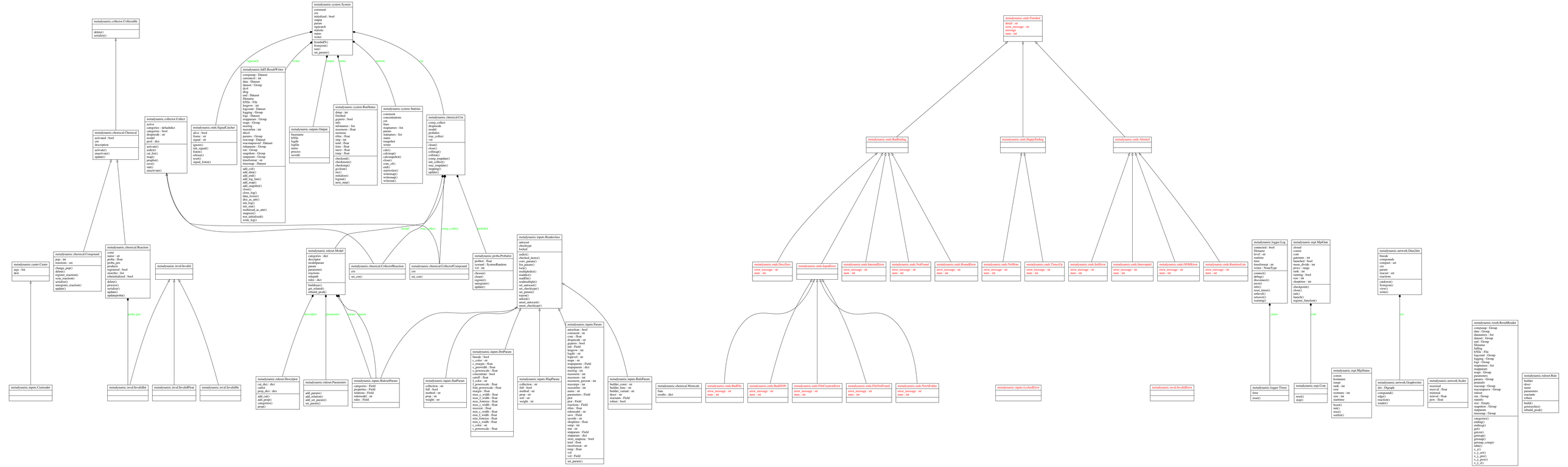
metadynamic.collector.Collectable
delete()
serialize()
metadynamic.system.System
comment
cwd
initialized : bool
output
param
signcatch
stderr
status
writer
fromhdf5()
fromjson()
run()
set_param()
metadynamic.hdf5.ResultWriter
compmap : Dataset
currentcol : int
data : Group
dataset : Group
dcol
dbg
end : Dataset
fatalerr
h5file : File
longrow : int
logcount : Dataset
logging : Group
log_count : int
mapparam : Group
maps : Group
maxlog
recorders : int
root : Group
params : Group
reacmap : Dataset
reacmapcurrent : Dataset
rnkparam : Group
rnk_count : int
snapshots : Group
statparam : Group
timeformat : str
timemap : Dataset
add_col()
add_data()
add_log()
add_log_line()
add_map()
add_snapshot()
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data_row()
data_resize()
dict_as_attr()
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snapsize()
test_initialized()
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metadynamic.collector.Collect
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categories : defaultdict
categorize : bool
dropnode : str
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pool : dict
activate()
add_pool()
cat_list()
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metadynamic.ends.SignalCatcher
alive : bool
frame : str
signal : str
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signal_trans()
metadynamic.outputs.Output
basename
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name
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metadynamic.system.RunStatus
disup : int
disup_ref
gcpeto : bool
info
infonames : list
maxmem : float
maxtime : float
rfim : float
step : int
tend : float
time : float
tmax : float
tstep : float
checkend()
checkmem()
checkstep()
gcclean()
inc()
initialize()
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next_step()
metadynamic.system.Statistic
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magnumnes : list
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statnames : list
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conc_of()
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startwriter()
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metadynamic.chemical.Chemical
activated : bool
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description
activate()
unactivate()
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metadynamic.chemical.Ctrs
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pool : dict
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initialize_pandas()
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reac_toupdate()
stepping()
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metadynamic.chemical.Compound
pop : int
reactions : set
change_pop()
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register_reaction()
set_reaction()
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metadynamic.chemical.Reaction
const
name : str
proba : float
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reversible : bool
reactlist : list
toheminalized : bool
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metadynamic.caster.Caster
args : list
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metadynamic.inputs.Castreader
metadynamic.inval.Invalid
metadynamic.inval.InvalidIn
metadynamic.inval.InvalidFloat
metadynamic.inval.InvalidStr
metadynamic.ruleset.Model
categories : dict
descriptor
modelparam
param
parameters
reactions
rulepath
rules : dict
buildreac()
get_relatedr()
rebuild_prod()
metadynamic.ruleset.Descriptor
cat_dict : dict
name
prop_dict : dict
add_cat()
add_prop()
categories()
prop()
metadynamic.ruleset.Parameters
add_param()
add_setparam()
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metadynamic.inputs.RulesetParam
categories : Field
properties : Field
relatives : Field
rulepath : Field
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metadynamic.chemical.CollectorReaction
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metadynamic.chemical.CollectorCompound
ctrs
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metadynamic.inputs.StatParam
collection : str
full : bool
method : str
prop : str
weight : str
metadynamic.inputs.DotParam
binode : bool
c_color : str
c_margin : float
c_powwidth : float
c_powscale : float
concentrate : bool
cutoff : float
f_color : str
f_powwidth : float
f_powscale : float
margin : float
max_c_width : float
max_f_width : float
max_fontsize : float
max_n_width : float
maxsize : float
min_c_width : float
min_f_width : float
min_fontsize : float
min_n_width : float
n_color : str
n_powscale : float
metadynamic.inputs.MapParam
collection : str
full : bool
method : str
prop : str
sort : str
weight : str
metadynamic.inputs.ReaderClass
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set_autocast()
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metadynamic.probs.Probalist
probtot : float
rcvseed : SystemRandom
vol : int
choose()
clean()
register()
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update()
metadynamic.inputs.Param
autoclean : bool
autocast : bool
conc : float
dropnode : str
ggperto : bool
int : Field
longrow : int
log : Field
loglevel : str
maps : str
mapparam : Field
mapparam : dict
max : Field
maxmem : int
maxmem : int
maximum_percent : int
maxtaps : int
minimum : int
name : str
parameters : Field
plot : bool
pool : Field
prop : Field
rfim : float
referenced : str
save : Field
seredir : str
sigfigs : int
sorp : int
stat : str
statparam : Field
statparam : dict
stepping_number : bool
total : float
timeformat : str
tmap : float
vol
write : Field
set_param()
metadynamic.inputs.RulesParam
builder_conv : str
builder_func : str
builder_variant : str
descr : str
reactants : Field
robust : bool
metadynamic.chemical.Memcalc
func
results : dict
metadynamic.ends.Finished
detail : str
error_message : str
name : str
num : int
metadynamic.ends.BadEnding
metadynamic.ends.HappyEnding
metadynamic.ends.Aborted
metadynamic.ends.DescZero
error_message : str
num : int
metadynamic.ends.InputError
metadynamic.ends.InternalError
error_message : str
num : int
metadynamic.ends.NotFound
error_message : str
num : int
metadynamic.ends.RoundError
error_message : str
num : int
metadynamic.ends.NoMore
error_message : str
num : int
metadynamic.ends.TimeUp
error_message : str
num : int
metadynamic.ends.InitError
error_message : str
num : int
metadynamic.ends.Interrupted
error_message : str
num : int
metadynamic.ends.OOMError
error_message : str
num : int
metadynamic.ends.RuntimeLim
error_message : str
num : int
metadynamic.ends.BadFile
error_message : str
num : int
metadynamic.ends.BadJSON
error_message : str
num : int
metadynamic.ends.FileCreationError
error_message : str
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metadynamic.ends.FileNotFound
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num : int
metadynamic.ends.NotAFolder
error_message : str
num : int
metadynamic.inputs.LockedError
metadynamic.inval.InvalidError
metadynamic.logger.Log
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settlevel()
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metadynamic.logger.Timer
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metadynamic.mpi.MpiGate
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comm
cost
gatenum : int
mpi_rank : int
mem_divide : int
procs : range
rank : int
running : bool
size : int
sleeptime : int
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register_function()
metadynamic.mpi.Cost
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rank : int
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rootsize : int
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metadynamic.network.DataZlib4
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compounds
compsel : set
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reacset : set
reactions
cmdrows()
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write()
metadynamic.network.GraphwriterDot
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reaction()
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metadynamic.network.Scaler
maximal
maxval : float
minimal
minval : float
pow : float
metadynamic.result.ResultReader
compmap : Group
data : Group
datanames : list
dataset : Group
dcol : Group
dbgmsg
fatlog
h5file : File
logcount : Group
logging : Group
log_count : int
mapnames : list
mapparam
maps : Group
parameters
parameters : Group
protmin
reacmap : Group
reacmapcur : Group
ruleset
rnk : Group
runinfo
size : Empty
snapshots : Group
statparam
timemap : Group
categories()
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endmsg()
get()
getctrl()
getmap()
getsnap()
gotmap_compt()
table()
x_y()
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metadynamic.ruleset.Rule
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