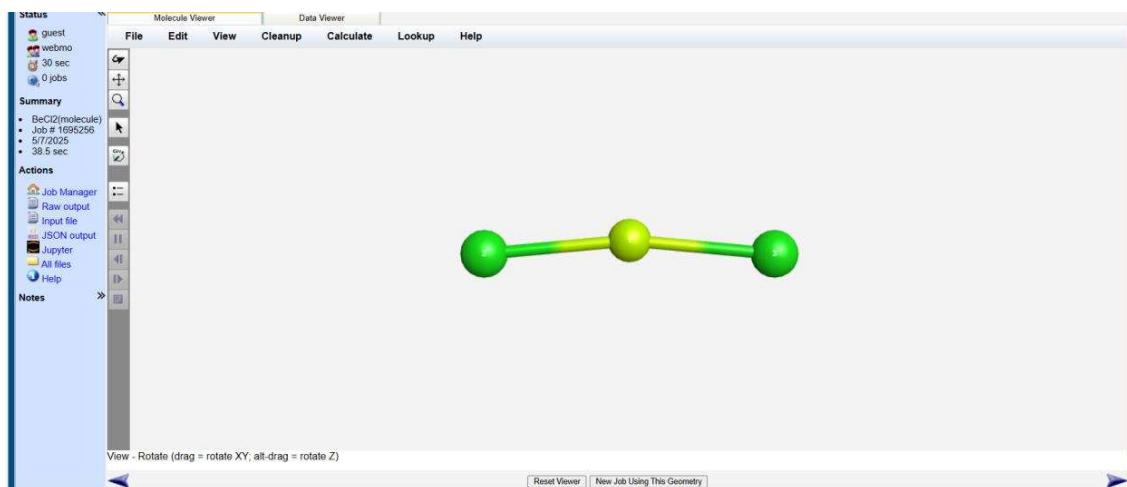
1. Determine the molecule whether linear or non-linear molecule.
2. Calculate how many atoms in the given molecule.
3. Substitute the number in “N” value and solve.

3. Calculating the number of vibrations in BeCl₂ molecule:

- BeCl₂ molecule is a linear molecule.
- The molecule has 3 atoms.
- According to formula:
 - $3N-5$
 - $(3 \times 3)-5 = 4$
- The number of modes of vibrations in BeCl₂ molecule is 3

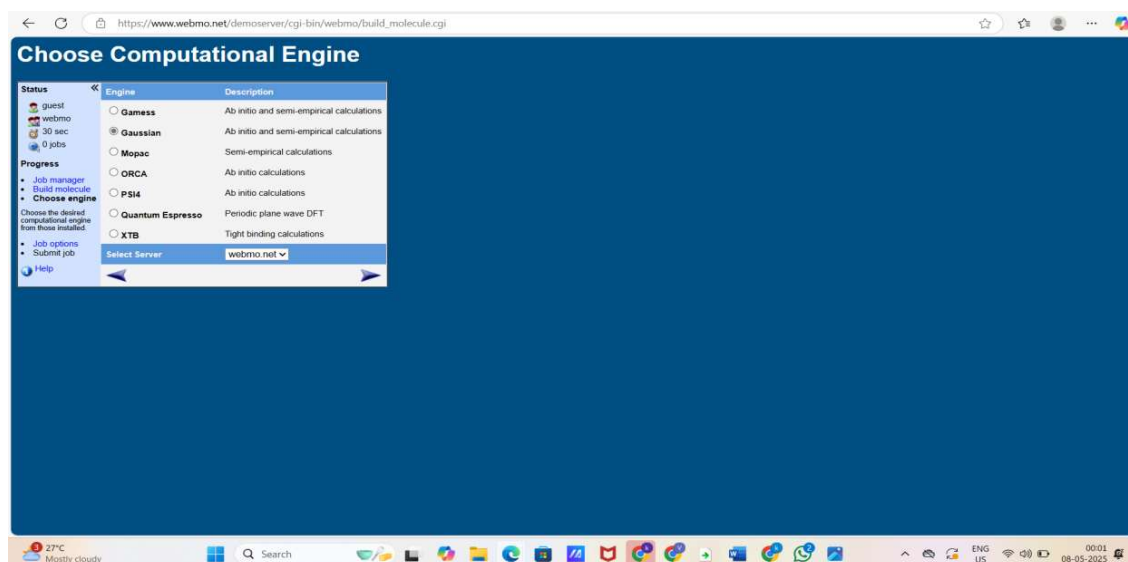
4. Drawing the 3D structure of BeCl₂ molecule in webmo interface:

- Open webmo interface select the webmo demo server
- login to the webmo demo server create username and password
- Create new file and select build (others)
- Select element in the periodic table beryllium and attach the chlorine atoms to the both sides of beryllium atom

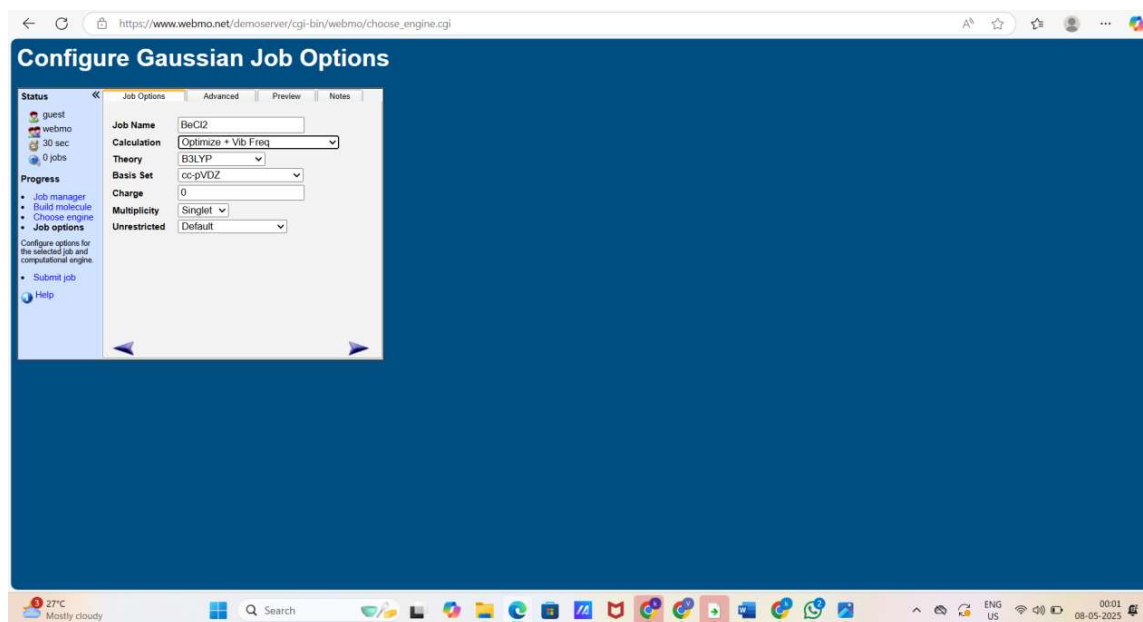


5.Importing the molecule to the Gaussian engine in WebMo

- Open the WebMO web page <https://www.webmo.net/>
- Click on the DEMO icon
- Login into demo server
<https://www.webmo.net/demoserver/cgi-bin/webmo/login.cgi>
- Click on the new job option-select-create new job
- Now build molecule page opens
- Create the molecule BeCl_2
- Proceed to the next step (Right side bottom corner arrow mark)
- Then next page opens Configure Gaussian Job Options(then fill as shown)



- And then,go to the next arrow to proceed as follows



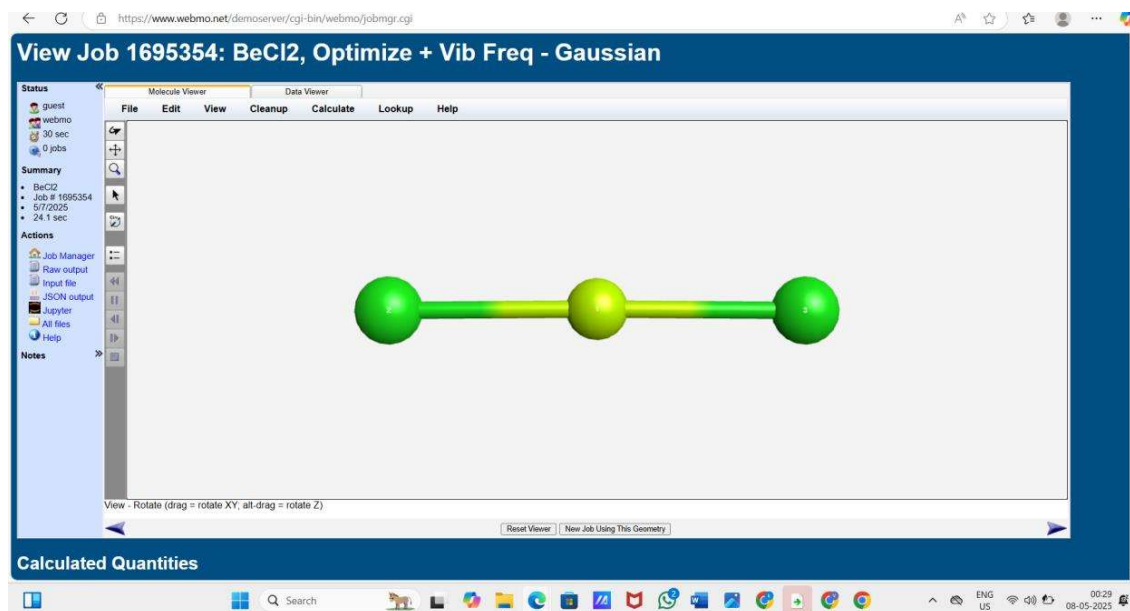
- Job Name: BeCl₂,
- Calculation: Optimize + Vib Freq
- Theory: B3LYP
- Basic Set: cc-pVDZ
- Charge: 0
- Multiplicity: Singlet
- Unrestricted: Defa

➤ Proceed to the next arrow mark then it opens to the WebMO job manager

WebMO Job Manager

Number	Name	Description	Date	Status	Time	Actions
1695354	BeCl2	Optimize + Vib Freq - Gaussian	5/7/2025 18:31	Complete	24.1 sec	[Download] [Delete]
1695353	CHCl3	Vibrational Frequencies - Gaussian	5/7/2025 18:25	Complete	18.8 sec	[Download] [Delete]
1695352	CHCl3	Molecular Energy - Gaussian	5/7/2025 18:23	Complete	25.0 sec	[Download] [Delete]
1695351	ClO4N2Fe	Geometry Optimization - XTB	5/7/2025 18:22	Complete	0.2 sec	[Download] [Delete]
1695350	C2H2F2	Vibrational Frequencies - Gaussian	5/7/2025 18:19	Complete	17.1 sec	[Download] [Delete]
1695349	H3N	Molecular Orbitals - Gaussian	5/7/2025 18:18	Complete	0.9 sec	[Download] [Delete]
1695348	C2H2F2	Vibrational Frequencies - Gaussian	5/7/2025 18:18	Failed	0.0 sec	[Download] [Delete]
1695347	C2H2F2	Vibrational Frequencies - Gaussian	5/7/2025 18:16	Complete	17.9 sec	[Download] [Delete]
1695346	CHCl3	Vibrational Frequencies - Gaussian	5/7/2025 18:15	Complete	24.8 sec	[Download] [Delete]
1695345	CHCl3	Molecular Energy - Gaussian	5/7/2025 18:14	Complete	3.2 sec	[Download] [Delete]
1695344	nbo	Import - Gaussian	5/7/2025 18:13	Complete	8.0 sec	[Download] [Delete]
1695343	Cl4	Molecular Energy - Gaussian	5/7/2025 18:11	Complete	2.8 sec	[Download] [Delete]
1695342	ClH18	Molecular Orbitals - Gaussian	5/7/2025 18:09	Complete	8.5 sec	[Download] [Delete]
1695341	H3N	Molecular Energy - Gaussian	5/7/2025 18:02	Complete	0.9 sec	[Download] [Delete]
1695340	I3	Geometry Optimization - Gaussian	5/7/2025 18:01	Failed	0.3 sec	[Download] [Delete]
1695339	ClH18	Natural Bond Orbitals - Gaussian	5/7/2025 18:00	Complete	8.9 sec	[Download] [Delete]
1695338	H3N	Geometry Optimization - Gaussian	5/7/2025 17:59	Complete	4.5 sec	[Download] [Delete]
1695337	ClH14	Natural Bond Orbitals - Gaussian	5/7/2025 17:56	Complete	4.8 sec	[Download] [Delete]
1695336	ClH14	NMR - Gaussian	5/7/2025 17:53	Complete	11.2 sec	[Download] [Delete]

➤ Now, open the page with job number, job name and job details appears as shown below



➤ Now, scroll down to see the details of optimization and vibrational modes and so on....

Calculated Quantities

Collapse all

Overview

Quantity	Value
Route	#N B3LYP/cc-pVDZ OPT FREQ
Method	B3LYP
Stoichiometry	BeCl ₂
Symmetry	CS
Basis	CC-pVDZ
RB3LYP Energy	-935.338585205 Hartree
ZPE	0.004023 Hartree
Conditions	298.150K, 1.00000 atm
Internal Energy	-935.330981 Hartree
Enthalpy	-935.329946 Hartree
Free Energy	-935.357314 Hartree
C _v	9.478 cal/mol-K
Entropy	57.600 cal/mol-K
Dipole Moment	0.0356 Debye
Server	webmo.net (261623)
CPU time	24.1 sec

Geometry Sequence Energies

https://www.webmo.net/demoserver/cgi-bin/webmo/jobmgr.cgi

Geometry Sequence Energies

Step	Energy (au)
0	-935.325100355
1	-935.337355236
2	-935.338573826
3	-935.338583267
4	-935.338585205
5	-935.338585205
6	-935.338585205

Animation speed: 5
Loop: None

Rotational Constants

Constant	Frequency (GHz)	Frequency (cm ⁻¹)
a	409643.72905	13670.91529531998
b	2.20734	0.07362893699
c	2.20732	0.07362826986

Partial Charges

Atom	Symbol	Charge
1	Be	0.137380
2	Cl	-0.068244
3	Cl	-0.069136

Vibrational Modes

Show all

Vibrational Modes

Show all

Mode	Symmetry	Frequency (cm ⁻¹)	IR Intensity	Actions
1	A'	239.1459	42.5688	
2	A'	394.3066	0.0408	
3	A'	1132.5340	433.2430	

Frequency Scale Factor: 1

Normal Mode Amplitude: 1.0

Animation Speed: 50

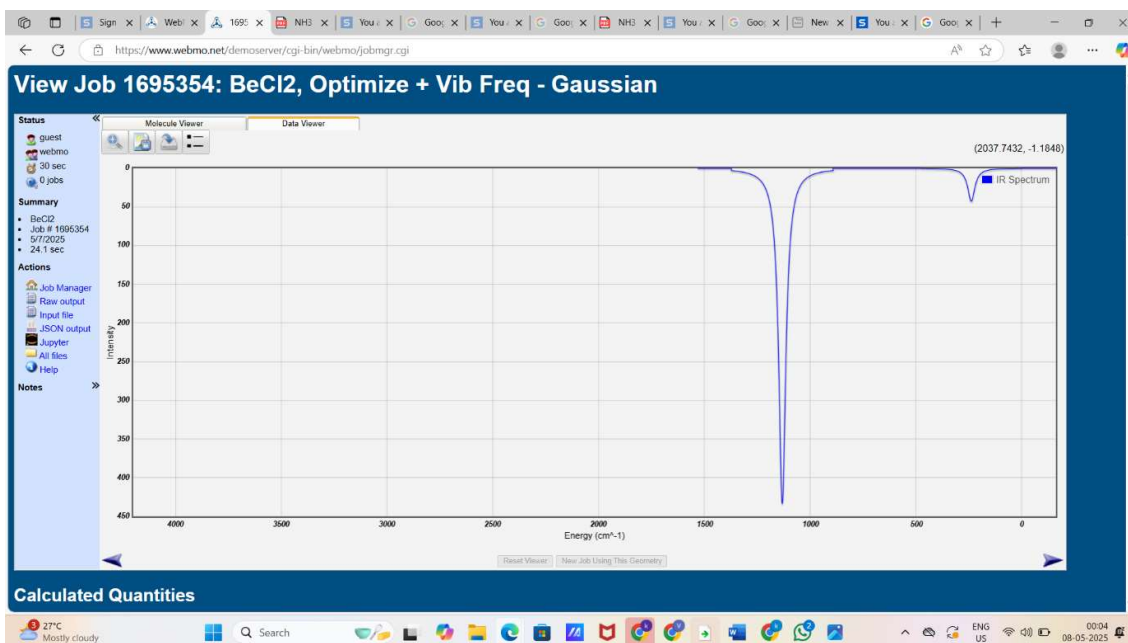
IR Spectrum:

Peak Width (cm⁻¹): 40

Quote

WE HAVE LEARNED THAT NOTHING IS SIMPLE AND RATIONAL EXCEPT WHAT WE OURSELVES HAVE INVENTED; THAT GOD THINKS IN TERMS NEITHER OF EUCLID OR RIEMANN; THAT SCIENCE HAS "EXPLAINED" NOTHING; THAT THE MORE WE KNOW THE MORE FANTASTIC THE WORLD BECOMES AND THE PROFOUNDER THE SURROUNDING DARKNESS. - ALDOUS HUXLEY

- For the above information, open the IR Spectrum to view peak graphs



- Though we get 4 modes of vibrations for BeCl₂ molecule, but only two peaks are obtained in the stimulated FTIR spectra.

6. Comparing the number of modes of vibrations obtained using the formula to the peaks obtained in the stimulated FTIR Spectra:

- Comparison of Theoretical and Simulated Vibrational Modes of BeCl₂
- For a linear triatomic molecule such as BeCl₂, the number of vibrational modes can be determined using the formula:
- Number of Vibrational Modes = $3N - 5$
- Where N is the number of atoms. For BeCl₂ (N = 3), this yields $3(3) - 5 = 4$ vibrational degrees of freedom,
- of which 3 are vibrational modes (after excluding translational and rotational motion).
- These three fundamental vibrational modes include:
 1. Symmetric Stretch – IR inactive

2. Asymmetric Stretch – IR active
 3. Bending Mode – IR active
- When analyzing the simulated FTIR spectrum generated via molecular modeling (e.g., using Jmol or Gaussian), only the IR-active modes are expected to appear as peaks. In the case of BeCl_2 , the simulated FTIR spectrum typically shows two distinct peaks, corresponding to:
 - The asymmetric stretching mode, and
 - The bending vibration.
 - BeCl_2 is a linear triatomic molecule with symmetry. Based on group theory and the IR selection rules, a vibrational mode is IR active only if it causes a change in the dipole moment of the molecule.
 - The 3 vibrational modes of BeCl_2 are:
 1. Symmetric Stretch – Both Cl atoms move in and out simultaneously while Be remains stationary. No net change in dipole moment (the molecule remains symmetrical). IR inactive.
 2. Asymmetric Stretch – One Cl moves in while the other moves out. Creates a changing dipole moment. IR active.
 3. Bending Mode – The molecule bends from its linear shape, creating an angle. Changes the overall dipole moment.

Acknowledgement

I would like to express my sincere gratitude to KARE Management for their valuable guidance, support, and encouragement throughout the course of this project. Their insightful feedback and expertise greatly contributed to my understanding of molecular vibrations and spectroscopy.

I also extend my thanks to Dr.D.Geetha for providing access to the necessary software tools, including Jmol and FTIR simulation platforms, which made the theoretical and practical aspects of this project possible. Thank you for all KARE Management towards this project guide and for their encouragement and support.