QCSchema

circa 9 Jan 2026, v0.50rc1

ACCESS QCSchema v1 in QCElemental
(PYDANTIC v1 API; c. 2019 field layout)

```
# longstanding until v0.70
> from qcelemental.models import Molecule

# longstanding until v0.70 but remove ASAP!
> from qcelemental.models.molecule import Molecule

# v0.50a1 until v1.0
> from qcelemental.models.v1 import Molecule
```

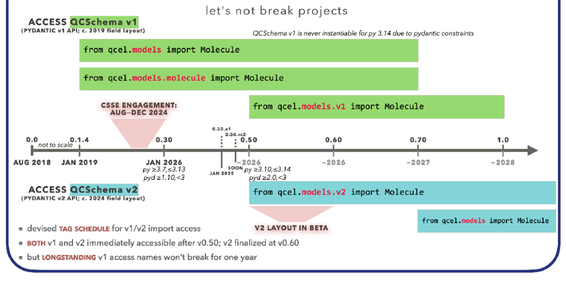
ACCESS QCSchema v2 in QCElemental
(PYDANTIC v2 API; c. 2024 field layout)

```
# v0.50a1 until v0.60 (beta layout)
# v0.60a1 onwards (final layout)
> from qcelemental.models.v2 import Molecule

# v0.70a1 onwards
> from qcelemental.models import Molecule
```

same info, two representations

QCSchema ACCESS PLAN
let's not break projects



Legend

ResultSchemaClass
field: brief field description
fixed_value_field: **True**
required_field: description
example: 'content'
field_with_options: shows choices for values. In this case: a string, a list of schema, a dictionary of schema (dummy key), and a rare-to-use choice.
- **gradient**
- [**AtomicResult**]
- {sub id: **ManyBodyResult** }
- OptimizationResult

field_holding subschema: description

InputSchemaClass
field: description
another_field: description

another_field: description

V1_InputSchemaClass
field: description
another_field: note that fields of this class left-align with outer child class **ResultSchemaClass** since in v1, **<>Result** inherits from **<>Input**.

tentative_or_inherited_field: description

*light blue dotted – **input** schema*
*dark blue solid – **output** schema*

Main Models in QCSchema (v2 names)

AtomicResult	OptimizationResult	TorsionDriveResult	ManyBodyResult	v1 inherited	v2	
AtomicInput	OptimizationInput	TorsionDriveInput	ManyBodyInput	v1	v2	
AtomicSpecification	OptimizationSpecification	TorsionDriveSpecification	ManyBodySpecification	v1	–	
AtomicKeywords	OptimizationKeywords	TorsionDriveKeywords	ManyBodyKeywords	–	–	
AtomicProtocols	OptimizationProtocols	TorsionDriveProtocols	ManyBodyProtocols	–	–	
AtomicProperties	OptimizationProperties	TorsionDriveProperties	ManyBodyProperties	–	–	
WavefunctionProperties				–	–	schema_version present?
			Molecule	v1	v2	
			BasisSet	v1	v2	
			FailedOperation	–	v2	

RUN QCEngine CMDLINE

```
# run with full local resources. use run-procedure for opt/td/mbe in v1
sh> qcengine run cmscode qcskin

# run with restricted resources: 4 cores, 4 GiB
sh> qcengine run cmscode qcskin  --ncores 4 --memory 4

# run with restricted resources: 4 cores, 4 GiB. available to sub-qcng calls
sh> cat qcengine.yaml
all:
  hostname_pattern: "*"
  ncores: 4
  memory: 4
sh> qcengine run cmscode qcskin
```

RUN QCEngine PyAPI

```
# run with full local resources. use compute_procedure for opt/td/mbe in v1
> qcengine.compute(qcskin, cmscode)

# run with restricted resources: 4 cores, 4 GiB
> qcengine.compute(qcskin, cmscode, task_config={"nnodes": 4, "memory": 4})

# run with restricted resources: 4 cores, 4 GiB. available to sub-qcng calls
sh> cat qcengine.yaml
all:
  hostname_pattern: "*"
  nnodes: 4
  memory: 4
> qcengine.compute(qcskin, cmscode)
```

Version Handling in QCEngine

```
> *Result v1 = qcengine.compute( *Input v1 )          no v1 models for py≥3.14
> *Result v2 = qcengine.compute( *Input v2 )
> *Result v2 = qcengine.compute( *Input v1, return_version=2)
> *Result v1 = qcengine.compute( *Input v2, return_version=1)
```

object, unless `return_dict=True` *object or dict*

QC Job Models

Comparing v1 & v2 QCSchema

Trace the same data horizontally between v1/v2 pairs and, to some degree, between schema.

any SP program in QCEngine

adcc · cfour · gamess · entos · mrchem · qchem · torchani · terachem terachem_pbs · nwchem · xtb · turbomole · mace · molpro · psi4 · s-dftd3 dftd3 · mopac · aimnet2 · dftd4 · rdkit · openmm · mp2d · mctc-gcp gcp

RUN QCSchema v1

any program in QCEngine

```
> qcng.compute( AtomicInput , ... )
```

RUN QCSchema v2

```
> qcengine.compute(atin, ... )
> qcengine.compute(atin)  (nyi in QCEngine)
```

QCSchema v1 ⟷ QCSchema v2 (convert_v(v))

AtomicResult

AtomicInput
schema_version: **1**
provenance: creator, version, & RT info
QCElemental, 0.28.0
id: tracker for databases
extras: free-form storage
molecule: **Molecule**
specification: *how* to run single-point
protocols: customize return layout
AtomicResultProtocols
stdout: save text output
wavefunction: save orbital info
native_files: save raw prog. files
error_correction: auto-edit&rerun
driver: single-point derivative
- energy
- gradient E G H
- Hessian
- properties

model: model chemistry or FF
method: B3LYP-D3, CCSD(T)
basis: 6-31G*, cc-pV5Z BasisSet
keywords: knobs in SP program
{scftyp: uhf, cc_conv: 7, docc: [4,1]}

success: True
provenance: *(overwrites input)*
xtb, 1.0.0, psinet, CPU E5-2630
stdout: program's text output for humans
stderr: anything in error channel
native_files: requested raw program files
extras: *(merges with input)*
molecule: *(overwrites inp w/result frame)*
return_result: single-point derivative
E · G H
properties: key results for single-point

AtomicResultProperties (abr.)
calcinfo_natom
calcinfo_nmo
nuclear_repulsion_energy
return_energy: E ·
return_gradient: G
scf_total_*egh*: ref. energy, gradient, etc.
***mtd*_correlation_energy:** post-scf energy
***mtd*_iterations:** count to convergence
***mtd*_mpole_moment:** dipole etc. array

wavefunction: orbital-level results

WavefunctionProperties (abr.)
basis: **BasisSet**
restricted: alpha == beta
orbitals_a/b
density_a/b
fock_a/b
eigenvalues_a/b
occupations_a/b

error: hold **ComputeError** for success=F

AtomicResult
schema_version: **2**
input_data: record of starting conditions

AtomicInput
schema_version: **2**
provenance: creator, version, & RT info
QCElemental, 0.28.0
id: tracker for databases
molecule: **Molecule**
specification: *how* to run single-point
AtomicSpecification
program: any SP in QCEngine
protocols: customize return layout
AtomicProtocols
stdout: save text output
wavefunction: save orbital info
native_files: save raw prog. files
error_correction: auto-edit&rerun
extras: free-form storage
driver: single-point derivative
- energy
- gradient E G H
- Hessian
- properties

model: model chemistry or FF
method: B3LYP-D3, CCSD(T)
basis: 6-31G*, cc-pV5Z BasisSet
keywords: knobs in SP program
{scftyp: uhf, cc_conv: 7, docc: [4,1]}

success: **True**
provenance: creator, version, & RT info
xtb, 1.0.0, psinet, CPU E5-2630
id: tracker for databases
stdout: program's text output for humans
stderr: anything in error channel
native_files: requested raw program files
extras: free-form storage
molecule: orientation & frame for results
return_result: single-point derivative
E · G H
properties: key results for single-point

AtomicProperties (abr.)
calcinfo_natom
calcinfo_nmo
nuclear_repulsion_energy
return_energy: E ·
return_gradient: G
scf_total_*egh*: ref. energy, gradient, etc.
***mtd*_correlation_energy:** post-scf energy
***mtd*_iterations:** count to convergence
***mtd*_mpole_moment:** dipole etc. array

wavefunction: orbital-level results

WavefunctionProperties (abr.)
basis: **BasisSet**
restricted: alpha == beta
orbitals_a/b
density_a/b
fock_a/b
eigenvalues_a/b
occupations_a/b

any optimizer procedure in QCEngine
optking · geometric · nwchemdriver · berny

RUN QCSchema v1

any optimizer in QCEngine

```
>qcengine.compute_procedure(optin, )
```

RUN QCSchema v2

```
> qcengine.compute(optin, )
> qcengine.compute(optin)  (nyi in QCEngine)
```

QCSchema v1 ⟷ QCSchema v2 (convert_v(v))

OptimizationResult

OptimizationInput
schema_version: **1**
provenance: creator name and version info
QCElemental, 0.28.0
id: tracker for databases
extras: free-form storage
initial_molecule: **Molecule**
protocols: customize opt return layout
OptimizationProtocols
trajectory: save fewer opt steps
keywords: knobs in the geo opt program
{coordsys: tric, program: }
input_specification: how to run *gradients* for opt
QCInputSpecification
schema_version: **1**
extras: free-form storage
driver: single-point derivative
- energy
- gradient E G H
- Hessian
- properties

model: model chemistry or FF
method: B3LYP-D3, CCSD(T)
basis: 6-31G*, cc-pV5Z
keywords: knobs in SP program
{scftyp: uhf, cc_conv: 7, docc: [4,1]}

success: True
provenance: *(overwrites input)*
geomeTRIC, 1.0.2, psinet, CPU E5-2630
stdout: Opt program's text output for humans
stderr: anything in error channel
extras: *(merges with input)*
final_molecule: optimized geom. for results
energies: energy for opt steps
[E ·]
trajectory: full results for opt steps
[**AtomicResult**]

error: hold **ComputeError** for success=F

OptimizationResult
schema_version: **2**
input_data: record of starting conditions

OptimizationInput
schema_version: **2**
provenance: creator name and version info
QCElemental, 0.28.0
id: tracker for databases
initial_molecule: **Molecule**
specification: how to run *geometry opts*
OptimizationSpecification
program: any optimizer in QCEngine
protocols: customize opt return layout
OptimizationProtocols
trajectory_results: save any opt steps
extras: free-form storage
keywords: knobs in the geo opt program
{coordsys: tric, maxiter: 100}
specification: how to run *gradients* for opt
- single-point

AtomicSpecification
program: any SP in QCEngine
protocols: customize return layout
AtomicProtocols
stdout: save text output
wavefunction: save orbital info
native_files: save raw prog. files
error_correction: auto-edit&rerun
extras: free-form storage
driver: single-point derivative
- energy
- gradient E G H
- Hessian
- properties

model: model chemistry or FF
method: B3LYP-D3, CCSD(T)
basis: 6-31G*, cc-pV5Z BasisSet
keywords: knobs in SP program
{scftyp: uhf, cc_conv: 7, docc: [4,1]}
- MBE
ManyBodySpecification

success: **True**
provenance: creator, version, & RT info
geomeTRIC, 1.0.2, psinet, CPU E5-2630
id: tracker for databases
stdout: Opt program's text output for humans
stderr: anything in error channel
native_files: requested raw program files *(nyi)*
extras: free-form storage
final_molecule: optimized geom. for results
properties: key results for optimization

OptimizationProperties
nuclear_repulsion_energy
return_energy: E ·
return_gradient: G
optimization_iterations: count to geo conv.
final_rms_force: measure of convergence *(nyi)*
opt_coordinate_system: intrnl, Cart., tric *(nyi)*
trajectory_properties: key results for opt steps
- [**AtomicProperties**]
- [**ManyBodyProperties**]

trajectory_results: full results for opt steps
- [**AtomicResult**]
- [**ManyBodyResult**]

any TD procedure in QCEngine
torsiondrive

RUN QCSchema v1

any TD in QCEngine

```
> qcengine.compute_procedure(tdin, )
```

RUN QCSchema v2

```
> qcengine.compute(tdin, )
> qcengine.compute(tdin)  (nyi in QCEngine)
```

QCSchema v1 ⟷ QCSchema v2 (convert_v(v))

TorsionDriveResult

TorsionDriveInput
schema_version: **1**
provenance: creator name and version info
QCElemental, 0.28.0
extras: free-form storage
initial_molecule: **Molecule**
keywords: knobs in the TD program
TDKeywords
dihedrals: dimensions to scan
dihedral_ranges: limits of scan
grid_spacing: IE dihedral steps of scan
energy_decrease_thresh: point trigger
energy_upper_limit: new point trigger
optimization_spec: how to run *geometry opts*
OptimizationSpecification
schema_version: **1**
procedure: any optimizer in QCEngine
protocols: customize opt return layout
OptimizationProtocols
trajectory: save fewer opt steps
keywords: knobs in the geo opt program
{coordsys: tric, program: ...}
input_specification: how to run *gradients* for opt
QCInputSpecification
schema_version: **1**
extras: free-form storage
driver: single-point derivative
- energy
- gradient E G H
- Hessian
- properties

model: model chemistry or FF
method: B3LYP-D3, CCSD(T)
basis: 6-31G*, cc-pVQZ BasisSet
keywords: knobs in SP program
{scftyp: uhf, cc_conv: 7, docc: [4,1]}

success: True
provenance: *(overwrites input)*
torsiondrive, 1.1.0, psinet, CPU E5-2630
stdout: TD program's text output for humans
stderr: anything in error channel
extras: *(merges with input)*
final_molecules: optimized molecules for angles
{dihedral id: **Molecule** }
final_energies: optimized energy for angles
{dihedral id: E · }
optimization_history: full results for all opts
{dihedral id: [**OptimizationResult**] }

error: hold **ComputeError** for success=F

TorsionDriveResult
schema_version: **2**
input_data: record of starting conditions

TorsionDriveInput
schema_version: **2**
provenance: creator name and version info
QCElemental, 0.28.0
id: tracker for databases
initial_molecule: [**Molecule**]
specification: *how* to run *torsion drive* opts
TorsionDriveSpecification
program: any TD in QCEngine
protocols: customize TD return layout
TorsionDriveProtocols
scan_results: save any optimization data
extras: free-form storage
keywords: knobs in the TD program
TorsionDriveKeywords
dihedrals: dimensions to scan
dihedral_ranges: limits of scan
grid_spacing: IE dihedral steps of scan
energy_decrease_thresh: point trigger
energy_upper_limit: new point trigger
specification: how to run *geometry opts*
OptimizationSpecification
program: any optimizer in QCEngine
protocols: customize opt return layout
OptimizationProtocols
trajectory_results: save any opt steps
extras: free-form storage
keywords: knobs in the geo opt program
{coordsys: tric, maxiter: 100}
specification: how to run *gradients* for opt
- single-point

AtomicSpecification
program: any SP in QCEngine
protocols: customize return layout
AtomicProtocols
stdout: save text output
wavefunction: save orbital info
native_files: save raw prog. files
error_correction: auto-edit&rerun
extras: free-form storage
driver: single-point derivative
- energy
- gradient E G H
- Hessian
- properties

model: model chemistry or FF
method: B3LYP-D3, CCSD(T)
basis: 6-31G*, cc-pV5Z BasisSet
keywords: knobs in SP program
{scftyp: uhf, cc_conv: 7, docc: [4,1]}
- MBE
ManyBodySpecification

success: **True**
provenance: creator, version, & RT info
torsiondrive, 1.1.0, psinet, CPU E5-2630
id: tracker for databases
stdout: TD program's text output for humans
stderr: anything in error channel
native_files: requested raw program files *(nyi)*
extras: free-form storage
final_molecules: optimized molecules for angles
{dihedral id: **Molecule** }
properties: key results for torsion drive
TorsionDriveProperties
calcinfo_ngrid: count dihedral scan pts optimized
scan_properties: key results for best opt steps
{dihedral id: **OptimizationProperties** }
scan_results: full results for all opts
{dihedral id: [**OptimizationResult**] }

any MBE procedure in QCEngine
qcmanybody

RUN QCSchema v1

any TD in QCEngine

```
> qcengine.compute_procedure(mbein, )
```

RUN QCSchema v2

```
> qcengine.compute(mbein, )
> qcengine.compute(mbein)  (nyi in QCEngine)
```

QCSchema v1 ⟷ QCSchema v2 (convert_v(v))

ManyBodyResult

ManyBodyInput
schema_version: **1**
extras: free-form storage
molecule: **Molecule**
specification: *how* to run MBE single-point
ManyBodySpecification
schema_version: **1**
protocols: customize MBE return layout
ManyBodyProtocols
component_results: save any sub data
extras: free-form storage
driver: MBE target derivative
- energy
- gradient E G H
- Hessian

keywords: knobs in the MBE program
ManyBodyKeywords
schema_version: 1
bsse_type: any combination of
- nocp/mbe
- cp/ssfc
- vmfc

embedding_charges
return_total_data: IE or total
levels:
- {2: hi, 4: lo}
- {1: hi, 2: md, supersystem: lo}

max_nbody: truncate MBE early
supersystem_ie_only: no MBE analysis
specification: how to run MBE *subsystems*
- single

AtomicSpecification*
schema_version: **1**
program: any SP in QCEngine
protocols: customize return layout
AtomicResultProtocols
stdout: save text output
wavefunction: save orbital info
native_files: save raw prog. files
error_correction: auto-edit&rerun
extras: free-form storage
driver: single-point derivative
- energy
- gradient E G H
- Hessian
- properties

model: model chemistry or FF
method: B3LYP-D3, CCSD(T)
basis: 6-31G*, cc-pV5Z BasisSet
keywords: knobs in SP program
{scftyp: uhf, cc_conv: 7, docc: [4,1]}
- mapping
{hi: **AtomicSpecification** ,
lo: **AtomicSpecification** }

success: True
provenance: creator, version, & RT info
QCManyBody, 0.3.0, psinet, CPU E5-2630
id: tracker for databases
stdout: program's text output for humans
stderr: anything in error channel
extras: free-form storage
return_result: MBE derivative
E · G H
properties: key results for MBE

ManyBodyResultProperties
schema_version: 1
calcinfo_nfr: M
return_energy: E ·
return_gradient: G
***bsse_corrected_interaction_egh_through_m_body*:**
- defined as E^{m}_{IE}
- defined for all *bsse* as **bsse_type** allows
- defined for all *egh* as **driver** allows
- def. for all *m* as **max_nbody/levels** allows

***bsse_corrected_total_egh_through_m_body*:**
- defined as E^{m}

***bsse_corrected_m_body_contribution_to_egh*:**
- defined as $E^{(m)}$

component_properties: key results for subsys
{cluster id: **AtomicResultProperties** }
component_results: full results for subsystems
{cluster id: **AtomicResult** }

ManyBodyResult
schema_version: **2**
input_data: record of starting conditions

ManyBodyInput
schema_version: **2**
provenance: creator name and version info
QCManyBody, 0.5.0
id: tracker for databases
molecule: **Molecule**
specification: *how* to run MBE single-point
ManyBodySpecification
program: any MBE speaking QCSchema
protocols: customize MBE return layout
ManyBodyProtocols
cluster_results: save any sub data
extras: free-form storage
driver: MBE target derivative
- energy
- gradient E G H
- Hessian

keywords: knobs in the MBE program
ManyBodyKeywords
bsse_type: any combination of
- nocp/mbe
- cp/ssfc
- vmfc

embedding_charges
return_total_data: IE or total
levels:
- {2: hi, 4: lo}
- {1: hi, 2: md, supersystem: lo}

max_nbody: truncate MBE early
supersystem_ie_only: no MBE analysis
specification: how to run MBE *subsystems*
- single

AtomicSpecification
program: any SP in QCEngine
protocols: customize return layout
AtomicProtocols
stdout: save text output
wavefunction: save orbital info
native_files: save raw prog. files
error_correction: auto-edit&rerun
extras: free-form storage
driver: single-point derivative
- energy
- gradient E G H
- Hessian
- properties

model: model chemistry or FF
method: B3LYP-D3, CCSD(T)
basis: 6-31G*, cc-pV5Z BasisSet
keywords: knobs in SP program
{scftyp: uhf, cc_conv: 7, docc: [4,1]}
- mapping
{hi: **AtomicSpecification** ,
lo: **AtomicSpecification** }

success: **True**
provenance: creator, version, & RT info
QCManyBody, 0.5.0, psinet, CPU E5-2630
id: tracker for databases
stdout: program's text output for humans
stderr: anything in error channel
native_files: requested raw program files
extras: free-form storage
molecule: orientation & frame for results
return_result: MBE derivative
E · G H
properties: key results for MBE

ManyBodyProperties
calcinfo_nfr: M
return_energy: E ·
return_gradient: G
***bsse_corrected_interaction_egh_through_m_body*:**
- defined as E^{m}_{IE}
- defined for all *bsse* as **bsse_type** allows
- defined for all *egh* as **driver** allows
- def. for all *m* as **max_nbody/levels** allows

***bsse_corrected_total_egh_through_m_body*:**
- defined as E^{m}

***bsse_corrected_m_body_contribution_to_egh*:**
- defined as $E^{(m)}$

cluster_properties: key results for subsystems
{cluster id: **AtomicProperties** }
cluster_results: full results for subsystems
{cluster id: **AtomicResult** }

live at GH:MolSSI/QCManyBody repo

Listed below are the **schema_name** *values for major models in the respective columns above. Changes bolded.*

qcschema_output
qcschema_input

qcschema_atomic_result
qcschema_atomic_input
qcschema_atomic_specification
qcschema_atomic_protocols
qcschema_atomic_properties
qcschema_wavefunction_properties

qcschema_optimization_output
qcschema_optimization_input

qcschema_input

qcschema_optimization_result
qcschema_optimization_input
qcschema_optimization_specification
qcschema_optimization_protocols
qcschema_atomic_specification
qcschema_optimization_properties

qcschema_torsion_drive_output
qcschema_torsion_drive_input

qcschema_optimization_specification
qcschema_input

qcschema_torsion_drive_result
qcschema_torsion_drive_input
qcschema_torsion_drive_specification
qcschema_torsion_drive_protocols
qcschema_torsion_drive_keywords
qcschema_optimization_specification
qcschema_atomic_specification

qcschema_manybodyoutput
qcschema_manybodyinput
qcschema_manybodyspecification

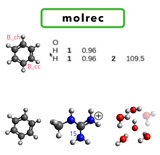
qcschema_manybodykeywords
qcschema_atomicspecification
qcschema_manybodyproperties

qcschema_many_body_output
qcschema_many_body_input
qcschema_many_body_specification
qcschema_many_body_protocols
qcschema_many_body_keywords
qcschema_atomic_specification
qcschema_many_body_properties

Molecule Models

Comparing v1 & v2 QCSchema

molrec



Molecule v2

Molecule v3

(nyi)

Molecule ("molrec")
schema_version: **psi4**
provenance: creator info

name: user label
comment: further user text
elem: elemental symb. for atoms
geom: Cartesian coord. in **units**
molecular_charge: net elst. charge
molecular_multiplicity: total **int** mult.
mass: per atom atomic masses
real: per atom real vs. ghost/virtual
elbl: further per atom labels
elez: per atom atomic numbers
elea: per atom isotope #

fragment_separators: gr'p atoms **idx**
fragment_charges: partitioned chg
fragment_multiplicities: ptn'd **int** mult
fix_com: conserve input COM
fix_orientation: conserve input frame
fix_symmetry: use lesser point group
connectivity: bond info **(unused)**

units: Bohr or Ångstrom for **geom**
input_units_to_au: conversion factor
geom_unsettled: replaces **geom** for Z-matrices or Cartesian w/variables
variables: names & vals, complete?

not QCSchema *but parseable in QCElemental*

Molecule
schema_version: **2** *(used w/QCSk v**1**)*
provenance: creator info
id: tracker for databases
extras: free-form storage
name: user label
comment: further user text
symbols: elemental symb. for atoms
geometry: Cartesian coord. in Bohr
molecular_charge: net elst. charge
molecular_multiplicity: total mult.
masses: per atom atomic masses
real: per atom real vs. ghost/virtual
atom_labels: further per atom labels
atomic_numbers: per atom numbers
mass_numbers: per atom isotope #

fragments: group atoms into fragmts
fragment_charges: partitioned chg
fragment_multiplicities: ptn'd mult
fix_com: conserve input COM
fix_orientation: conserve input frame
fix_symmetry: use lesser point group
connectivity: bond info
validated: passed physics checks
identifiers: registration/classification

Identifiers (abr.)
molecular_formula
smiles
inchi
canonical_isomeric_smiles
canonical_smiles
pubchem_cid
pubchem_conformerid

qcschema_molecule

Molecule
schema_version: **3** *(used w/QCSk v**2**)*
provenance: creator info
id: tracker for databases
extras: free-form storage
name: user label
comment: further user text
symbols: elemental symb. for atoms
geometry: Cartesian coord. in Bohr
molecular_charge: net elst. charge
molecular_multiplicity: total mult.
masses: per atom atomic masses
real: per atom real vs. ghost/virtual
atom_labels: further per atom labels
atomic_numbers: per atom numbers
mass_numbers: per atom isotope #
abc: periodic box vectors *(nyi)*
fragments: group atoms into fragmts
fragment_charges: partitioned chg
fragment_multiplicities: ptn'd mult
fix_com: conserve input COM
fix_orientation: conserve input frame
fix_symmetry: use lesser point group
connectivity: bond info
validated: passed physics checks
identifiers: registration/classification

Identifiers (abr.)
molecular_formula
smiles
inchi
canonical_isomeric_smiles
canonical_smiles
pubchem_cid
pubchem_conformerid

qcschema_molecule

Basis Set Models

Comparing v1 & v2 QCSchema

BasisSet
schema_version: **1**
name: BSE standard name, e.g., cc-pVDZ
description: text of characteristics
nbf: basis function count
atom_map: center & mol. correspondence
center_data: merged for all atoms/centers
{center_id:
BasisCenter
electron_shells: elec. shells for this center
[
ElectronShell
angular_momentum: *d*=[2]; *sp*=[0,1]
harmonic_type: shell repr. for AM≥2
- **spherical**
- **cartesian**

exponents: exp. for contracted shell
coefficients: nested list of coeff. Outer generalized; inner segmented.
]
ecp_electrons: #e^- replaced by field pots
ecp_potentials: field pots for this center
[
ECPPotential
angular_momentum: *d*=[2]; *sp*=[0,1]
ecp_type:
- **scalar**
- **spinorbit**

r_exponents: exp. of *r* term
gaussian_exponents: exp. of e^{-r^2} term
coefficients: nested list of coeff. Outer generalized; inner segmented.
]
}

qcschema_basis_set

BasisSet
schema_version: **2**
name: BSE standard name, e.g., cc-pVDZ
description: text of characteristics
nbf: basis function count
atom_map: center & mol. correspondence
center_data: merged for all atoms/centers
{center_id:
BasisCenter
electron_shells: elec. shells for this center
[
ElectronShell
angular_momentum: *d*=[2]; *sp*=[0,1]
harmonic_type: shell repr. for AM≥2
- **spherical**
- **cartesian**

exponents: exp. for contracted shell
coefficients: nested list of coeff. Outer generalized; inner segmented.
normalization_scheme: lbl conv. *(nyi)*
- **bse** *(nyi)*
- **cca** *(nyi)*

]
ecp_electrons: #e^- replaced by field pots
ecp_potentials: field pots for this center
[
ECPPotential
angular_momentum: *d*=[2]; *sp*=[0,1]
ecp_type:
- **scalar**
- **spinorbit**

r_exponents: exp. of *r* term
gaussian_exponents: exp. of e^{-r^2} term
coefficients: nested list of coeff. Outer generalized; inner segmented.
]
}

qcschema_basis_set

Error Handling Models

Comparing v1 & v2 QCSchema

FailedOperation
input_data: dict record of starting conditions
- **AtomicInput**
- **OptimizationInput**
- **TorsionDriveInput**
- **ManyBodyInput**

success: False
id: tracker for databases
extras: free-form storage
error: components to build error object

ComputeError
error_type: classification
- **Input:** bad user param, unrecoverable
- **Resource:** insufficient memory, cores, disk; likely recoverable on diff. node
- **Random:** likely recoverable from segfault, disk I/O
- **Unknown:** cannot classify

error_message: user text
extras: free-form storage

FailedOperation
schema_version: **2**
input_data: record of starting conditions
- **AtomicInput**
- **OptimizationInput**
- **TorsionDriveInput**
- **ManyBodyInput**

success: **False**
id: tracker for databases
extras: free-form storage
error: components to build error object

ComputeError
error_type: classification
- **Input:** bad user param, unrecoverable
- **Resource:** insufficient memory, cores, disk; likely recoverable on diff. node
- **Random:** likely recoverable from segfault, disk I/O
- **Unknown:** cannot classify

error_message: user text
extras: free-form storage

qcschema_failed_operation

`Return of qcengine.compute()`

good_calc	raise_error	return_dict	output
T	F (def)	F (def)	``AtomicResult`` object
T	T	F (def)	``AtomicResult`` object
T	T	T	dict of ``AtomicResult``
T	F (def)	T	dict of ``AtomicResult``
F	F (def)	F (def)	``FailedOperation`` object
F	T	F (def)	raises ``InputError`` (type encoded in FailedOp)
F	T	T	raises ``InputError`` (type encoded in FailedOp)
F	F (def)	T	dict of ``FailedOperation``