

1. [CCCBDB](#)
2. [Usage](#)
3. [Compare](#)
4. [Quantum 1](#)
5. [Quantum 2](#)
6. [Calcs](#)
7. [Cost](#)
8. [Energetic](#)
9. [Geometric](#)
10. [Vibrational](#)
11. [Electrostatic](#)
12. [Molecules](#)
13. [Molecules 2](#)
14. [Compare 1](#)
15. [Compare](#)
16. [Classify](#)

Computational Chemistry Comparison and Benchmark Database

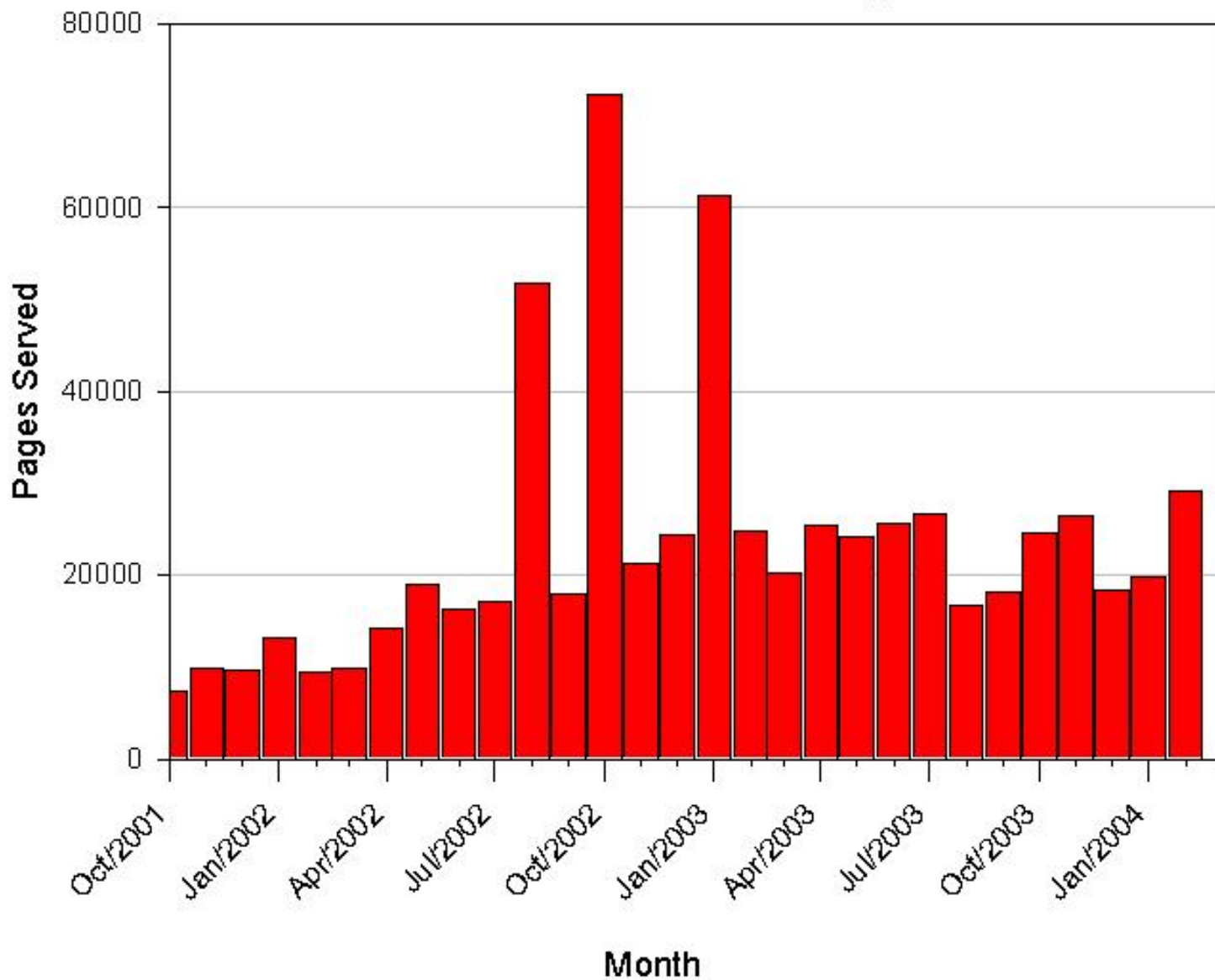
The database/website contains:

- Gas-phase thermochemical properties for 647 molecules.
- 76000 quantum chemical calculations on those molecules.

CCCBDB goal:
How good is that quantum chemical calculation?

It has been online since November 1999. <http://srdata.nist.gov/cccbdb>

CCCBDB Usage



There are 400 requests/month for molecules *not* in the CCCBDB.

Comparisons

- Compare experiment to quantum calculations for the vibrational frequencies of H₂S.
- Compare bond lengths for C-F bonds calculated at HF/6-31G*
- Compare experiment to quantum calculations for the atomization enthalpy of organic alcohols.

Quantum Mechanics

There is a wavefunction, Ψ , which describes the molecule. The properties of the molecule can be obtained from the appropriate operator function.

For the energy of a molecule the operator is the Hamiltonian:

$$H \Psi = E \Psi$$

- H is Hamiltonian (The energy of a system of particles described by their positions and momenta)
- Ψ is the wavefunction
- E is the Energy of the system

Quantum Mechanics 2

But we don't know Ψ , so the quantum chemical programs approximate it from linear combinations of atomic orbitals. Even then we can't solve the eigenvalue problem without throwing out some of the terms in H .

Calculations in CCCBDB

Theory

Basis sets

AMBER, MM+, OPLS

3-21G, 3-21G*

AM1, PM3

6-31G, 6-31G*

HF, ROHF

6-311G*

MP2, MP4

6-31G**

BLYP, B3LYP, B3PW91, MPW1PW91, PBE 6-31+G**

CID, CISD

6-31G(2df,p)

QCISD, QCISD(T)

cc-pVDZ, aug-cc-pVDZ

CCD, CCSD, CCSD(T)

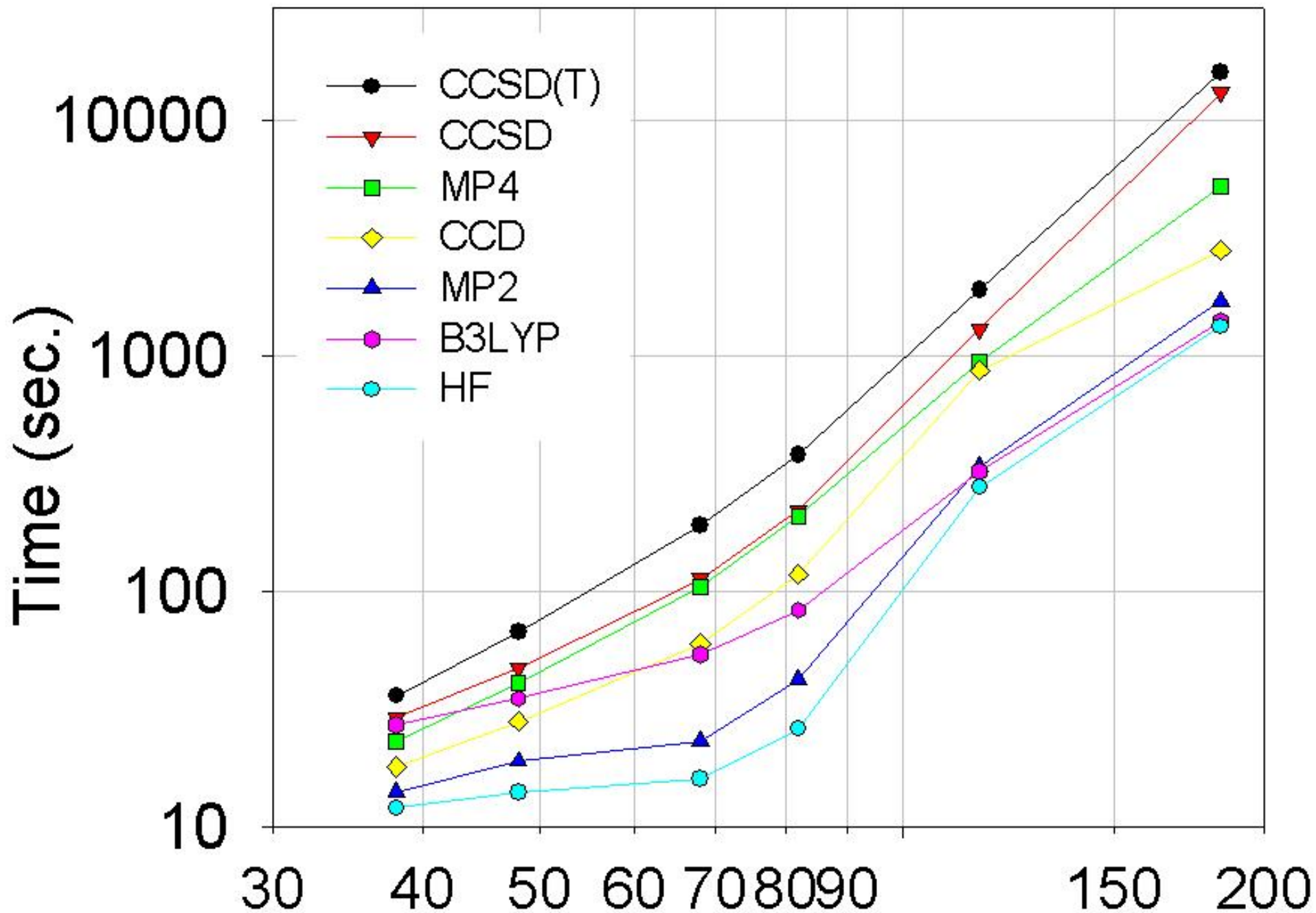
cc-pVTZ

G1, G2, G2MP2, CBS-Q

ECPs

A quantum chemistry *model* is a combination of a **theory** and a **basis set**.

Cost



Properties in CCCBDB

Energetics

- Enthalpies of formation, Enthalpies of atomization, Enthalpies of reaction
- Entropies, Heat capacities, Integrated heat capacities
- Barriers to internal rotation
- Transition States

Properties in CCCBDB

Geometric data

- Bond lengths, angles and dihedrals
- Rotational constants, moments of inertia
- Cartesian coordinates
- Point groups

Properties in CCCBDB

Vibrational data

- Vibrational frequencies, intensities, reduced masses, zero-point energies
- Vibrational scaling factors

Properties in CCCBDB

Electrostatic data

- Atom charges, Dipole moments, Quadrupole moments, Polarizabilities
- Ionization Energies, Nuclear Repulsion Energies

Molecules in CCCBDB

The initial set of molecules was chosen from the NIST webbook with the constraints:

- The uncertainty in the experimental enthalpy of formation is better than 10 kJ/mol.
- No elements heavier than Chlorine.
- No more than 6 heavy (non-hydrogen) atoms.
- No more than 20 atoms total.

Molecules 2

Types of molecules:

- 20 atoms, 81 diatomics, 546 polyatomics, 647 total
- 453 organic molecules (contain carbon)
- 194 inorganic molecules
- 96 radicals (molecular fragments)

Comparisons

3 dimensions of comparisons -

1. Property

- For example: Rotational Constant

2. Molecule(s)

- For example: H₂O

3. Quantum chemical model

- For example: MP2/6-31+G**

Classify Molecules

A given quantum chemical model will perform differently for different molecules.

- Molecules that are similar chemically will have similar bias in results from a quantum chemical model.
- The CCCBDB allows users to compare different classifications of molecules.

**Overall goal:
Assign uncertainties to quantum chemical calculations.**



IV.C.1 Vibrational Frequency Comparison

Please enter the chemical formula

Rules for chemical formula

- Enter a sequence of element symbols followed by numbers to specify the amounts of desired elements (e.g., C6H6).
- Elements may be in any order.
- If only one of a given atom is desired, you may omit the number after the element symbol.
- Parentheses may be used to group atoms.
- Multiple specifications for an atom will be added. This means that **CH3 (CH2) 4CH3** will be treated the same as **C6H14**.
- To specify one or more of a given atom, use a question mark (?) after the element symbol.
- To specify any number (including zero) of given element, use an asterisk (*) after the element symbol.
- A comma delimited list of several species may be entered.

Species in the CCCBDB

- No atoms with atomic number greater than 18 (Argon).
- Six or fewer heavy atoms and twenty or fewer total atoms. *Exception:* Release version 8 and higher have a few substituted benzenes with more than six heavy atoms.



IV.C.1 Vibrational frequency comparison for H₂S (Hydrogen sulfide)

Experimental vibrational frequencies (cm⁻¹)

mode number	symmetry	Frequency
1	A1	2,615
2	A1	1,183
3	B2	2,626

rms differences (cm⁻¹) from experimental frequencies are shown in the following tables.
Click on an entry for details.

d.p.g. = different point group

Methods with predefined basis sets

semi-empirical	AM1	78
	PM3	693
	MNDOd	d.p.g.
molecular mechanics	AMBER	d.p.g.
	DREIDING	128
	UFF	d.p.g.
	MM+	d.p.g.
	MM3	d.p.g.
	BIO+	d.p.g.
	OPLS	d.p.g.

Methods with standard basis sets

		3-21G	3-21G*	6-31G	6-31G*	6-31G**	6-31+G**	6-311G*	6-31G (2df, p)	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-311+G (3df,2p)
hartree fock	HF	178	44	164	28	16	16	49	16	15	16	61	33
density functional	BLYP	197	32	168	28	20	22	72		42	24		
	B3LYP	189	27	160	20	17	20	66	29	42	30	47	
	B3PW91	183	18	143	9	11	13	55		35	28		
	MPW1PW91	164			8	14	11	40		25	19		
	PBEPBE	2,246		2,246	49		65			2,246			
Moller Plesset perturbation	MP2FC	211	33	177	30	42	39	48		27	29	45	
	MP2FU	214			28	63	60	51		34			
	MP4	278			28			112					
Configuration interaction	CID				46			119			46		
	CISD				56						56		
Quadratic configuration interaction	QCISD	277	d.p.g.		17	38	34	91		14	d.p.g.		
	QCISD(T)				24	30	25	110		21	27		
Coupled Cluster	CCD	284			27	23	20	105		24	28		
	CCSD				34	13	13	115		29	33		
	CCSD(T)				46	5	5	132		41	49		

Methods with effective core potentials

		CEP-31G	CEP-31G*	CEP-121G	CEP-121G*	LANL2DZ	SDD
hartree fock	HF	165	22	165	51	152	183
density functional	B3LYP	179	40	183	59	163	169
Moller Plesset perturbation	MP2FC	179	10	184	31	147	178

For descriptions of the methods (AM1, HF, MP2, ...) and basis sets (3-21G, 3-21G*, 6-31G, ...) see the [glossary](#) in section I.C. Predefined means the basis set used is determined by the method.

A large rms difference may be due to different vibrational numbering between experiment and theory. Sometimes this is due to the theory giving a geometry described by a different point group, and sometimes it is because the calculation was run with the wrong geometry (usually at a lower symmetry). We are rerunning calculations to correct this latter problem.



IV.D.4 Comparison of experiment and theory for rCF

Species with coordinate rCF

Species	Name
CH2CHF	Ethene, fluoro-
CH2F2	Methane, difluoro-
CH3CHF2	Ethane, 1,1-difluoro-
CH2CF2	Ethene, 1,1-difluoro-
CHF3	Methane, trifluoro-
CFCI3	Trichloromonofluoromethane
CF2Cl2	difluorodichloromethane
CF4	Carbon tetrafluoride
C2F6	hexafluoroethane
C2F4	Tetrafluoroethylene
CF2O	Carbonic difluoride
CF3CN	Acetonitrile, trifluoro-
CH3CF3	Ethane, 1,1,1-trifluoro-
CH3COF	Acetyl fluoride
CH3F	Methyl fluoride
CF2	Difluoromethylene
CF3	Trifluoromethyl radical
CF	Fluoromethylidyne
HCF	Fluoromethylene

rms differences (calculated - experiment) in Å

The small subscript is the number of bonds with completed calculations.
Click on an entry for a histogram of the difference distribution.

Methods with predefined basis sets

semi-empirical	AM1	0.030 42
	PM3	0.015 42
	MNDOd	

molecular mechanics	AMBER	0.138 37
	DREIDING	
	UFF	
	MM+	0.093 37
	MM3	
	BIO+	0.151 37
	OPLS	0.151 37

Methods with standard basis sets

		3-21G	3-21G*	6-31G	6-31G*	6-31G**	6-31+G**	6-311G*	6-31G (2df, p)	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	6-311+G (3df,2p)
hartree fock	HF	0.016 43	0.016 43	0.028 43	0.017 43	0.017 43	0.015 43	0.022 43	0.026 43	0.018 43	0.024 43	0.014 43	0.024 8
	ROHF	0.022 4			0.015 4	0.015 4	0.014 4	0.021 4		0.016 4	0.023 4		
density functional	BLYP	0.055 43	0.056 36	0.071 42	0.028 43	0.028 43	0.035 43	0.029 36		0.030 43	0.027 33		
	B3LYP	0.036 43	0.038 43	0.053 43	0.012 43	0.012 43	0.016 43	0.011 40	0.008 43	0.012 40	0.009 43	0.020 14	
	B3PW91	0.035 43	0.036 43	0.049 43	0.009 43	0.009 43	0.012 36	0.007 43		0.009 43	0.007 43		
	MPW1PW91	0.031 43	0.036 6	0.049 6	0.007 43	0.007 43	0.008 43	0.007 43		0.007 43	0.005 26		
	PBEPBE	0.048 43		0.064 43	0.021 43		0.026 43			0.022 40			
Moller Plesset perturbation	MP2FC	0.043 43	0.043 43	0.068 43	0.014 43	0.014 42	0.020 43	0.006 43		0.011 36	0.006 28	0.023 28	
	MP2FU	0.046 26	0.048 6	0.070 6	0.013 36	0.013 36	0.019 36	0.006 43		0.010 26	0.005 6		
	MP4	0.056 8	0.065 2		0.022 8			0.010 3					
Configuration interaction	CID				0.005 36			0.007 3					
	CISD	0.045 8			0.005 24	0.008 8							

Quadratic configuration interaction	QCISD	<u>0.054</u> 8	<u>0.057</u> 2	<u>0.085</u> 2	<u>0.014</u> 36	<u>0.017</u> 8	<u>0.024</u> 8	<u>0.004</u> 20		<u>0.015</u> 2	<u>0.002</u> 2		
	QCISD(T)				<u>0.021</u> 3			<u>0.008</u> 3					
Coupled Cluster	CCD	<u>0.048</u> 2	<u>0.048</u> 2	<u>0.075</u> 2	<u>0.011</u> 30	<u>0.013</u> 2	<u>0.016</u> 2	<u>0.002</u> 5		<u>0.008</u> 2	<u>0.004</u> 2		
	CCSD				<u>0.015</u> 8			<u>0.003</u> 3					
	CCSD(T)				<u>0.018</u> 7	<u>0.018</u> 8		<u>0.007</u> 3					

Methods with effective core potentials

		CEP-31G	CEP-31G*	CEP-121G	CEP-121G*	LANL2DZ	SDD
hartree fock	HF	<u>0.037</u> ₄₃	<u>0.011</u> ₄₃	<u>0.036</u> ₄₃	<u>0.011</u> ₄₃	<u>0.034</u> ₄₃	<u>0.034</u> ₄₃
density functional	B3LYP	<u>0.071</u> ₄₃	<u>0.022</u> ₄₃	<u>0.069</u> ₄₃	<u>0.022</u> ₄₃	<u>0.064</u> ₄₃	<u>0.064</u> ₄₃
Moller Plesset perturbation	MP2FC	<u>0.089</u> ₄₃	<u>0.022</u> ₄₃	<u>0.086</u> ₄₃	<u>0.021</u> ₄₃	<u>0.084</u> ₄₃	<u>0.084</u> ₄₃

For descriptions of the methods (AM1, HF, MP2, ...) and basis sets (3-21G, 3-21G*, 6-31G, ...) see the [glossary](#) in section I. C. Predefined means the basis set used is determined by the method.

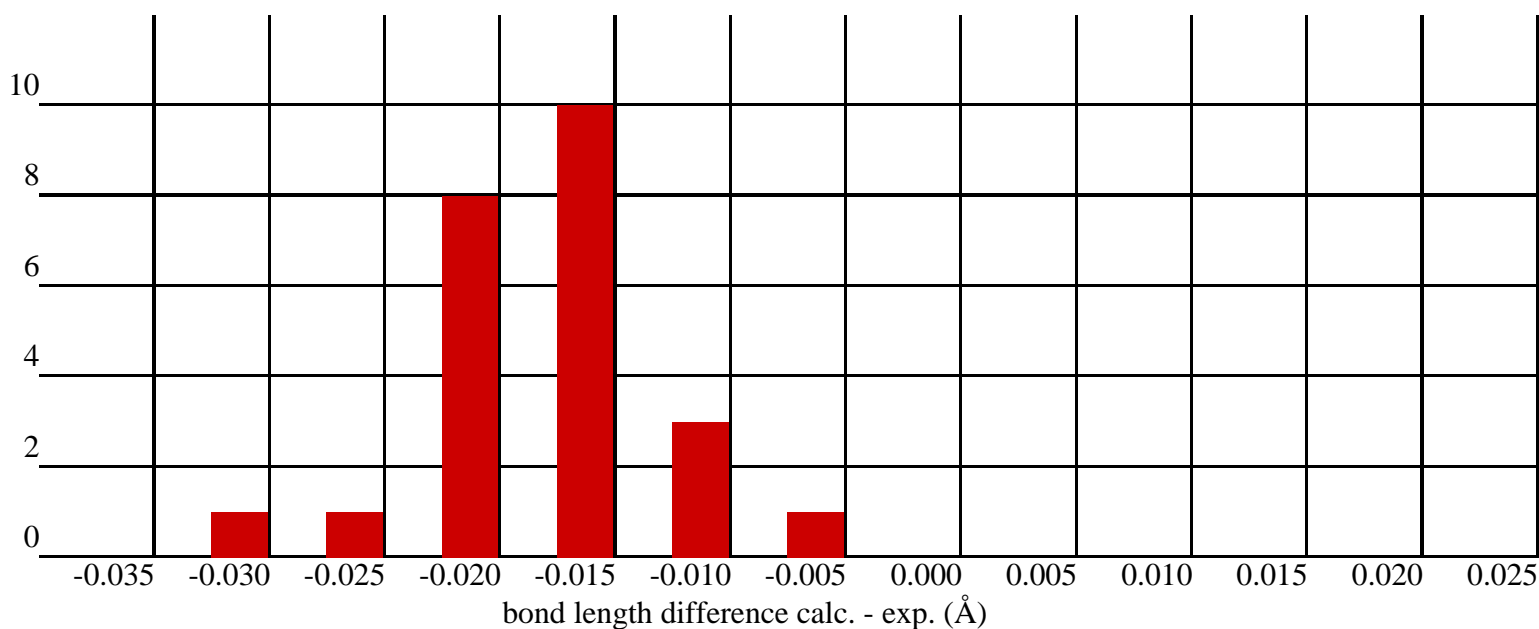


IV.D.4 Compare Bonds

HF/6-31G* for rCF

Histogram of Bond length differences (in Å) vs number of species

Differences greater than 0.025 are in the 0.025 bin. Differences less than -0.035 are in the -0.035 bin.



	Species	Name	Difference (Å)
Most negative difference	CF ₂ Cl ₂	difluorodichloromethane	-0.032
Most positive difference	CF	Fluoromethylidyne	-0.005

Bond lengths

Click on entry for experimental details.

Species	Name	Experimental (Å)	Difference (Å)
CF ₂ Cl ₂	difluorodichloromethane	1.345	-0.032
CFCl ₃	Trichloromonofluoromethane	1.345	-0.023
CF ₂ O	Carbonic difluoride	1.312	-0.022
CH ₃ COF	Acetyl fluoride	1.348	-0.022

CH ₂ CF ₂	Ethene, 1,1-difluoro-	1.323	-0.020
CF ₃ CN	Acetonitrile, trifluoro-	1.328	-0.019
CF ₃ CN	Acetonitrile, trifluoro-	1.328	-0.019
CH ₃ F	Methyl fluoride	1.383	-0.018
CH ₂ CHF	Ethene, fluoro-	1.347	-0.018
CH ₃ CHF ₂	Ethane, 1,1-difluoro-	1.364	-0.018
C ₂ F ₄	Tetrafluoroethylene	1.319	-0.017
CF ₃	Trifluoromethyl radical	1.318	-0.017
CF ₃	Trifluoromethyl radical	1.318	-0.017
CHF ₃	Methane, trifluoro-	1.332	-0.015
CHF ₃	Methane, trifluoro-	1.332	-0.015
CH ₃ CF ₃	Ethane, 1,1,1-trifluoro-	1.340	-0.015
CH ₃ CF ₃	Ethane, 1,1,1-trifluoro-	1.340	-0.015
CF ₂	Difluoromethylene	1.297	-0.014
CF ₄	Carbon tetrafluoride	1.315	-0.013
CH ₂ F ₂	Methane, difluoro-	1.351	-0.013
HCF	Fluoromethylene	1.305	-0.009
C ₂ F ₆	hexafluoroethane	1.320	-0.009
C ₂ F ₆	hexafluoroethane	1.320	-0.009
CF	Fluoromethylidyne	1.272	-0.005



IV.A.2 Heats of Atomization Comparison at 298.15K - Theory versus Experiment

Select a species by entering a chemical formula.

or choose by chemical [groups](#).

Entering a formula will return all species with the same empirical formula. The characters * and ? can be used to indicate (0 or more) or (1 or more). For example C₂H*F? will return all species with two C, zero or more H and one or more F and *no other elements*. A list of species that match the formula criteria is returned and one or more may be selected.

Going to the group selection page allows the selection of molecules with certain chemical groups, such as C=O bonds or NH₂ groups. A list of species that match the group criteria is returned and one or more may be selected.

Caution! Choosing a long list may take a long time to to load. For example: 150 species takes about a minute.



Select group of species

Select from the following tables to search for the species of interest. The search performs a boolean AND so that if both C-N bond is selected and C-F bond is selected the search will return only species with both C-N and C-F bonds. "#" indicates a triple bond.

Bonds														
A-H bonds				C-A bonds								Other		
C-H		Si-H		CC any		CN any		CO any		CS any		CX any		N-O
N-H		P-H		C-C		C-N		C-O		C-S		C-F		N-S
O-H		S-H		C=C		C=N		C=O		C=S		C-Cl		C-P
				C#C		C#N								

Groups							
alkane		C-O-H alcohol		r-N=O		OOH peroxy	3 membered ring
alkene		C-O-C ether		r-NO2 nitro		NH2 amine	4 membered ring
alkyne		COOH acid		r-ONO nitrite			5 membered ring
diene		C(O)OC ester		r-ONO2 nitrate		RCH3	6 membered ring
		CC(O)C ketone		C(O)N amide		R2CH2	aromatic
		CC(O)H aldehyde				R3CH	
		COC epoxide				R4C	
substituted methanes, etc.							
methanes		ethanes		propanes		butanes	pentanes

			ethenes					hexanes
--	--	--	---------	--	--	--	--	---------

Elements				
Must contain these elements				
Must NOT contain these elements				
only first row (H thru Ne)				

Atom Count
Total number of atoms
Heavy (non-hydrogen) atoms

Experimental Uncertainty in Enthalpy of formation (<i>kJ/mol</i>)			
Less or equal to	kJ/	More than	kJ/
mol		mol	

Radicals	
	Must be a radical (unpaired electrons)
	Exclude all radicals

G2 Set (no ions, no excited states)	
	G2-1 set (53 species)
	G2/97 set extended (146 species)

Constraints from experimental vibrational frequencies	
	experimetal frequencies are present
	species that are good for determing scaling factors



Choose which species

Checked species in the following table will be kept



Choose which species				
1		67561	CH3OH	Methyl alcohol
2		64175	CH3CH2OH	Ethanol
3		107211	C2H6O2	1,2-Ethanediol
4		107186	C3H6O	2-Propen-1-ol
5		71238	C3H7OH	1-Propanol
6		67630	CH3CHOHCH3	Isopropyl alcohol
7		504632	C3H8O2	1,3-Propanediol
8		57556	C3H8O2	Propylene glycol
9		2919235	C4H8O	Cyclobutanol
10		71363	C4H10O	1-Butanol
11		78831	C4H10O	1-Propanol, 2-methyl-
12		15892236	C4H10O	2-Butanol, (.+/-)-
13		75650	C4H10O	Ethanol, 1,1-dimethyl-
14		56815	C3H8O3	1,2,3-Propanetriol
15		107880	C4H10O2	1,3-Butanediol
16		110634	C4H10O2	1,4-Butanediol
17		96413	C5H10O	Cyclopentanol

18		137326	C5H12O	1-Butanol, 2-methyl-
19		123513	C5H12O	1-Butanol, 3-methyl-
20		71410	C5H12O	1-Pentanol
21		598754	C5H12O	2-Butanol, 3-methyl-
22		6032297	C5H12O	2-Pentanol
23		108952	C6H6O	phenol

Constraints chosen: COH_alcohol, no radicals



IV.A.2 Heats of Atomization Comparison 298.15K - Theory versus Experiment

23 species with data at 298K.

Experimental Atomization Energies at 298.15K

Species	Name	Atomization Energy kJ mol ⁻¹	Uncertainty
C ₃ H ₈ O ₃	1,2,3-Propanetriol	5,219.5	1.1
C ₃ H ₈ O ₂	Propylene glycol	4,822.2	4.1
CH ₃ CH ₂ OH	Ethanol	3,225.5	
CH ₃ OH	Methyl alcohol	2,038.9	0.6
CH ₃ CHOHCH ₃	Isopropyl alcohol	4,415.9	
C ₃ H ₇ OH	1-Propanol	4,398.4	
C ₄ H ₁₀ O	1-Butanol	5,570.5	
C ₅ H ₁₂ O	1-Pentanol	6,744.2	0.7
C ₄ H ₁₀ O	Ethanol, 1,1-dimethyl-	5,608.3	
C ₄ H ₁₀ O	1-Propanol, 2-methyl-	5,579.7	0.9
C ₅ H ₁₀ O	Cyclopentanol	6,255.1	1.7
C ₃ H ₆ O	2-Propen-1-ol	3,830.8	1.5
C ₂ H ₆ O ₂	1,2-Ethenediol	3,627.2	
C ₄ H ₁₀ O ₂	1,3-Butanediol	5,978.1	2.9
C ₆ H ₆ O	phenol	5,953.6	0.6
C ₄ H ₁₀ O ₂	1,4-Butanediol	5,971.8	2.5
C ₅ H ₁₂ O	1-Butanol, 3-methyl-	6,749.9	1.5
C ₅ H ₁₂ O	1-Butanol, 2-methyl-	6,750.6	1.5
C ₃ H ₈ O ₂	1,3-Propanediol	4,784.4	3.3
C ₅ H ₁₂ O	2-Butanol, 3-methyl-	6,765.0	1.8
C ₄ H ₈ O	Cyclobutanol	5,004.7	
C ₅ H ₁₂ O	2-Pentanol	6,762.4	1.1

C ₄ H ₁₀ O	2-Butanol, (+/-)-	5,588.6	0.3
----------------------------------	-------------------	---------	-----

RMS Atomization Energies Differences (kJ mol⁻¹)

Click on entry for details.

Methods with predefined basis sets

semi-empirical	AM1	356
	PM3	261
	MNDOd	5,472 ¹⁴
composite	G1	21 ¹⁵
	G2MP2	8 ¹⁵
	G2	7 ¹⁵
	G3	4 ²²
	CBS-Q	1,233 ¹⁴

Methods with standard basis sets

		3-21G	3-21G*	6-31G	6-31G*	6-31G**	6-31+G**	6-311G*	6-31G (2df, p)	cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	aug-cc-pVTZ
hartree fock	HF	1,724	1,724	1,736	1,515	1,461	1,480	1,568	1,452	1,551 ₂₂	1,475 ₂₂	1,518 ₂₂	
	ROHF												
density functional	BLYP	134	119 ₁₄	192	69	23	66	113 ₁₄		139	72 ¹⁶		
	B3LYP	151	151	197	50	12	37 ²²	110	9	116 ₂₀	38	72 ⁷	
	B3PW91	130	130	176	30	28	8 ¹⁴	83		79	15		
	MPW1PW91	144			43	24	23	100		95	28 ⁷		
	PBEPBE												
Moller Plesset perturbation	MP2FC	797	797	794	436 ₂₂	222	228	445 ₂₂		282 ₁₃	38 ⁴	180 ⁷	
	MP2FU	577 ⁶			420 ₂₂	181 ₁₃	188 ₁₂	439 ₁₉		232 ⁶			
	MP4	553 ²	615 ¹		300 ³			219 ¹					
Configuration	CID				752 ₁₂			312 ¹					

interaction	CISD				<u>750</u> 12								
Quadratic configuration interaction	QCISD	<u>739</u> 15		<u>677</u> ²	<u>406</u> ⁷	<u>261</u> ³	<u>237</u> ³	<u>428</u> ⁷		<u>311</u> ²			
	QCISD(T)				<u>218</u> ¹			<u>226</u> ¹					
Coupled Cluster	CCD	<u>674</u> ²	<u>674</u> ²	<u>682</u> ²	<u>464</u> 11	<u>267</u> ²	<u>204</u> ¹	<u>417</u> ³		<u>269</u> ¹			
	CCSD				<u>231</u> ¹			<u>244</u> ¹					
	CCSD(T)				<u>287</u> ²	<u>147</u> ²		<u>225</u> ¹					

Methods with effective core potentials

		CEP-31G	CEP-31G*	CEP-121G	CEP-121G*	LANL2DZ	SDD
hartree fock	HF	<u>1,823</u> ²²	<u>1,592</u> ²²	<u>1,854</u> ²²	<u>1,616</u> ²²	<u>1,785</u> ²²	<u>1,784</u> ²²
density functional	B3LYP	<u>408</u> ²²	<u>252</u> ²²	<u>452</u>	<u>286</u>	<u>226</u>	<u>229</u>
Moller Plesset perturbation	MP2FC	<u>944</u> ²²	<u>541</u> ²²	<u>895</u> ²²	<u>513</u> ²²	<u>852</u>	<u>849</u>

Single point energy calculations

		cc-pVDZ	cc-pVTZ	aug-cc-pVDZ	aug-cc-pVTZ	6-311+G (3df,2p)
Moller Plesset perturbation	MP2FC//HF/6-31G*	<u>350</u> ²²	<u>712</u> ²²	<u>809</u> ⁶	<u>20</u> ²	<u>850</u> ⁶
	MP2FC//B3LYP/6-31G*	<u>528</u> ²²	<u>857</u> ⁶	<u>810</u> ⁶	<u>19</u> ²	<u>38</u> ²
	MP2FC//MP2FC/6-31G*	<u>321</u> ⁹	<u>42</u> ⁴	<u>260</u> ²²		
Coupled Cluster	CCSD//HF/6-31G*	<u>403</u> ¹²	<u>134</u> ⁴			
	CCSD(T)//HF/6-31G*	<u>350</u> ¹³	<u>88</u> ⁴	<u>171</u> ²	<u>38</u> ¹	<u>66</u> ²
	CCSD(T)//B3LYP/6-31G*	<u>909</u> ⁶	<u>64</u> ²	<u>126</u> ¹		
	CCSD//MP2FC/6-31G*	<u>277</u> ²	<u>126</u> ²			
	CCSD(T)//MP2FC/6-31G*	<u>250</u> ²	<u>82</u> ²			

If not all the species have calculated data the entry will be followed by a superscript indicating how many of the 23 species have calculated data.

For descriptions of the methods (AM1, HF, MP2, ...) and basis sets (3-21G, 3-21G*, 6-31G, ...) see the [glossary](#) in section I.C. Predefined means the basis set used is determined by the method.

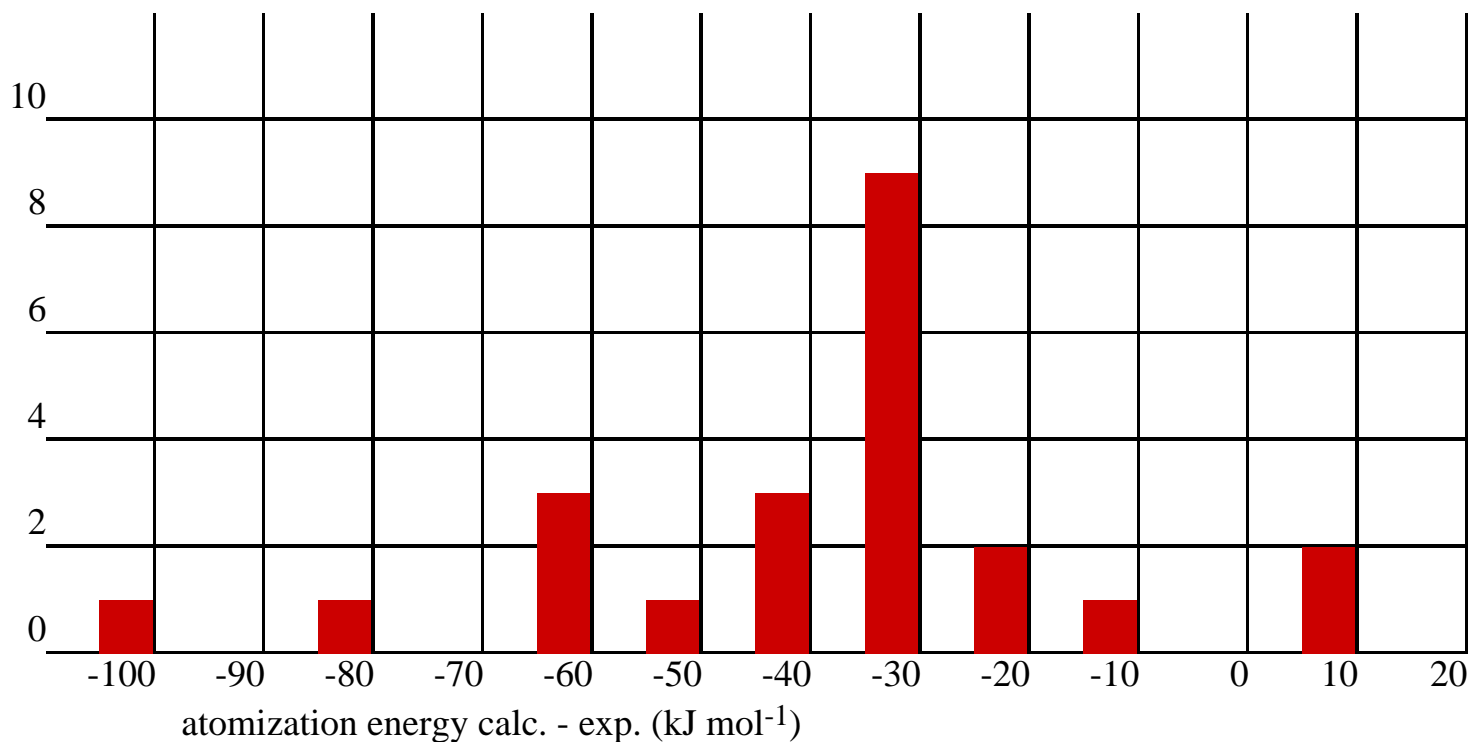


IV.A.2.a Heats of Atomization Comparison at 298.15K - Theory versus Experiment

MPW1PW91/6-31G*

Histogram of Atomization Energy differences vs number of species

Differences greater than 20 are in the 20 bin. Differences less than -100 are in the -100 bin.



23 species have completed calculations from a selection of 23.

	Species	Name	Difference
Most negative difference	C ₃ H ₈ O ₃	1,2,3-Propanetriol	-96
Most positive difference	C ₄ H ₁₀ O	1-Butanol	13

Atomization Energies (kJ mol⁻¹)

Click on entry for details.

Species	Name	Experimental	unc.	Theory	Difference
C ₃ H ₈ O ₃	1,2,3-Propanetriol	5,219	2	5,124	-96
C ₂ H ₆ O ₂	1,2-Ethandiol	3,627		3,552	-75
C ₄ H ₁₀ O ₂	1,4-Butanediol	5,972	3	5,909	-62
C ₃ H ₈ O ₂	Propylene glycol	4,822	4	4,761	-61
C ₃ H ₈ O ₂	1,3-Propanediol	4,784	4	4,729	-56
C ₄ H ₁₀ O ₂	1,3-Butanediol	5,978	3	5,927	-52
C ₃ H ₆ O	2-Propen-1-ol	3,831	2	3,790	-41
CH ₃ OH	Methyl alcohol	2,039	1	1,998	-40
CH ₃ CH ₂ OH	Ethanol	3,226		3,190	-35
C ₅ H ₁₂ O	1-Butanol, 3-methyl-	6,750	3	6,717	-33
C ₄ H ₁₀ O	Ethanol, 1,1-dimethyl-	5,608		5,575	-33
CH ₃ CHOHCH ₃	Isopropyl alcohol	4,416		4,385	-31
C ₃ H ₇ OH	1-Propanol	4,398		4,368	-31
C ₄ H ₁₀ O	1-Propanol, 2-methyl-	5,580	2	5,550	-30
C ₅ H ₁₂ O	1-Butanol, 2-methyl-	6,751	3	6,722	-29
C ₅ H ₁₂ O	2-Butanol, 3-methyl-	6,765	3	6,738	-27
C ₅ H ₁₂ O	2-Pentanol	6,762	3	6,736	-26
C ₄ H ₁₀ O	2-Butanol, (+/-)-	5,589	2	5,563	-26
C ₅ H ₁₂ O	1-Pentanol	6,744	2	6,722	-22
C ₄ H ₈ O	Cyclobutanol	5,005		4,987	-18
C ₅ H ₁₀ O	Cyclopentanol	6,255	3	6,243	-13
C ₆ H ₆ O	phenol	5,954	3	5,962	8
C ₄ H ₁₀ O	1-Butanol	5,570		5,583	13
rms					42.6
average of absolute values					37.2

average value

-35.4
