main:711:execute 514.154606 100.00% (0.024353) (0.00%) 1×
reactors:505:to_rms 4.236508 0.82% (4.134255) (0.81%) 14964×
0.17% 6906×
11.27% 1×
39.26% 270×
6.92% 136×
1.77% 2×
model:589:enlarge 201.864581 39.26% (0.026310999999999998) (0.01%) 275×
main:1954:save_everything 35.594888999999995 6.92% (0.0015589999999999998) (0.00%) 136×
main:1692:generate_cantera_files 9.117654 1.77% (8.3e-05) (0.00%) 2×
main:467:initialize 57.947624999999995 11.27% (0.000523) (0.00%) 1×
0.96% 139×
26.07% 136×
11.63% 756×
3.50% 136×
3.42% 136×
1.77% 2×
model:1107:add_species_to_core 4.9591449999999995 0.96% (0.691018) (0.13%) 139×
react:99:react_all 134.04831099999998 26.07% (0.044121) (0.01%) 136×
model:799:process_new_reactions 59.794835 11.63% (0.125959) (0.02%) 756×
main:1948:save_profiler_info 17.998413 3.50% (0.892245) (0.17%) 136×
util:110:notify 17.594858 3.42% (9.387551) (1.83%) 136×
ck2yaml:2039:convert_mech 9.103181 1.77% (0.000352) (0.00%) 2×
10.97% 1×
26.06% 136×
10.98% 6694×
3.27% 136×
1.55% 2×
main:374:load_database 56.381944 10.97% (0.000384) (0.00%) 1×
react:42:react 134.003048 26.06% (0.00146) (0.00%) 136×
model:449:make_new_reaction 56.440256 10.98% (0.372909) (0.07%) 6694×
cProfile:54:snapshot_stats 16.818583 3.27% (10.553659999999999) (2.06%) 136×
ck2yaml:1900:write_yaml 7.984229999999999 1.55% (0.0006299999999999999) (0.00%) 2×
4.07% 1×
2.40% 36×
26.06% 782×
1.80% 5151×
8.26% 6330×
0.87% 136×
1.55% 12×
rmg:74:load 20.921518 4.07% (3.1e-05) (0.00%) 1×
family:1360:fill_rules_by_averaging_up 12.324555 2.40% (0.013231) (0.00%) 36×
react:77:_react_species_star 133.98916 26.06% (0.0010969999999999999) (0.00%) 782×
model:492:<listcomp> 9.242690999999999 1.80% (0.013193) (0.00%) 5151×
0.72% 2516×
model:929:apply_kinetics_to_reaction 42.48312 8.26% (0.0247) (0.00%) 6330×
~:0:<method 'getstats' of '_lsprof.Profiler' objects> 4.44851 0.87% (4.44851) (0.87%) 136×
main:560:dump 7.9800489999999999 1.55% (1.6e-05) (0.00%) 12×
2.73% 1×
2.39% 36×
1.80% 9977×
8.25% 6330×
1.55% 12×
rmg:143:load_kinetics 14.044252 2.73% (7e-06) (0.00%) 1×
rules:454:fill_rules_by_averaging_up 12.311245999999999 2.39% (5.605201) (1.09%) 897753×
2.39% 277×
4.50% 36×
react:82:react_species 133.98806299999998 26.06% (0.0040939999999999995) (0.00%) 782×
model:274:make_new_species 13.146325 2.56% (0.462669) (0.09%) 24421×
model:951:generate_kinetics 42.442797 8.25% (0.094465) (0.02%) 6330×
main:576:dump_all 7.980033 1.55% (4.9999999999999996e-05) (0.00%) 12×
39.53% 270×
2.73% 1×
26.06% 782×
2.23% 576×
8.23% 7348×
1.55% 12×
database:105:load 14.044224999999999 2.73% (1.2e-05) (0.00%) 1×
database:474:generate_reactions_from_families 133.982917 26.06% (0.066311) (0.01%) 782×
model:889:generate_thermo 11.938849999999999 2.32% (0.030784) (0.01%) 1147×
family:2621:get_kinetics 42.309255 8.23% (0.032459) (0.01%) 7348×
main:910:dump 7.9796059999999995 1.55% (0.005702) (0.00%) 12×
2.73% 1×
10.52% 1090×
2.12% 576×
7.90% 7348×
1.55% 12×
database:147:load_families 14.032345999999999 2.73% (0.00043799999999999997) (0.00%) 1×
family:1166:add_rules_from_training 23.135157 4.50% (0.773783) (0.15%) 36×
2.73% 1205×
database:555:react_molecules 54.083017999999996 10.52% (0.055055) (0.01%) 1090×
thermoengine:173:submit 10.93789 2.13% (0.001046) (0.00%) 582×
family:2580:get_kinetics_from_depository 40.621626 7.90% (40.521366) (7.91%) 7348×
representer:78:represent 7.973235 1.55% (0.003189) (0.00%) 12×
2.73% 51×
0.34% 100×
12.69% 782×
10.51% 55590×
2.13% 582×
1.30% 12×
family:700:load 14.028545 2.73% (0.005405) (0.00%) 51×
family:1907:calculate_degeneracy 63.615568999999994 12.37% (0.11240399999999999) (0.02%) 5251×
family:1818:add_reverse_attribute 14.04516 2.73% (0.017685) (0.00%) 1205×
family:1769:generate_reactions 54.023485 10.51% (0.122649) (0.02%) 55590×
thermoengine:147:evaluator 10.936843999999999 2.13% (0.09140899999999999) (0.02%) 582×
serializer:100:serialize 6.682238 1.30% (0.0011589999999999999) (0.00%) 12×
2.29% 51×
1.27% 5251×
0.41% 5251×
12.03% 5151×
10.67% 10145×
0.10% 1205×
0.21% 1205×
2.41% 1205×
10.48% 100280×
2.47% 295×
2.07% 582×
1.28% 12×
depository:128:load 11.760572 2.29% (0.191818) (0.04%) 51×
common:226:find_degenerate_reactions 65.814146 12.80% (5.325489999999999) (1.04%) 7238×
family:1978:_generate_reactions 121.175366 23.57% (2.88509) (0.56%) 111630×
thermoengine:106:generate_thermo_data 10.648316 2.07% (0.005821) (0.00%) 582×
serializer:153:serialize_node 6.5849079999999995 1.28% (0.499517) (0.10%) 72616×
1.28% 36×
0.42% 102×
1.19% 6841×
common:186:ensure_independent_atom_ids 8.090819 1.57% (2.7460359999999997) (0.54%) 7238×
2.11% 51×
0.13% 51×
15.22% 108885×
6.21% 51874×
0.98% 155266×
1.83% 581×
0.90% 84524×
base:293:get_species 10.834721 2.11% (0.9651689999999999) (0.19%) 51×
base:203:load 9.703604 1.89% (0.0021809999999999998) (0.00%) 181×
0.18% 31409×
family:1633:_generate_product_structures 78.253728 15.22% (0.714218) (0.14%) 108885×
family:2730:get_reaction_template_labels 32.002884 6.22% (0.055) (0.01%) 51974×
family:1734:_match_reactant_to_template 5.0162939999999999 0.98% (4.614458) (0.90%) 155266×
thermo:1247:get_thermo_data 22.085193999999998 4.30% (0.68217299999999999) (0.13%) 876×
emitter:251:emit 4.6158209999999995 0.90% (0.178457) (0.03%) 84572×
1.59% 7687×
1.81% 181×
0.19% 21212×
12.97% 108510×
1.83% 393282×
6.21% 51974×
3.97% 773×
~:0:<method 'simulate' of 'rmgpy.solver.base.ReactionSystem' objects> 203.25036 39.53% (153.852261) (30.04%) 270×
adjlist:465:from_adjacency_list 11.706074 2.28% (5.516907) (1.08%) 22664×
~:0:<built-in method builtins.exec> 514.154709 100.00% (1.293407) (0.25%) 188×
family:1373:apply_recipe 66.80899999999999 12.99% (33.230239) (6.49%) 108691×
family:1686:is_molecule_forbidden 9.401999 1.83% (0.503011) (0.10%) 393282×
family:2551:get_reaction_template 38.058073 7.40% (0.063951) (0.01%) 58815×
thermo:1884:get_thermo_data_from_groups 20.401761 3.97% (0.037702) (0.01%) 773×
0.16% 7687×
0.15% 7687×
0.15% 124359×
2.17% 1329926×
3.46% 2910618×
2.58% 431463×
0.91% 156733×
0.41% 40964×
3.38% 392514×
1.72% 352753×
7.39% 58815×
3.93% 1212×
<__array_function__ internals>:2:sum 11.140583999999999 2.17% (0.864244) (0.17%) 1330270×
<__array_function__ internals>:2:zeros_like 17.928361 3.49% (1.4764169999999999) (0.29%) 2920484×
fragment:466:detect_cutting_label 19.71756 3.83% (10.83531) (2.12%) 627751×
Graph:45:from_edges 22.316799 4.34% (1.60946) (0.31%) 481644×
base:1326:is_molecule_forbidden 8.852995 1.72% (7.483726) (1.46%) 352897×
groups:111:get_reaction_template 37.994122 7.39% (0.645728) (0.13%) 58815×
thermo:2122:estimate_thermo_via_group_additivity 20.200272 3.93% (0.009785) (0.00%) 1212×
0.37% 1965690×
2.41% 1970253×
1.96% 1330270×
3.14% 2920484×
0.17% 627751×
0.97% 72819116×
0.11% 352897×
3.93% 4547933×
0.64% 37599×
3.37% 988×
~:0:<built-in method numpy.core._multiarray_umath.implement_array_function> 27.71782 5.39% (7.688002) (1.50%) 10426094×
<frozen importlib:1009:_handle_fromlist 4.60942 0.90% (1.0854789999999999) (0.21%) 4106483×
~:0:<method 'append' of 'list' objects> 5.912561999999999 1.15% (5.912561999999999) (1.15%) 81675895×
Graph:81:add_edge 20.227798 3.93% (9.178796) (1.79%) 4547933×
copy:132:deepcopy 22.190029 4.32% (10.063563) (1.97%) 9646441×
0.43% 351866×
thermo:2021:estimate_radical_thermo_via_hbi 17.564141 3.42% (0.42277499999999996) (0.08%) 1990×
0.55% 224×
2.89% 2920484×
1.81% 1330270×
1.50% 9095866×
1.25% 5883190×
2.20% 2949231×
numeric:76:zeros_like 14.834719999999999 2.89% (3.208164) (0.63%) 2920484×
fromnumeric:2123:sum 9.305121999999999 1.81% (1.617788) (0.32%) 1330270×
Graph:75:_add_or_get_node_index 7.719544999999999 1.50% (6.769372) (1.32%) 9095866×
copy:237:_deepcopy_dict 11.31866 2.20% (3.9504219999999997) (0.77%) 2949366×
2.67% 988×
0.56% 2922931×
0.47% 2926193×
thermo:2143:compute_group_additivity_thermo 16.558602 3.22% (0.291222) (0.06%) 1212×
0.46% 13156×
6.59% 109167×
0.95% 2920484×
0.82% 2920484×
1.43% 1330270×
1.53% 36430×
1.28% 155×
thermo:2535:_add_group_thermo_data 10.197735 1.98% (0.415207) (0.08%) 49586×
thermo:2270:_add_polycyclic_correction_thermo_data 6.591991999999999 1.28% (0.0018969999999999998) (0.00%) 155×
0.33% 453×
<__array_function__ internals>:2:empty_like 4.895726 0.95% (1.6783789999999998) (0.33%) 2922931×
<__array_function__ internals>:2:copyto 4.215485999999999 0.82% (1.408353) (0.28%) 2926193×
fromnumeric:69:_wrapreduction 7.433469 1.45% (2.188421) (0.43%) 1343326×
0.15% 8062261×
0.81% 155×
thermo:2433:_add_ring_correction_thermo_data_from_tree 8.147545 1.58% (0.016319) (0.00%) 798×
1.87% 49586×
0.82% 1334622×
~:0:<method 'reduce' of 'numpy.ufunc' objects> 5.190341 1.01% (5.190341) (1.01%) 1646087×
1.47% 6324×
base:1026:descend_tree 51.60019 10.04% (2.21215) (0.43%) 630751×
6.78% 96884×
9.56% 3909584×
base:943:match_node_to_structure 49.172945999999996 9.56% (42.772697) (8.35%) 4544585×
0.68% 35241622×
~:0:<built-in method builtins.isinstance> 6.894323 1.34% (6.874002) (1.34%) 61312473×