Galaxy A set of Gaussian basis functions into information that we could access easily on a computer and in particular at the end of the video we had programmed are Gaussian basis functions for the 6-31G basis set for the hydrogen and helium atoms.Now that we have our basic functions, were running to start using them to make matrices that will need to solve in order to calculate the total electronic energy.In this series of video we're going to build the two simplest matrices, the overlap or ask me tricks and kinetic energy or he matrix. If you recall from quantum mechanics or our first video, each matrix will have will be a matrix of size number of bases.James, Times the number of bases function there will be square matrix and the each individual element of a given matrix would say oh so MN will be the overlap integral of basis function. Oh times an operator O.So basic function M times operator oh times basis function N.I will need to evaluate this for each combination of basis functions in our basis function set.Now, if you would like to know more about this, I highly recommend the article Gaussian basis set selected integral by helicopter and healer. It's a very thorough and relatively easy to read description of how to calculate these integrales. Will just be giving an overview here in this set.In this video will give an overview of our strategy is going to be calculate the overlap matrix, the kinetic energy matrix, and then the two videos following that will actually write the code that allows us to calculate those matrix values.So just an assigned. One of the questions you might be asking is why are we starting with the overlap matrix, the kinetic energy matrix? And the reason is those are the two simplest matrices that we need to calculate.He overlapped matrix is just the overlap of each basis function, every other basis function, or just the overlap integral. And we need this because our basis functions aren't all auto normal to each other.The kinetic energy operator is also extremely easy to calculate an atomic unit. The kinetic energy operator is just minus the Laplacian or minus the quantity DX squared plus B y ^2 + B square.The reason that this is easy to calculate as then we apply this operator to the nth basis function. What we're going to get out as a series of polynomials times the basis function, and then that overlap integral between the resulting functions in the IMP basis function is again easy to.So why are these integral is easy to compute? Well, that's the whole reason why we're using Gaussian basis set. And when it comes down to is 2 quantities. First, the Gaussian basis functions are separable, so right now we're looking at us or medals which are spherically symmetric and we can write them as a Gaussian in.Spherical quarters of E to the minus alpha, R minus **** today squared, but we can split that up into three individual Gaussians. A Gaussian in the X coordinate, a Gaussian into one coordinate, times of Gaussian the Z coordinate.We can therefore split are integral overall space into 31 dimensional integrales.And we have something called the Gaussian product. Here the Gaussian product theorem states that if I have a Gaussian at function Gaussian location A and the Galaxy and with the location B9 multiply them together, the resulting function 8 * B is another Gaussian with a different exponent.Centred somewhere between 8:00 and B.Everyone knows that our function the resulting function of agencies and other county, and we can apply the Gaussian integral theorem to numerically evaluate it very simply. Okay for the very simple result. So that's what we're going to do for the overlap matrix. All we need to do for.Each combination of 1 dimensional Gaussian functions what is the new Galaxy and and then what is the interval for that? And so if I have two girls skins at 1A and expert alpha in the Gaussian it be an exponent beta. I'm multiplying them together, I will get a new Galaxy and with exponent.Lower HP which is just out looks lost data and it will be the geometric mean will be its new location, so it's weighted weighted mean by the exponent. So alpha times A plus beta times be over alpha plus beta will give me the location of my new centre, my new Gaussian function.Amplitude of that new Gaussian function will be given by a product of two

factors, either minus lower case too, which is just alpha, beta over a + b to the geometric mean in the exponent times the midpoint of the two galaxians a -, B.And so the resulting integral will just be the new amplitude factories in my SQ square behind the interval. Overall space in this little little smaller Gaussian could be described in Highbridge.I mean not now. This situation changes significant looms refinishing angular momentum. Because we introduce angular momentum of basis function, AM based function B are no longer, we don't, we no longer have everything centred at point P we have these things that are centred at the original add appointment.Home.Dealing with these polynomials is the whole reason why we're ignoring angular momentum for now and will come back to that which we written the programme and have a better understanding of what's going on. Xo calculate the overlap matrix. We need to loop over each basis set each function of the base assessment.Now we're going to get loop over each function the basic set a second time. So at this plane in my 424 groups will have basis functioning am basis functions B and then need to loop over the each primitive Gaussian inside egg which were going to call. We're going to effect NBA for the number basis a.Man primitive Gaussian in BB inside basis function be.We're going to split that into its XY&Z component. For each XY&Z component were going to determine the new Galaxy and location exponent P and then will apply the Gaussian integral theorem for that. Well then for each AMB bases loaded some overall the primitive Gaussians.They come out of that, we're going to wait them by their appropriate normalisation, Constance contraction coefficients and some. Then we'll get our matrix element for SA baby.At least the kinetic energy make expected some more. Again we're going to lose overall basis functions. Rental look over the mall against we have double for loop, so we have another set of four loops will look over the primitive Gaussian functions.And then we're going to apply the Dell squared operator onto Gaussian function be the primitive Gaussian inside that.It means.Mummy do that. Take herbal passing over going to get our free new Gaussian function 36 new Galaxy functions. Three of them are the same and then three of them are Gaussian functions that are multiplied by a polynomial and will deal with these polynomials individually.What we having you a moment in the factory? Easier. Once we've written the code to deal with things on that. This will be a little bit easier than the fray. Now, I don't want to get too bogged down into this, but will calculate what these new new functions are as our overlap with every primitive Gaussian in a given basis function A, and then will some over those multiplied by their contracting coefficients.The normalisation concert to get the matrix element. He's a baby.sweet sweet that's all we need to do to calculate our overlapping kinetic energy matrices take him with me to the next video and will write the code that we need to calculate the matrix elements for matrix ask the overlapping thanks see you