I'm human

Basis set

Basis set extrapolation. Basis sets in quantum chemistry. Basis set superposition error. Basis set exchange. Basis set linear algebra. Basis set orca. Basis set calculator. Basis set ventures fund size. Basis set for iodine. Basis set gaussian. Basis sets in computational chemistry. Basis set ventures. Basis set superposition error gaussian. Basis set chemistry. Basis set meaning.

Most methods need a basis set specified; if no keyword is given in the route section, then STO-3G will be used. Exceptions are some methods where the basis set is part of the method itself. These include all semi-empirical methods and molecular mechanics methods. Some compound model chemistries like Gn, CBS, and W1 also have their basis sets defined within them. Basis sets other than listed ones can still be input using ExtraBasis and Gen keywords. The ChkBasis keyword allows reading the basis set from a checkpoint file. Internally stored basis sets include STO-3G, 3-21G, 6-21G, 4-31G, 6-31G, 6-31G†, 6-31G‡, and more, with some allowing for diffuse functions or f functions to be added. The 6-311G basis set is specified for first-row atoms, while second-row atoms use a McLean-Chandler basis set. Other basis sets include D95V, D95, SHC, CEP-4G, CEP-31G, and CEP-121G for various elements, and LanL2MB which uses STO-3G on first row and Los Alamos ECP for others. **Basis Sets** The text discusses various basis sets used in quantum chemistry calculations. These include: * **SDD**: A basis set developed by Stuttgart/Dresden group, which is used for atoms up to Ar. * **CC-pVDZ**, **CC-pVTZ**, **CC-pVQZ**, **CC-pV5Z**, and **CC-pV6Z**: Correlation consistent basis sets developed by Dunning's group, which are double, triple, quadruple, quintuple-zeta, and sextuple-zeta respectively. * **Ahlrichs' Basis Sets**: A series of basis sets developed by Ahlrichs and coworkers, including SV, SVP, TZV, and TZVP. These have been redefined in more recent papers with the prefixes Def2SV, Def2SVP, etc. **Atomic Polarization Functions** The text also discusses the atomic polarization functions present in each of these basis sets: * **CC-pVDZ**: 2s,1p for H; 3s,2p,1d for Li-Be * **CC-pVTZ**: 4s,3p,2d,1f for B-Ne; 5s,4p,2d,1f for Na-Ar * **CC-pVQZ**: 6s,5p,3d,2f,1g for B-Kr **Other Basis Sets** The text also mentions other basis sets: * **EPR-II and EPR-III**: Basis sets developed by Barone for the computation of hyperfine coupling constants. * **MidiX**: A basis set developed by Truhlar and coworkers. Note that this paraphrased version still conveys the same information as the original text, but in a more concise and readable format. The basis sets used in this context are described by a single set of f-polarization functions and an improved s-part for the nuclear region, using (6,2)/[4,2] for H and (11,7,2,1)/[7,4,2,1] for B to F. The universal Gaussian basis set, UGBS, can be augmented by adding polarization functions with a suffix like UGBSnP[V|O], where n specifies the number of additional functions, P adds them to all functions, V adds them to valence functions, and O uses the scheme from Gaussian 03. For example, UGBS1P adds one polarization function to all orbitals, while UGBS2V adds two polarization functions to valence orbitals. Diffuse functions can also be added using + or ++, and specific diffuse functions like 2+ for heavy atoms. calender basis set variations are available. The naming of these sets originates from the cc-pV*Z series with added polarization functions, known as Aug-cc-pV*Z. Truhlar observed that "Aug" is also related to August and suggested a new method for augmenting these basis sets using month names. These modified basis sets have diffuse functions removed from the original Aug basis set. For example, Jul-cc-pV*Z has the diffuse function from H and He removed, Jun-cc-pV*Z removes all but the highest angular momentum diffuse function, May-cc-pV*Z removes two high-order ones, and Apr-cc-pV*Z removes three. Despite this, some atoms still have at least s or p diffuse functions included in these sets by default to avoid inconsistencies with Truhlar's original definitions. To specify these sets as used originally, use TJul, TJun, etc. The addition of a single polarization function to 6-311G results in different d or f functions for first and second-row atoms and third-row atoms respectively. A frozen core calculation using the D95 basis set freezes both occupied and virtual core orbitals. EPR-II, EPR-III H, B, C, N, O, F, UGBS(1,2,3)P +,+,2+,2+ MTSmall H-Ar DGDZVP H-Xe DGDZVP2 H-F, Al-Ar, Sc-Zn included in definition. Cartesian vs. pure basis sets offer 5D and 6D functions for d orbitals, 7F and 10F for f orbitals. Additional keywords like 5D, 6D, 7F, and 10F adjust the basis set. Users should note that built-in basis sets use pure f functions, while most use pure d functions except for certain sets. The default setting can be overridden using preceding keywords. When reading a wavefunction from a checkpoint file, the basis function type is automatically converted if necessary. In a job, all d functions must be 5D or 6D and all f and higher functions must be pure or Cartesian. When using ExtraBasis and Gen or GenECP keywords, the basis set specified in the route section determines the default form of the basis functions. For example, adding basis functions from one set to another will use the same type of d or f function as the original set. Gaussian 16 provides a density fitting approximation for pure DFT calculations, which expands the density in atom-centered functions when computing the Coulomb interaction. This approach offers significant performance gains without degrading accuracy. Gaussian 16 can automatically generate an appropriate fitting basis from the AO basis or select one of the built-in sets. The desired fitting basis is specified as a third component of the model chemistry, for example, BLYP/TZVP/TZVPFit. Note that slashes must be used to separate characters between the method, basis set, and fitting set when specifying a density fitting basis. Gaussian 16 provides two fitting sets: DGA1 and DGA2. DGA1 is applicable for H to Xe, while DGA2 is suitable for H, He, and B to Ne. The SVPFit set corresponds to the SVP basis set, whereas TZVPFit corresponds to the TZVP basis set. The fitting set can be selected using the Fit keyword. If no fitting set matches the specified basis set, an error will occur. The NoFit keyword disables the use of fitting sets, allowing for override of the DensityFit keyword in the Default.Route file. For Auto generation, a fitting set is created automatically from the AO primitives within the basis set. This process truncates the set at a reasonable angular momentum by default, using Max(MaxTyp+1,2*MaxVal), where MaxTyp and MaxVal are specific values. The DensityFit keyword can be used to control various aspects of the fitting set. It can also be made the default for jobs using pure DFT functionals by adding it to the route section (-#-) line in the Default.Route file. The development of quantum chemistry has been marked by significant advances over several decades. Key studies have emerged that have shaped our understanding of molecular behavior. Notable papers from leading researchers include: * Hehre et al.'s (1969) work on ab initio calculations, which laid the foundation for modern quantum chemistry. * Pople's contributions to the development of Hartree-Fock methods and their applications in chemical physics. * Ahlrichs' studies on basis sets and density functional theory, which have had a lasting impact on the field. More recent research has focused on improving computational methods, including: * The development of more accurate and efficient algorithms for calculating molecular properties. * Advances in density functional theory, which has enabled more precise predictions of chemical behavior. * Studies on the accuracy and reliability of quantum mechanical calculations for large molecules. These studies have led to significant improvements in our understanding of molecular behavior and have had a profound impact on various fields, including chemistry and physics. A plethora of research papers on computational atomic structure have been published in reputable journals and publications. These studies date back to the 1920s with Hartree's work on the Proc Cambr Phil Soc, followed by contributions from Frose-Fischer et al. in 1997. The topic has continued to evolve over the years, with notable contributions from Laaksonen et al. in 1986, Losilla and Sundholm in 2012, Enkovaara et al. in 2010, and Rescigno and McCurdy in 2000.