Reference Program for Molecular Calculations with Slater-Type Orbitals

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ABSTRACT: A program for computing all the integrals appearing in molecular calculation with Slater-type orbitals is reported. The program is mainly intended as a reference for testing and comparing other algorithms and techniques. An analysis of the performance of the program is presented, paying special attention to the computational cost and the accuracy of the results. Results are also compared with others obtained with Gaussian basis sets of similar quality. © 1998 John Wiley & Sons, Inc.   J Comput Chem 19: 1284–1293, 1998

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Introduction

The use of exponential-type orbitals (ETOs) in molecular calculations is a challenging problem in computational chemistry.[1] Although there is general agreement in the best quality of these functions for describing the electronic function in atoms and molecules, the difficulties in solving some molecular integrals (in particular the three- and four-center two-electron repulsion integrals) has restricted their use to atoms and small molecules. In addition, almost all the calculations in molecular systems are done in terms of Gaussian-type orbitals (GTOs).

However, the interest in extending the use of ETOs to calculations on larger molecular systems has increased in the last few years.[2] There are a variety of reasons for these renewed efforts. The increase in the power of computers, the possibility of applying sophisticated computations [such as configuration interaction (CI)] beyond the Hartree–Fock (HF) level to complex systems, and the development of new promising algorithms for computing the many-center molecular integrals involving ETOs have encouraged the researchers in this field and allowed them to expect that efficient programs for molecular calculations with exponential-type functions will be available in the near future.

In view of this, we implemented a program for molecular calculations with Slater-type orbitals (STOs). This has been designed to be used for

testing the numerical results obtained with new algorithms and to be useful as a reference on their performances.

Given the aim of this program, we placed our emphasis on the reliability of the calculation, the possibility of carrying out calculations with any STO basis sets, and the accuracy of the results; the efficiency was considered a less important feature. Nevertheless, molecular calculations on medium-sized molecules (about 100 basis functions at most) can be carried out at an acceptable computational cost; therefore, other possibilities are open for STO such as large CI calculations, basis set optimization for molecules, calculation of properties other than energy, comparison with the results obtained with GTOs, etc. The next section presents a description of the main features of the program.

Algorithms

We prepared two versions of the program. One works with real spherical STOs defined as

$$\chi_{NLM}(\zeta, \mathbf{r}) = e^{-\zeta r} r^{N-1} (-1)^M P_L^{|M|}(\cos\theta) \Phi_M(\phi). \tag{1}$$

$P_L^{|M|}$ are the corresponding Legendre functions,[3] and the functions Φ are defined as

$$\Phi_M(\phi) = \begin{cases} \cos M\phi & \text{for } M \geq 0, \\ \sin|M|\phi & \text{for } M < 0. \end{cases} \tag{2}$$

The other version uses Cartesian STOs, defined as

$$\chi_{Nijk}(\zeta, \mathbf{r}) = e^{-\zeta r} r^{N-(i+j+k+1)} x^i y^j z^k. \tag{3}$$

To compute the molecular integrals, we combined different techniques for the different types of integrals. Thus, the one-center integrals (overlap, kinetic energy, nuclear attraction, and electron repulsion) are obtained quickly by standard techniques.[4] In these integrals there is no limitation to the quantum numbers and a standard accuracy of about 14 significant figures is ensured.

The two- and three-center one-electron integrals overlap, kinetic energy, and nuclear attraction) are calculated by means of recursion algorithms as detailed in ref. 5. The two-center two-electron integrals are solved according to the techniques of ref. 6. Limits in the values of the quantum numbers are $N < 8$, $L < 5$ for the three-center nuclear attraction integrals and only $L < 5$ for the two-center integrals. In these integrals the accuracy is slightly

lower than in the one-center integrals (about 12 decimal places).

Finally, the three- and four-center electron repulsion integrals are computed by means of Gaussian expansions of the STO. This method was proposed in the 1960s by Hehre et al.[7] and is used here according to Foster and Boys' suggestion,[8] (i.e., as a provisional solution until a better solution is available) and implemented following a version of Saunders'[9] algorithms with slight modifications.[10]

In order to increase the accuracy, we obtained further STO-nG expansions than previously reported[7,11,12] for all the STOs with $N < 8$ and $L < 7$. The largest expansion for each STO was chosen to reach a least square error (Δ^2) below 10^{-13} in function from $L = 0$ to $L = 3$ and below 10^{-10} in the remaining ones; the general trend is that the higher the N quantum number, the shorter the expansion required to achieve a given accuracy. For instance, an STO-23G expansion is needed for a least squares error of 10^{-15} in the $1s$ STO whereas a STO-12G is enough to reach the same error for a $7f$ STO. We found empirically that in STOs from $L = 0$ to $L = 3$ the largest expansions enabled us to attain an accuracy of about 10 decimal places in the integrals, which was even higher in many cases. It should be noted, however, that the number of correct significant figures in the energy is usually higher than in the many-center integrals, because the one- and two-center integrals (which have a higher standard accuracy) have a large weight in the final result. Furthermore, such high accuracy is not usually required in actual calculations; therefore, the largest expansions are not necessary for such calculations. This point will be illustrated in the next section.

The standard limits for the three- and four-center integrals are $N < 8$ and $L < 5$ (and can be easily extended to $L < 7$ by just modifying the dimensions of some arrays in the program). The version in terms of Cartesian STOs is limited to functions with $N < 8$ and $L < 4$.

In the present versions for STOs defined in terms of real spherical harmonics, the quantum numbers of the STOs in the three-center electron repulsion integrals of type ($AB|CC$) are limited to $N < 5$ and $L < 4$ because a single expansion is used for the one-center density $|CC)$ to save computational time. However, this limitation can be removed by also using a double expansion in the one-center density.

Because the computation of the repulsion integrals by means of Gaussian expansions is a rather

slow process, we implemented some methods to reduce the overall computational cost. For instance, as previously mentioned, single Gaussian expansions instead of double expansions were used for one-center densities in ($AB|CC$) type integrals, planar geometry was used in the calculation of the three-center integrals followed by a rotation of the final integrals to the molecular axes system, and a simple test was implemented to estimate the order of magnitude in the integrals and reject without calculation the negligible ones (according to a pre-fixed threshold). A test to avoid the calculation of negligible Gaussian contributions to a given set of integrals in three- and four-center electron repulsion integrals is also included.

Finally, we stress that the program has a modular structure that was prepared for the easy replacement subroutines as soon as other more efficient algorithms are available.

Results

We first analyzed the performance of the program (computational cost and accuracy of the results) by computing the pure electronic energy (without the nuclear repulsion) of different molecules. The results collected in Tables I and II

are representative of this analysis and can be useful for testing the efficiency and accuracy of alternative algorithms. The first molecules presented in these tables (from BH_3 to HCN) were chosen because calculations with STOs single-zeta basis sets were carried previously.[13] Two more systems were added (SF_6 and Zn_3) to show the behavior of the program in larger systems or systems with heavy atoms. Tables I and II summarize the results with STO single- and double-zeta basis sets, respectively.

To simplify the analysis, we took in each sample the same length of the Gaussian expansion for all the STOs, despite the fact that the expansions required to achieve a given precision are smaller as the N quantum number of the STO increases.[10] For some STOs appearing in the SF_6 and Zn_3 systems, the three- and four-center repulsion integrals were calculated with Gaussian expansions shorter than STO-21G; in these cases the longest expansion available was used instead. All the computational times were measured on a Digital AlphaServer 8400. No vector facilities were used in any case. Details on basis sets and geometries are given in the Appendix.

In Tables I and II, the computational cost in the calculation of all the molecular integrals (in seconds) and the average time per integral (in mil-

TABLE I.
Computational Cost and RHF Electronic Energy[b]: Single-Zeta Basis Sets of STOs.

Molecule	Basis Set Size	Direct. Int. Timing[a] s[d]	ms[e]	(9G)[b] Timing[c] s[d]	ms[e]	Energy	(12G)[b] Timing[c] s[d]	ms[e]	Energy	(21G)[b] Timing s[d]	ms[e]	Energy
BH_3	8	0.05	0.16	1.0	6.8	-33.77424164	3.4	23.3	-33.7742681	13.1	89.7	-33.77424726
B_2H_6	16	0.35	0.13	26.8	5.5	-84.42645106	65.9	13.4	-84.42649449	387.3	78.8	-84.42649808
CH_4	9	0.06	0.09	2.3	5.6	-53.49344166	5.1	12.4	-53.4934807	31.6	76.9	-53.49344892
C_2H_2	12	0.13	0.14	3.9	8.9	-101.35594072	8.2	18.7	-101.3559543	48.0	109.	-101.35595557
C_2H_4	14	0.22	0.13	11.1	5.3	-111.21675020	28.6	13.9	-111.21677417	162.7	78.9	-111.21677693
C_2H_6	16	0.38	0.13	24.2	4.1	-121.00138675	61.0	10.2	-121.00142107	366.9	62.7	-121.00142560
HCN	11	0.09	0.13	1.5	8.7	-116.46664220	3.2	18.6	-116.4666903	17.9	104.1	-116.46664960
SF_6	39	2.61	0.10	322.	2.2	-1569.13899221	785.1	5.3	-1569.13933834	4138.	27.8	-1569.13932560
Zn_3	48	21.9	0.22	43.6	1.2	-5849.75004643	101.9	2.6	-5849.75008095	503.8	12.8	-5849.75008440

All times were measured on a Digital AlphaServer 8400. The energy is in hartrees (nuclear repulsion not included). Italic numbers are those differing from the most accurate result corresponding to the longest expansion used.
[a] Computational cost for directly computed integrals (all the one- and two-center integrals plus the three-center nuclear attraction integrals).
[b] Length of the Gaussian expansions used in the computation of three- and four-center electron repulsion integrals.
[c] Computational cost for integrals computed by Gaussian expansions (three- and four-center two-electron integrals).
[d] Total time in seconds for the full set of the corresponding integrals.
[e] Average time in milliseconds per integral actually computed.

TABLE II.
Computational Cost and RHF Electronic Energy Double-Zeta Basis Sets of STOs.

| Molecule | Basis Set Size | Direct. Int. Timing[a] | | (9G)[b] | | | (12G)[b] | | | (21G)[b] | | |
| | | Timing[a] | | Timing[c] | | | Timing[c] | | | Timing[c] | | |
		s[d]	ms[e]	s[d]	ms[e]	Energy	s[d]	ms[e]	Energy	s[d]	ms[e]	Energy
BH_3	16	0.32	0.09	13.0	5.9	−33.811354945	37.7	17.1	−33.81136477	207.4	94.3	−33.81136513
B_2H_6	32	3.09	0.13	370.1	4.9	−84.50625680	959.2	12.7	−84.50628605	6087.5	80.4	−84.50628782
CH_4	18	0.49	0.05	30.3	4.6	−53.57544746	79.2	12.3	−53.57545347	395.6	61.3	−53.57545398
C_2H_2	24	1.24	0.12	50.7	7.7	−101.54108572	127.1	19.2	−101.54110906	750.0	113.	−101.54111037
C_2H_4	28	1.90	0.11	166.4	5.3	−111.38724624	426.2	13.5	−111.38727066	2589.2	82.0	−111.38727226
C_2H_6	32	3.03	0.11	388.2	4.2	−121.13224948	976.3	10.6	−121.13227996	6114.6	66.5	−121.13228206
HCN	22	1.04	0.12	19.7	7.6	−116.71007148	47.8	18.5	−116.71008492	277.1	107.	−116.71008543
SF_6	78	33.9	0.12	4828.	2.2	−1572.99347805	19658.	9.1	−1572.99365215	64998.	30.2	−1572.99363143
Zn_3	114	531.	0.16	2814.	1.3	−5869.12961531	6372.	3.0	−5869.12961719	22042.	10.4	−5869.12961809

All times were measured on a Digital AlphaServer 8400. The energy is in hartrees (nuclear repulsion not included). Italic numbers are those differing from the most accurate result corresponding to the longest expansion used.
[a] Computational cost for directly computed integrals (all the one- and two-center integrals plus the three-center nuclear attraction integrals).
[b] Length of the Gaussian expansions used in the computation of three- and four-center electron repulsion integrals.
[c] Computational cost for integrals computed by Gaussian expansions (three- and four-center two-electron integrals).
[d] Total time in seconds for the full set of the corresponding integrals.
[e] Average time in milliseconds per integral actually computed.

liseconds) are analyzed for the directly computed integrals (i.e., all the one- and two-center integrals plus the three-center nuclear attraction integrals), as well as for the integrals computed by means of Gaussian expansion (i.e., the three- and four-center two-electron integrals). In the latter, computational cost and values of the pure electronic energy are given for three different lengths in the Gaussian expansions. It is important to note that the average time per integral refers to only the integrals that are actually computed (i.e., the integrals that are found negligible without calculation are not taken into account). This is important in systems such as the Zn_3 where approximately two-thirds of the three-center integrals are lower than 10^{-10} and are therefore neglected without calculation.

We note that the computational cost of the three- and four-center repulsion integrals is about 2 or 3 orders of magnitude higher than for the directly computed ones. This fact spurs the interest to continue further search on algorithms for the direct and more efficient calculation of integrals with ETOs.

The energy values in Tables I and II correspond to pure electronic energy and are given for the three different Gaussian expansions above. The figures printed in italic are those differing from the most accurate result corresponding to the longest expansion used. These values show the effect of the length of the Gaussian expansions in the final results, because the accuracy in the directly computed integrals is higher. We recall that for most applications sufficient accuracy can be attained with relatively short expansions.

Tables III–IX compare some calculations with STO and GTO double-zeta basis sets on different molecular systems. The STO basis sets are described in the appendix. In the GTO[14] the basis sets by Dunning and Hay[15] were chosen. All the energies in these tables are measured in hartrees and the time is always in seconds.

No advantage of the local symmetry was taken in the integral evaluation with STOs. In the GTO, the integrals were computed with the HONDO[16] package. The calculations were performed both at the HF and the CI levels. In both cases the mini-

TABLE III.

BH_3 Methods and Basis Sets.

	RHF		CI-SD		MRDCI	
	STO	GTO	STO	GTO	STO	GTO
No. configs.[a]	—	—	1	1	7	13
SAF[b]	—	—	485	485	5383	9163
Energy	−26.37489	−26.37621	−26.45847	−26.45530	−26.46058	−26.45742
Comput. time	13.5	0.5	3.4	3.4	6.2	19.6

[a] Number of reference configurations chosen in the MRDCI calculation.
[b] Number of selected symmetry-adapted functions.

TABLE IV.

B_2H_6 Methods and Basis Sets.

	RHF		CI-SD		MRDCI	
	STO	GTO	STO	GTO	STO	GTO
No. configs.[a]	—	—	1	1	11	9
SAFT[b]	—	—	5959	5959	249567	155119
SAF[c]	—	—	5959	5959	108095	155119
Energy	−52.75799	−52.77082	−52.94313	−52.94375	−52.94994	−52.94796
Comput. time	380.3	3.6	17.1	15.0	682.5	1213.8

[a] Number of reference configurations chosen in the MRDCI calculation.
[b] Number of generated symmetry-adapted functions.
[c] Number of selected symmetry-adapted functions.

TABLE V.
CH$_4$ Methods and Basis Sets.

	RHF		CI-SD		MRDCI	
	STO	GTO	STO	GTO	STO	GTO
No. configs.[a]	—	—	1	1	10	19
SAF[b]	—	—	579	579	12465	21300
Energy	−40.18361	−40.18534	−40.30977	−40.30726	−40.31427	−40.31241
Comput. time	31.1	0.8	4.1	3.8	23.9	48.9

[a] Number of reference configuration chosen in the MRDCI calculation.
[b] Number of selected symmetry-adapted functions.

TABLE VI.
CH$_2$H$_2$ Methods and Basis Sets.

	RHF		CI-SD		MRDCI	
	STO	GTO	STO	GTO	STO	GTO
No. configs.[a]	—	—	1	1	15	25
SAF[b]	—	—	1372	1372	59806	95932
Energy	−76.80365	−76.79910	−77.01311	−77.00127	−77.03175	−77.01978
Comput. time	51.4	1.4	5.5	5.2	201.4	457.7

[a] Number of reference configurations chosen in the MRDCI calculation.
[b] Number of selected symmetry-adapted functions.

TABLE VII.
C$_2$H$_4$ Methods and Basis Sets.

	RHF		CI-SD		MRDCI	
	STO	GTO	STO	GTO	STO	GTO
No. configs.[a]	—	—	1	1	11	7
SAFT[b]	—	—	4363	4363	149996	85696
SAF[c]	—	—	4363	4363	65361	85696
Energy	−78.00480	−78.01100	−78.22441	−78.21923	−78.23782	−78.22948
Comput. time	167.9	2.8	11.3	13.0	390.2	362.7

[a] Number of reference configurations chosen in the MRDCI calculation.
[b] Number of generated symmetry-adapted function.
[c] Number of selected symmetry-adapted functions.

TABLE VIII.
C$_2$H$_6$ Methods and Basis Sets.

	RHF		CI-SD		MRDCI	
	STO	GTO	STO	GTO	STO	GTO
No. configs.[a]	—	—	1	1	5	9
SAFT[b]	—	—	11704	11704	210891	398342
SAF[c]	—	—	11704	11704	67590	128246
Energy	−79.19986	−79.20450	−79.42896	−79.42578	−79.43415	−79.43144
Comput. time	372.5	4.5	39.3	45.0	530.9	1320.0

[a] Number of reference configuration chosen in the MRDCI calculation.
[b] Number of generated symmetry-adapted functions.
[c] Number of selected symmetry-adapted functions.

TABLE IX.
HCN Methods and Basis Sets.

	RHF		CI-SD		MRDCI	
	STO	GTO	STO	GTO	STO	GTO
No. configs.[a]	—	—	1	1	19	19
SAF[b]	—	—	1999	1999	102333	102333
Energy	-92.83384	-92.83680	-93.06076	-93.05546	-93.08231	-93.07488
Comput. time	21.4	1.2	7.1	6.6	723.0	785.6

[a] Number of reference configurations chosen in the MRDCI calculation.
[b] Number of selected symmetry-adapted functions.

mization of the energy was accomplished with the MRDCI program by Buenker and Phillips.[17] The symmetry of the system simplified the CI procedure.

The CI calculations were done at two levels, which differed in the number of configurations of reference taken in each one. The first-level single and double excitations over a single reference determinant (CI-SD in tables) is intended to compare the quality of the results with STOs and GTOs at a similar CI computational cost for both. The second-level single and double excitations over a multireference function (MRDCI in tables) is presented to compare the results that can be expected in high quality calculations.

The computational time recorded as self-consistent field (SCF) time collects the total time for computing the integrals and carrying out the SCF process. The time recorded as *CI time* corresponds to the transformation of the integrals and the CI procedure. The time was measured with the same machine and conditions as mentioned above.

As can be seen in these tables, the CI energies are slightly better with STOs than with GTOs. Nevertheless, these results are not representative of the advantages of the exponential functions because STO basis sets are not optimized for molecular calculations and their best qualities are more evident in heavy atoms.

Table X illustrates the improvement in the quality of the results when the STO basis set is optimized for molecules with light atoms. It is interesting to note that, although the STO basis set was optimized at the restricted HF (RHF) level, the energy also improves in the CI level.

Tables XI and XII show the differences in the systems with heavier atoms. In table XII the STO basis set of ref. 8 was used; the GTO basis set and corresponding energies were taken from ref. 19. In both systems, frozen core CI calculations were carried out. It is evident that in these cases the

improvement in the energy is more important than in the previously mentioned ones. In particular, we note that the CI energy of the Zn_3 with the GTO lies above the RHF energy with the STO.

Remarks

A reference program for molecular calculations with STOs has been presented and its performance has been illustrated on several molecular systems. From the results of these calculations, it seems clear that the program can be regarded as a benchmark with sufficient accuracy and acceptable cost for the purpose of testing new molecular programs with STOs. All the integrals computed by direct methods in the present version have good cost/accuracy ratios. In contrast, those obtained from Gaussian expansions are much more expensive with cost/accuracy ratios higher by 2 or 3 orders. This fact should encourage further research on algorithms for direct computation of multicenter repulsion integrals between STOs.

TABLE X.
Effect of Basis Set Optimization in HCN Molecule.

Basis Set	GTO[a]	STO (Atomic)[b]	STO (Optimized)[c]
RHF	-92.83680	-92.83384	-92.84542
CI-SD[d]	-93.05546	-93.06076	-93.07668
MRDCI[d]	-93.07488	-93.08231	-93.09924

[a] Double-zeta basis set by Dunning.[15a]
[b] Clementi and Roetti's[21] double-zeta basis set for C and N plus $1s_H(1.0)$ and $1s'_H(1.2)$ for hydrogen.
[c] Optimized double-zeta basis set: $1s_H(1.01650)$, $1s'_H(1.24684)$, $1s_C(6.78273)$, $1s'_C(4.71395)$, $2s_C(1.89791)$, $2s'_C(1.35861)$, $2p_C(2.20483)$, $2p'_C(1.15633)$, $1s_N(8.24032)$, $1s'_N(5.88333)$, $2s_N(2.26019)$, $2s'_N(1.24653)$, $2p_N(3.25451)$, and $2p'_N(1.59522)$.
[d] Same configurations as in Table IX.

TABLE XI.
SF$_6$ Methods and Basis Sets.

	RHF		CI-SD		MRDCI	
	STO	GTO	STO	GTO	STO	GTO
No. configs.[a]	—	—	1	1	3	3
SAFT[b]	—	—	34500	34500	305251	305251
SAF[c]	—	—	34500	34500	128457	134621
Energy	−993.70444	−993.61804	−994.18281	−994.07010	−994.18500	−994.07074
Comput. time	4884.	66.5	316.6	310.8	1587.6	1545.3

[a] Number of reference configurations chosen in the MRDCI calculation. Frozen-core calculation with 34 valence electrons.
[b] Number of generated s ymmetry adapted functions.
[c] Number of selected symmetry-adapted functions.

TABLE XII.
Zn$_3$ Methods and Basis Sets.

	RHF		CI-SD		MRDCI
	STO	GTO	STO	GTO	STO
No. configs.[a]	—	—	1	1	4
SAFT[b]	—	—	198775	—	5034606
SAF[c]	—	—	31632	—	215984
Energy	−5332.98245	−5328.53737[d]	−5333.57044	−5328.53119[d]	−5333.58937
Comput. time	3019.	—	419.7	—	4842.2

[a] Number of reference configurations chosen in the MRDCI calculation. Frozen-core calculation with 36 valence electrons.
[b] Number of generated symmetry-adapted functions.
[c] Number of selected symmetry-adapted functions.
[d] Results of ref. 19.

The results also reinforce the general belief that the STOs are preferable to the GTOs for molecular calculations. This is evident in molecules with heavy atoms, but in molecules with only light atoms this is not so clear because the basis sets of STOs were not properly optimized. Moreover, the advantages of the STO can be greater in the study of the different properties of the energy, such as multipolar moments, force constants, electronic transition moments, etc. Some insight on these aspects could be obtained with this program.

A beta version of this program can be obtained upon request at rafa@qgc.qfa.uam.es.

Appendix: Basis Sets and Geometries

The geometries for the molecules from BH$_3$ to HCN were taken from ref. 13. For the SF$_6$ molecule, the geometry is that of ref. 20. Finally, the geometry of the Zn$_3$ system is the same as in ref. 19.

These geometries are summarized in Table A.I. The single-zeta basis sets for the carbon, boron, and nitrogen atoms were taken from ref. 13. In the case of hydrogen, a $1s$ function with exponent 1.2 was taken. The corresponding set for sulfur, fluorine, and zinc was that of the single-zeta basis set of Clementi and Roetti.[21] The double-zeta basis set is that of Clementi and Roetti in all cases except in hydrogen, where two $1s$ functions with exponents 1.0 and 1.2 were chosen; in zinc, where the basis function of ref. [18] was taken; and in the optimized basis set for HCN in Table X. In this latter case, the optimized basis set is described in the table footnote.

The RHF and correlation energies for the SF$_6$ molecule were studied in ref. 20. We did not use these results for comparison because the RHF energy was calculated with much larger basis sets (optimized basis sets of 278−406 contracted GTOs) and the correlation energy was estimated with the density functional theory method.

TABLE A.I.
Geometries Used for Molecular Calculations.

Molecule	Geometry	Bond Distances and Angles[a]		Nuclear Repulsion Energy[b]
BH_3	Planar	$R_{BH} = 2.25$		7.43646695
B_2H_6	See Fig. 1	$R_{BH} = 2.26013$	$R'_{BH} = 2.53037$	31.74826121
		$R_{BB} = 3.35430$	$\angle_{HBB} = 119°$	
CH_4	Regular tetrahedron	$R_{CH} = 2.0665$		13.39184014
C_2H_2	Linear	$R_{HC} = 2.002$	$R_{CC} = 2.281$	24.73744095
C_2H_4	Planar	$R_{HC} = 2.02203$	$R_{CC} = 2.55116$	33.38244969
		$\angle_{HCH} = 120°$		
C_2H_6	Alternate	$R_{HC} = 2.08250$	$R_{CC} = 2.91588$	41.93239182
		$\angle_{HCH} = 109.32°$	$\angle_{HCC} = 109.62°$	
HCN	Linear	$R_{HC} = 2.0$	$R_{CN} = 2.187$	23.87623099
SF_6	Regular octahedron	$R_{SF} = 2.88769$		579.28919908
Zn_3	Equilateral triangle	$R_{ZnZn} = 5.03593$		536.14717355

[a] Distances are in atomic units and angles in degrees.
[b] Energy is in hartrees.
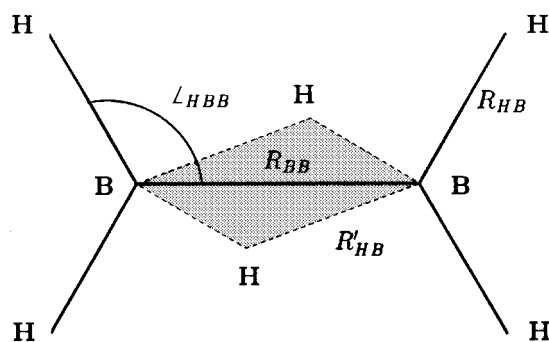
FIGURE 1. Geometry for the B_2H_6 molecule.

Acknowledgment

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