Geometries for Minnesota Database 2019

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Executive Summary

This document describes our deposit in Data Repository for the University of Minnesota (DRUM) of all the structures and input files used in Minnesota Database 2019.[1] For each structure we provide the geometry, charge, spin multiplicity, and *Gaussian*[2,3,4] settings used in our calculations. In addition we provide basis set information for cases where it is needed in the input files. All the geometries have been reported in literature in the past by us or by our co-workers, and here we put everything together for the convenience of the scientific community.

Citation

A recommended citation for data in this data depository is:

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Introduction to Minnesota Database 2019

Minnesota Database 2019 is subdivided into a primary set with 31 databases and an auxiliary set with 25 databases. The primary data was used for training and testing in Ref. 1, and the auxiliary data is called "additional test data" in Ref. 1. The descriptions of the primary and auxiliary data sets are in Ref. 1 and references cited therein, and the reference values (i.e., accurate values) are in the supporting information of Ref. 1.

The zip file deposited in DRUM contains another copy of the present document plus two folders. One of the folders, named "txt_files", has *Gaussian* input files in .txt format, and the other folder, named "basis_set_files", has basis set files in .gbs format.

There are 64 .txt files that correspond to (a) 30 databases in the primary set, (b) 24 databases in the auxiliary set, and (c) 10 files of S66x8 database. In comparing these databases to Ref. 1, one should note the following small difference. The S66x8 database has 528 data that are here reported as a single database, but in Ref. 1 this data was split into the two databases: S6x6 in the primary set with 36 data and S492 in the auxiliary set with the remaining 492 data. Thus Database 2019 in Ref. 1 has 56 databases, although there are only 55 if one merges S6x6 and S492 into a single database.

Table 1 gives a basic description of each of the 56 databases that are part of Database 2019 and the names of .txt files that correspond to each of them in the "txt_files" folder.

For historical reasons, some users might be interested in the older Minnesota Database 2.0. The *Gaussian* input files for the databases of that database collection are currently given at
https://comp.chem.umn.edu/db/

Table 1. Description of Minnesota Database 2019.

Database	Description	text file name
	Ground-state energies	
SR-MGM-BE8	Single-reference main-group metal bond energies	SR-MGM-BE8_DRUM
SR-MGN-BE107	Single-reference main-group non-metal bond energies	SR-MGN-BE107_DRUM
SR-TM-BE15	Single-reference transition-metal bond energies	SR-TM-BE15_DRUM
MR-MGM-BE4	Multi-reference main-group metal bond energies	MR-MGM-BE4_DRUM
MR-MGN-BE17	Multi-reference main-group non-metal bond energies	MR-MGN-BE17_DRUM
MR-TM-BE12	Multi-reference transition-metal bond energies	MR-TM-BE12_DRUM
MR-TMD-BE3	Multi-reference transition-metal dimer bond energies	MR-TMD-BE3_DRUM
HTBH38/18	Hydrogen transfer barrier heights	HTBH38_DRUM
NHTBH38/18	Non-hydrogen transfer barrier heights	NHTBH38_DRUM
NCCE30/18	Noncovalent complexation energies	NCCE30_DRUM
NGD21/18	Noble gas dimer weak interactions	NGD21_DRUM
S6x6	Subset of S66x8 [Note that in Ref. 1, this database and the S492 database when combined give S66x8.]	S66_0.90_DRUM S66_0.95_DRUM S66_1.00_DRUM S66_1.05_DRUM S66_1.10_DRUM S66_1.25_DRUM S66_1.50_DRUM S66_2.00_DRUM S66_A_DRUM S66_B_DRUM
IP23	Ionization potentials	IP23_DRUM
EA13/03	Electron affinities	EA13_DRUM
PA8	Proton affinities	PA8_DRUM
2pIsoE4	2p isomerization energies	2pIsoE4_DRUM
4pIsoE4	4p isomerization energies	4pIsoE4_DRUM
IsoL6/11	Isomerization energies of large molecules	ISOL6_DRUM
πTC13	Thermochemistry of π systems	pTC13_DRUM
AE17	Atomic energies	AE17_DRUM
HC7/11	Hydrocarbon chemistry	HC7_DRUM
SMAE3/19	Sulfur molecules atomization energies	SMAE3_DRUM
DC9/19	Difficult cases	DC9_DRUM
ABDE13	Alkyl bond dissociation energies	ABDE13_DRUM
Al2X6	Dimerization energies of aluminum compounds	AL2X6_DRUM
BHDIV10	Barrier heights of diverse reactions	BHDIV10_DRUM
BHPERI26	Barrier heights of pericyclic reactions	BHPERI26_DRUM
BHROT27	Barrier heights for rotation around single bonds	BHROT27_DRUM
DIPCS10	Double-ionization potentials of closed-shell systems	DIPCS10_DRUM
HeavySB11	Dissociation energies in heavy-element compounds	HEAVYSB11_DRUM
PX13	Proton-exchange barriers in H_2O, NH_3, HF clusters	PX13_DRUM
SIE4x4	Self-interaction-error	SIE4x4_DRUM
YBDE18	Ylide bond-dissociation energy	YBDE18_DRUM
S492	Subset of S66x8 for noncovalent interaction energies [Note that in Ref. 1, this database and the S6x6 database when combined give S66x8.]	S66_0.90_DRUM S66_0.95_DRUM S66_1.00_DRUM S66_1.05_DRUM S66_1.10_DRUM

		S66_1.25_DRUM S66_1.50_DRUM S66_2.00_DRUM S66_A_DRUM S66_B_DRUM
TMBH22	Transition-metal reaction barrier heights of Mo, W, Zr, Re reactions	TMBH22_DRUM
WCCR10	Ligand dissociation energies of large cationic transition-metal complexes	WCCR10_DRUM
ASNC2	Atmospheric sulfur-nitrogen cluster binding energies	ASNC2_DRUM
	Ground-state noncovalent potential energy curves	
PEC4	Potential energy curves of Ar_2, Kr_2, KrHe, Ne_2	PEC4_DRUM
	Ground-state dipole moments	
DM79	Dipole moments	DM79_DRUM
	Test of ground-state delocalization error	
NaCl	Charge on Na in NaCl at 10 Å interatomic separation	NaCl_DRUM
	Ground-state bond lengths	
DGL6	Bond lengths for diatoms with light atoms	DGL6_DRUM
DGH4	Bond lengths for diatoms with one or more nonhydrogenic atom	DGH4_DRUM
TSG48	Transition state geometries	TSG48_DRUM
MGBL193	Bond lengths of main-group containing systems	MGBL193_DRUM
TMDBL10	Transition-metal dimer bond lengths	TMDBL10_DRUM
	Excitation energies calculated by ΔSCF	
3dEE8	Excitation energies involving 3d orbitals	3dEE8_DRUM
4dAEE5	4d transition-metal atomic excitation energies	4dAEE5_DRUM
pAEE5	p-block atomic excitation energies	pEE5_DRUM
	Excitation energies calculated by LR-TDDFT	
EE23	Excitation energies of molecules	EE23_DRUM
LRCTEE9	Excitation energies of long-range charge transfer complexes	LRCTEE9_DRUM
EEA11	Excitation energies of atoms	EEA11_DRUM
AEE15	Adiabatic excitation energies of molecules	AEE15_DRUM
EEAroT5	Excitation energies of aromatic molecule complexes with TCNE	EEAroT5_DRUM
EE69	Excitation energies of organic molecules	EE69_DRUM
EER5	Excitation energies of retinal and dihydroretinal	EER5_DRUM
LRCTEE2	Excitation energies of long-range charge transfer complexes	LRCTEE2_DRUM

Comments on stability checks and frequency calculations

When performing calculations on Minnesota Database 2019, frequency calculations and stability checks may or may not be required. Several input files have keywords corresponding to them, and these keywords may be removed at the discretion of the user.

Stability checks followed by reoptimization of the wave function are invoked via the stable = opt or stable = (opt, xqc) keyword; these two keywords can be used interchangeably and stable = (opt, xqc) may be used if stable = opt fails to converge.

Basis sets

Some basis sets are specified in the input file, while others are in a basis set file in the "basis_set_files" folder. The databases for which basis set files are provided are as follows:

- 4pIsoE4 – cc-pVQZ.gbs
- ABDE13 – def2-ma-TZVP.gbs
- AE17 – cc-p_5Z.gbs
- ASNC2 – MG3S.gbs
- DC9 – mg3s.gbs
- DGH4 – modified_basis.gbs
- EA13 – mg3s.gbs
- EE23 – jul-cc-pVT+dZ.gbs
- HTBH38 – mg3s.gbs
- IP23 – mg3s.gbs
- ISOL6 – MG3SXP.gbs
- MR-MGM-BE4 – aug-cc-pcvqz_f_o_s.gbs
- MR-MGN-BE17 – mg3s.gbs
- MR-TM-BE13 – def2-ma-TZVP.gbs, def2.gbs, HOSCl-avtz_TM-apwcvtz_NR.gbs,
- NCCE30 – mg3s.gbs
- NHTBH38 – mg3s.gbs
- PA8 – mg3s.gbs
- pEE5 – d-aug-cc-pvqz-dk.gbs
- pTC13 – mg3s.gbs
- SMAE3 – mg3s.gbs
- SR-MGN-BE107 – mg3s.gbs
- SR-TM-BE17 – def2.gbs, def2-ma-TZVP.gbs, HOSCl-avtz_TM-apwcvtz_NR.gbs
- TMBH22 – Mix_QZ_PP_Mo.gbs, Mix_ATZ_PP_W.gbs, Mix_QZ_PP_W.gbs, Mix_ATZ_PP_Mo.gbs, Mix_QZ_PP.gbs, Mix_TZ_PP_Re.gbs, Mix_QZ_PP_Zr.gbs
- TSG48 – mg3s.gbs

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References

1. Verma, P.; Wang, Y.; Ghosh, S.; He, X.; Truhlar, D. G. Revised M11 Exchange-Correlation Functional for Electronic Excitation Energies and Ground-State Properties. *J. Phys. Chem. A* **2019**, *123*, 2966–2990. doi.org/10.1021/acs.jpca.8b11499

2. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; et al. *Gaussian 09*, Revision C.01, Gaussian, Inc.: Wallingford CT, 2010.

3. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; et al. *Gaussian 16*, Revision A.03, Gaussian, Inc.: Wallingford CT, 2016.

4. Zhao, Y.; Peverati, R.; Yang, K. R.; Luo, S.; Yu, H. S.; He, X.; Wang, Y.; Verma, P.; Truhlar, D. G. *MN-GFM*, version 6.10: Minnesota–Gaussian Functional Module. (See https://comp.chem.umn.edu/mn-gfm/).