**Supporting Information File 2**

**Cartesian coordinates of all the stationary points discussed in the main text**

**1** (S0)

 ---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 2.313815 2.199899 0.000000

 2 6 0 1.163644 2.989069 0.000000

 3 6 0 -0.082170 2.343002 -0.000000

 4 7 0 0.000000 0.976132 -0.000000

 5 6 0 1.078281 0.135525 0.000000

 6 6 0 2.299495 0.780334 0.000000

 7 7 0 -1.390766 2.686558 -0.000000

 8 6 0 -2.090172 1.518370 -0.000000

 9 6 0 -1.236701 0.398700 -0.000000

 10 6 0 0.470554 -1.188346 0.000000

 11 6 0 -0.962957 -1.023604 -0.000000

 12 6 0 -1.787372 -2.151083 -0.000000

 13 6 0 -1.201987 -3.411203 -0.000000

 14 6 0 0.193169 -3.569839 0.000000

 15 6 0 1.034407 -2.464391 0.000000

 16 1 0 3.276797 2.695792 0.000000

 17 1 0 1.220977 4.068804 -0.000000

 18 1 0 3.227602 0.225334 0.000000

 19 1 0 -3.169530 1.526633 -0.000000

 20 1 0 -2.865400 -2.044957 -0.000000

 21 1 0 -1.835019 -4.290818 -0.000000

 22 1 0 0.617157 -4.566654 0.000000

 23 1 0 2.110737 -2.591556 0.000000

 ---------------------------------------------------------------------

**1** (S1)

 ---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 2.269672 2.271280 0.000000

 2 6 0 1.090943 3.045375 -0.000000

 3 6 0 -0.128685 2.317132 -0.000000

 4 7 0 0.000000 0.986054 -0.000000

 5 6 0 1.086460 0.161220 0.000000

 6 6 0 2.321799 0.866821 0.000000

 7 7 0 -1.483437 2.612683 -0.000000

 8 6 0 -2.152273 1.448329 -0.000000

 9 6 0 -1.244906 0.343410 -0.000000

 10 6 0 0.521343 -1.160690 0.000000

 11 6 0 -0.942584 -1.049966 -0.000000

 12 6 0 -1.746055 -2.188483 -0.000000

 13 6 0 -1.140056 -3.453175 0.000000

 14 6 0 0.256477 -3.559238 0.000000

 15 6 0 1.094482 -2.431997 0.000000

 16 1 0 3.214578 2.803749 0.000000

 17 1 0 1.107755 4.123410 -0.000000

 18 1 0 3.267700 0.346361 0.000000

 19 1 0 -3.230091 1.416707 -0.000000

 20 1 0 -2.825657 -2.095135 -0.000000

 21 1 0 -1.750117 -4.346723 0.000000

 22 1 0 0.709587 -4.544079 0.000000

 23 1 0 2.170606 -2.555543 0.000000

 ---------------------------------------------------------------------

**2**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 2.652359 -1.788447 -0.238304

 2 6 0 3.189395 -0.416717 0.273562

 3 6 0 2.191741 0.674667 0.027304

 4 7 0 0.913866 0.258206 -0.077769

 5 6 0 0.327442 -1.009882 -0.002331

 6 6 0 1.167281 -2.053911 -0.020053

 7 7 0 2.222661 1.997933 0.045604

 8 6 0 0.896538 2.419786 -0.030178

 9 6 0 0.048994 1.326120 -0.090234

 10 6 0 -1.116487 -0.702186 0.022694

 11 6 0 -1.282476 0.718559 -0.049866

 12 6 0 -2.559655 1.265847 -0.055552

 13 6 0 -3.661778 0.410225 0.009492

 14 6 0 -3.498062 -0.974546 0.076883

 15 6 0 -2.220450 -1.539518 0.081256

 16 1 0 2.837325 -1.853562 -1.320180

 17 1 0 3.243973 -2.586727 0.214891

 18 1 0 4.149406 -0.194076 -0.193910

 19 1 0 3.367566 -0.470208 1.355392

 20 1 0 0.809077 -3.074335 0.016729

 21 1 0 0.653108 3.469589 -0.031775

 22 1 0 -2.699377 2.338667 -0.110328

 23 1 0 -4.661193 0.829332 0.006244

 24 1 0 -4.369074 -1.616699 0.126472

 25 1 0 -2.095551 -2.614930 0.133577

 ---------------------------------------------------------------------

**3**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 2.604477 -1.838988 -0.110322

 2 6 0 3.134131 -0.577777 -0.134364

 3 6 0 2.227311 0.543335 -0.015627

 4 7 0 1.002189 0.179081 0.556918

 5 6 0 0.389686 -1.021864 0.275220

 6 6 0 1.192397 -2.092782 0.004162

 7 7 0 2.287023 1.760975 -0.432826

 8 6 0 0.912199 2.321542 -0.338246

 9 6 0 0.104090 1.333832 0.563111

 10 6 0 -1.039619 -0.722075 0.147729

 11 6 0 -1.212378 0.680437 0.210911

 12 6 0 -2.470720 1.239166 0.045375

 13 6 0 -3.554945 0.394544 -0.205174

 14 6 0 -3.383503 -0.991018 -0.268136

 15 6 0 -2.124627 -1.561411 -0.091456

 16 1 0 3.264247 -2.683334 -0.277569

 17 1 0 4.174858 -0.398580 -0.366297

 18 1 0 0.783256 -3.070152 -0.206847

 19 1 0 0.930353 3.319361 0.100048

 20 1 0 0.495188 2.404770 -1.349315

 21 1 0 0.044415 1.739001 1.581143

 22 1 0 -2.613535 2.312377 0.101313

 23 1 0 -4.541624 0.817979 -0.351648

 24 1 0 -4.239623 -1.627604 -0.457482

 25 1 0 -1.993013 -2.635850 -0.141080

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**4**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 2.714009 -1.733111 0.178623

 2 6 0 3.085500 -0.364276 -0.454494

 3 6 0 2.040973 0.676391 -0.159197

 4 7 0 0.994452 0.260217 0.695068

 5 6 0 0.413656 -0.989507 0.318577

 6 6 0 1.236379 -2.011763 0.047491

 7 7 0 1.932049 1.839603 -0.665793

 8 6 0 0.640771 2.408345 -0.232034

 9 6 0 -0.014767 1.342042 0.706054

 10 6 0 -1.019617 -0.749267 0.138733

 11 6 0 -1.278149 0.623687 0.296554

 12 6 0 -2.559840 1.125571 0.117909

 13 6 0 -3.586758 0.244200 -0.226167

 14 6 0 -3.331392 -1.121760 -0.377418

 15 6 0 -2.046755 -1.629211 -0.196029

 16 1 0 3.309741 -2.523472 -0.280569

 17 1 0 2.986399 -1.705655 1.241703

 18 1 0 3.165118 -0.450799 -1.540912

 19 1 0 4.058258 -0.023673 -0.089410

 20 1 0 0.865014 -2.964344 -0.304639

 21 1 0 0.805578 3.348640 0.298001

 22 1 0 0.031124 2.626491 -1.113909

 23 1 0 -0.121452 1.742194 1.718558

 24 1 0 -2.764883 2.183284 0.241522

 25 1 0 -4.592070 0.621107 -0.373357

 26 1 0 -4.141711 -1.792109 -0.638892

 27 1 0 -1.850697 -2.688441 -0.314630

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**5**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 1.319264 -2.093397 -0.000162

 2 1 0 0.976485 -3.119199 -0.009772

 3 6 0 0.420001 -1.032843 -0.042763

 4 7 0 1.029385 0.192998 -0.020776

 5 6 0 0.190222 1.268633 -0.053852

 6 6 0 -0.983739 -0.707256 -0.095680

 7 6 0 -1.117190 0.692637 -0.099079

 8 6 0 -2.471042 1.318731 -0.235196

 9 1 0 -2.498539 2.312937 0.216821

 10 1 0 -2.682732 1.453419 -1.305531

 11 6 0 -3.550320 0.414588 0.390997

 12 1 0 -4.541430 0.763046 0.090556

 13 1 0 -3.509611 0.510896 1.486200

 14 6 0 2.699267 -1.805148 0.058418

 15 1 0 3.389371 -2.639808 0.089234

 16 6 0 3.234689 -0.506660 0.081325

 17 1 0 4.301461 -0.338555 0.128307

 18 6 0 2.341211 0.563564 0.041544

 19 7 0 2.390582 1.927026 0.046208

 20 6 0 1.109279 2.352251 -0.009592

 21 1 0 0.881704 3.407933 -0.015831

 22 6 0 -2.150614 -1.567807 -0.159681

 23 1 0 -2.021955 -2.625529 -0.361615

 24 6 0 -3.371663 -1.044981 0.038911

 25 1 0 -4.250711 -1.679178 0.012462

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**6**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 1.263396 -2.095408 -0.031503

 2 1 0 0.895276 -3.112263 -0.055088

 3 6 0 0.387408 -1.011415 -0.059530

 4 7 0 1.030778 0.200913 -0.024915

 5 6 0 0.222825 1.295462 -0.044265

 6 6 0 -0.999573 -0.658209 -0.103820

 7 6 0 -1.105012 0.744059 -0.098223

 8 6 0 2.648687 -1.842480 0.034315

 9 1 0 3.317779 -2.694415 0.056333

 10 6 0 3.217413 -0.557842 0.077642

 11 1 0 4.287922 -0.418403 0.132611

 12 6 0 2.352464 0.536183 0.049512

 13 7 0 2.436791 1.896373 0.075363

 14 6 0 1.165424 2.354739 0.022696

 15 1 0 0.964113 3.415635 0.031941

 16 6 0 -2.223410 -1.512831 -0.246753

 17 1 0 -2.080163 -2.496537 0.207467

 18 1 0 -2.419313 -1.684675 -1.314697

 19 6 0 -3.439709 -0.811700 0.387646

 20 1 0 -3.383473 -0.905955 1.482355

 21 1 0 -4.360057 -1.316970 0.084517

 22 6 0 -3.511743 0.659641 0.051623

 23 1 0 -4.486410 1.135535 0.042755

 24 6 0 -2.402876 1.389996 -0.152691

 25 1 0 -2.460433 2.455883 -0.341243

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**7**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -1.343277 -2.091345 -0.041480

 2 1 0 -0.982776 -3.111057 -0.062388

 3 6 0 -0.462617 -1.015923 -0.020851

 4 7 0 -1.093351 0.198277 0.004696

 5 6 0 -0.271870 1.282148 0.025115

 6 6 0 0.938864 -0.673160 -0.014376

 7 6 0 1.053989 0.719582 0.011465

 8 6 0 2.114746 -1.604430 -0.038237

 9 1 0 2.235132 -2.027714 -1.044245

 10 1 0 1.944077 -2.453455 0.631808

 11 6 0 2.370428 1.434538 0.031740

 12 1 0 2.342360 2.299261 -0.638677

 13 1 0 2.548700 1.835390 1.038118

 14 6 0 3.515747 0.486607 -0.359742

 15 1 0 4.477041 0.957151 -0.136660

 16 1 0 3.488513 0.316132 -1.442292

 17 6 0 3.399871 -0.861612 0.363397

 18 1 0 4.271346 -1.485219 0.146669

 19 1 0 3.392776 -0.688414 1.445883

 20 6 0 -2.731199 -1.826687 -0.036383

 21 1 0 -3.407462 -2.673107 -0.053075

 22 6 0 -3.288775 -0.539263 -0.011846

 23 1 0 -4.359540 -0.390354 -0.009990

 24 6 0 -2.413383 0.548925 0.010133

 25 7 0 -2.483450 1.908296 0.035394

 26 6 0 -1.202830 2.351486 0.044388

 27 1 0 -0.990713 3.410180 0.064275

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**8**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 2.190960 -0.143137 -0.000000

 2 1 0 3.260159 0.020412 -0.000000

 3 6 0 1.357507 0.934932 -0.000000

 4 1 0 1.694185 1.962332 -0.000000

 5 7 0 0.000000 0.732933 0.000000

 6 6 0 -1.054243 1.623131 0.000000

 7 1 0 -0.902634 2.688841 0.000000

 8 6 0 -2.190372 0.841619 0.000000

 9 1 0 -3.213021 1.187702 0.000000

 10 7 0 -1.894056 -0.489018 0.000000

 11 6 0 -0.567007 -0.558065 0.000000

 12 6 0 1.660525 -1.463965 -0.000000

 13 1 0 2.337922 -2.308530 -0.000000

 14 6 0 0.305113 -1.668041 -0.000000

 15 1 0 -0.133107 -2.657004 -0.000000

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**9**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -1.987207 0.885130 0.016048

 2 1 0 -2.876798 1.499279 -0.041239

 3 6 0 -0.790763 1.454235 -0.143832

 4 1 0 -0.635970 2.507319 -0.335713

 5 7 0 0.373656 0.669981 -0.064024

 6 7 0 1.561132 -1.205175 0.033996

 7 6 0 0.351834 -0.707579 -0.071081

 8 6 0 -2.111620 -0.587099 0.327848

 9 1 0 -2.118426 -0.715451 1.419017

 10 1 0 -3.067106 -0.974183 -0.033000

 11 6 0 -0.954215 -1.401664 -0.281215

 12 1 0 -0.903848 -2.405151 0.142172

 13 1 0 -1.119142 -1.514138 -1.360809

 14 6 0 1.700839 1.054545 0.053352

 15 1 0 1.992476 2.090104 0.099293

 16 6 0 2.409442 -0.114472 0.115864

 17 1 0 3.475451 -0.240008 0.218567

 ---------------------------------------------------------------------

**10**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -2.284199 0.082640 0.000000

 2 1 0 -3.325314 0.370124 0.000000

 3 6 0 -1.308621 1.034667 0.000000

 4 1 0 -1.516792 2.097370 0.000000

 5 7 0 -0.000000 0.676357 0.000000

 6 7 0 1.732339 -0.812172 0.000000

 7 6 0 0.453449 -0.660210 0.000000

 8 6 0 -1.890041 -1.294608 0.000000

 9 1 0 -2.659097 -2.059004 0.000000

 10 6 0 -0.580675 -1.664393 0.000000

 11 1 0 -0.271036 -2.700386 0.000000

 12 6 0 1.168756 1.564095 0.000000

 13 1 0 1.161483 2.200860 0.888202

 14 1 0 1.161483 2.200860 -0.888202

 15 6 0 2.336830 0.528082 0.000000

 16 1 0 2.974952 0.649622 -0.880086

 17 1 0 2.974952 0.649622 0.880086

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**11**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -2.040618 0.900817 0.089230

 2 1 0 -2.914383 1.539059 0.116237

 3 6 0 -0.842066 1.439360 -0.170116

 4 1 0 -0.702769 2.499492 -0.344996

 5 7 0 0.315462 0.665591 -0.264845

 6 7 0 1.392158 -1.297832 0.110697

 7 6 0 0.275483 -0.721468 -0.123668

 8 6 0 1.659228 1.112317 0.120859

 9 1 0 1.636000 1.571700 1.116629

 10 1 0 2.059429 1.837855 -0.590128

 11 6 0 2.422823 -0.238931 0.118707

 12 1 0 3.042394 -0.347498 -0.777636

 13 1 0 3.076127 -0.350161 0.985564

 14 6 0 -2.183796 -0.576914 0.359448

 15 1 0 -2.168199 -0.757606 1.442606

 16 1 0 -3.151682 -0.941601 0.005501

 17 6 0 -1.055452 -1.381185 -0.316140

 18 1 0 -0.998815 -2.405642 0.050525

 19 1 0 -1.245053 -1.423889 -1.395178

 ---------------------------------------------------------------------

**12**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 0.051076 1.422065 0.110802

 2 1 0 0.013601 2.506307 0.112398

 3 6 0 -0.051076 0.730563 1.255119

 4 1 0 -0.188893 1.243185 2.201101

 5 6 0 0.051076 -0.730563 1.255119

 6 1 0 0.188893 -1.243185 2.201101

 7 6 0 -0.051076 -1.422065 0.110802

 8 1 0 -0.013601 -2.506307 0.112398

 9 6 0 -0.309576 -0.702356 -1.190108

 10 1 0 -1.398855 -0.624178 -1.331274

 11 1 0 0.068520 -1.280602 -2.037106

 12 6 0 0.309576 0.702356 -1.190108

 13 1 0 -0.068520 1.280602 -2.037106

 14 1 0 1.398855 0.624178 -1.331274

 ---------------------------------------------------------------------

**13**

---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -0.120665 -0.656064 1.303401

 2 1 0 -0.227666 -1.178502 2.250285

 3 6 0 0.120665 0.656064 1.303401

 4 1 0 0.227666 1.178502 2.250285

 5 6 0 0.253305 1.477288 0.046506

 6 1 0 1.305887 1.761185 -0.091600

 7 1 0 -0.292381 2.420002 0.164946

 8 6 0 -0.253305 0.723007 -1.189702

 9 1 0 0.056246 1.241425 -2.101754

 10 1 0 -1.349605 0.717297 -1.183107

 11 6 0 0.253305 -0.723007 -1.189702

 12 1 0 1.349605 -0.717297 -1.183107

 13 1 0 -0.056246 -1.241425 -2.101754

 14 6 0 -0.253305 -1.477288 0.046506

 15 1 0 0.292381 -2.420002 0.164946

 16 1 0 -1.305887 -1.761185 -0.091600

 ---------------------------------------------------------------------

**14**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -0.000000 1.394109 0.000000

 2 1 0 -0.000000 2.478130 0.000000

 3 6 0 1.207334 0.697054 0.000000

 4 1 0 2.146124 1.239065 0.000000

 5 6 0 1.207334 -0.697054 0.000000

 6 1 0 2.146124 -1.239065 0.000000

 7 6 0 -0.000000 -1.394109 0.000000

 8 1 0 -0.000000 -2.478130 0.000000

 9 6 0 -1.207334 0.697054 0.000000

 10 1 0 -2.146124 1.239065 0.000000

 11 6 0 -1.207334 -0.697054 0.000000

 12 1 0 -2.146124 -1.239065 0.000000

 ---------------------------------------------------------------------

**15a**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 8 0 -1.577182 0.000092 -0.700894

 2 8 0 -0.000000 -2.150065 0.024390

 3 8 0 1.577182 -0.000092 -0.700894

 4 8 0 0.000000 2.150065 0.024390

 5 6 0 1.251230 -2.394339 -0.660886

 6 6 0 1.703784 -1.204248 -1.491455

 7 6 0 1.699920 1.202329 -1.494705

 8 6 0 1.248635 2.394074 -0.665808

 9 6 0 -1.251230 2.394339 -0.660886

 10 6 0 -1.703784 1.204248 -1.491455

 11 6 0 -1.699920 -1.202329 -1.494705

 12 6 0 -1.248635 -2.394074 -0.665808

 13 1 0 1.169101 -3.284150 -1.289263

 14 1 0 1.971306 -2.614703 0.130057

 15 1 0 2.745678 -1.348334 -1.792740

 16 1 0 1.098920 -1.091593 -2.394837

 17 1 0 2.740743 1.346950 -1.799443

 18 1 0 1.092525 1.086585 -2.395996

 19 1 0 1.163034 3.281921 -1.296495

 20 1 0 1.971130 2.617558 0.121979

 21 1 0 -1.169101 3.284150 -1.289263

 22 1 0 -1.971306 2.614703 0.130057

 23 1 0 -2.745678 1.348334 -1.792740

 24 1 0 -1.098920 1.091593 -2.394837

 25 1 0 -2.740743 -1.346950 -1.799443

 26 1 0 -1.092525 -1.086585 -2.395996

 27 1 0 -1.163034 -3.281921 -1.296495

 28 1 0 -1.971130 -2.617558 0.121979

 29 56 0 -0.000000 0.000000 1.500210

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**15b**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 8 0 -1.035764 -2.029192 0.308120

 2 8 0 -2.416115 0.384164 -0.096724

 3 8 0 -0.379781 2.069781 0.471399

 4 8 0 2.139603 1.106290 0.176220

 5 8 0 1.594125 -1.516150 0.284950

 6 6 0 -2.611364 1.390389 0.923705

 7 6 0 -1.727875 2.573133 0.590713

 8 6 0 0.697561 3.030804 0.436023

 9 6 0 1.946680 2.328772 0.925082

 10 6 0 3.116788 0.234814 0.792951

 11 6 0 2.989399 -1.158169 0.208087

 12 6 0 1.210635 -2.898474 0.431588

 13 6 0 -0.164872 -2.900213 1.067144

 14 6 0 -2.323810 -1.838867 0.935878

 15 6 0 -3.128607 -0.859593 0.103551

 16 1 0 -3.659589 1.700511 0.936203

 17 1 0 -2.341772 0.980319 1.901168

 18 1 0 -1.782957 3.308705 1.397429

 19 1 0 -2.032849 3.051079 -0.346299

 20 1 0 0.478714 3.871418 1.099229

 21 1 0 0.812975 3.420690 -0.582169

 22 1 0 2.814661 2.983152 0.803762

 23 1 0 1.834917 2.072992 1.982630

 24 1 0 4.124610 0.624854 0.625074

 25 1 0 2.918759 0.200706 1.867953

 26 1 0 3.596691 -1.852151 0.793984

 27 1 0 3.327499 -1.203678 -0.833476

 28 1 0 1.912424 -3.421561 1.085812

 29 1 0 1.211618 -3.392250 -0.546197

 30 1 0 -0.571710 -3.915319 1.076772

 31 1 0 -0.105328 -2.525788 2.093578

 32 1 0 -2.857235 -2.792948 0.988291

 33 1 0 -2.167774 -1.470906 1.955401

 34 1 0 -4.096017 -0.669927 0.574346

 35 1 0 -3.316776 -1.261603 -0.894137

 36 56 0 0.011703 0.013517 -1.136061

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**15c**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 56 0 0.000123 -0.000423 -0.002400

 2 6 0 2.204945 2.910899 -0.322293

 3 8 0 0.846774 2.623554 0.067138

 4 8 0 2.695544 0.578392 -0.066210

 5 6 0 3.116775 1.900601 0.326369

 6 8 0 1.849036 -2.044770 0.068396

 7 6 0 3.204936 -1.749308 -0.322627

 8 6 0 3.622553 -0.453815 0.325708

 9 8 0 -0.847097 -2.623562 -0.067685

 10 6 0 0.087166 -3.649748 0.323456

 11 6 0 1.418181 -3.363604 -0.324077

 12 6 0 -0.087332 3.649624 -0.324806

 13 6 0 -1.418176 3.364432 0.323558

 14 8 0 -1.849274 2.044942 -0.066955

 15 6 0 -3.204582 1.749118 0.326334

 16 6 0 -3.623328 0.454123 -0.321843

 17 8 0 -2.694920 -0.578185 0.067581

 18 6 0 -3.117629 -1.900373 -0.322205

 19 6 0 -2.204409 -2.909486 0.325909

 20 1 0 2.287348 2.872319 -1.413985

 21 1 0 2.482932 3.913407 0.016377

 22 1 0 3.083782 1.984363 1.418147

 23 1 0 4.143036 2.077180 -0.009183

 24 1 0 3.262895 -1.680116 -1.414396

 25 1 0 3.870404 -2.549357 0.015084

 26 1 0 4.630487 -0.193651 -0.011038

 27 1 0 3.628195 -0.543554 1.417498

 28 1 0 0.175532 -3.665486 1.415242

 29 1 0 -0.272638 -4.626150 -0.014465

 30 1 0 2.147129 -4.106674 0.012753

 31 1 0 1.343631 -3.412944 -1.415908

 32 1 0 -0.176014 3.664287 -1.416599

 33 1 0 0.272784 4.626297 0.011980

 34 1 0 -2.147246 4.106978 -0.014186

 35 1 0 -1.343316 3.415292 1.415279

 36 1 0 -3.260484 1.679192 1.418162

 37 1 0 -3.870634 2.549468 -0.009528

 38 1 0 -4.630393 0.193476 0.017078

 39 1 0 -3.631362 0.544382 -1.413565

 40 1 0 -3.087610 -1.985882 -1.413928

 41 1 0 -4.143018 -2.076145 0.016408

 42 1 0 -2.483714 -3.912696 -0.009534

 43 1 0 -2.283712 -2.868016 1.417696

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**15d**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 8 0 0.688775 -2.474166 -0.736065

 2 8 0 2.370419 -1.275457 1.107103

 3 8 0 2.589161 1.309724 0.072627

 4 8 0 0.360413 2.654847 -0.842766

 5 8 0 -2.013046 1.893595 0.387504

 6 8 0 -2.258792 -0.670904 1.440460

 7 8 0 -1.790124 -1.321739 -1.258996

 8 6 0 1.596309 -3.277431 0.042473

 9 6 0 2.803774 -2.443226 0.386350

 10 6 0 -1.197727 -2.266241 -2.170885

 11 6 0 -0.300918 -3.242389 -1.440707

 12 6 0 -3.316449 1.448260 0.795363

 13 6 0 -3.128748 0.395829 1.870357

 14 6 0 3.444309 -0.394524 1.493530

 15 6 0 3.787543 0.578046 0.383937

 16 6 0 -0.718223 3.597733 -0.684663

 17 6 0 -2.035528 2.865089 -0.673869

 18 6 0 2.740140 2.291461 -0.968350

 19 6 0 1.641830 3.314315 -0.820448

 20 6 0 -2.874352 -1.834905 0.860457

 21 6 0 -3.038693 -1.711140 -0.647006

 22 1 0 1.920058 -4.145934 -0.538858

 23 1 0 1.087468 -3.629730 0.946520

 24 1 0 3.483805 -3.029918 1.011641

 25 1 0 3.328530 -2.147198 -0.527794

 26 1 0 -1.970920 -2.796994 -2.731029

 27 1 0 -0.614751 -1.676739 -2.881995

 28 1 0 0.186405 -3.908755 -2.160228

 29 1 0 -0.867274 -3.855306 -0.729697

 30 1 0 -3.884600 2.288892 1.207996

 31 1 0 -3.858515 1.059039 -0.072225

 32 1 0 -4.096184 -0.005894 2.181726

 33 1 0 -2.647579 0.837250 2.745052

 34 1 0 4.325413 -0.973539 1.782322

 35 1 0 3.091695 0.145858 2.374032

 36 1 0 4.566219 1.266844 0.727153

 37 1 0 4.150344 0.064657 -0.513403

 38 1 0 -0.707529 4.312639 -1.513580

 39 1 0 -0.579925 4.142697 0.255130

 40 1 0 -2.836103 3.590971 -0.502998

 41 1 0 -2.223540 2.358374 -1.627732

 42 1 0 3.704887 2.798249 -0.872983

 43 1 0 2.703747 1.797727 -1.946292

 44 1 0 1.701392 4.034002 -1.643143

 45 1 0 1.748782 3.850875 0.128258

 46 1 0 -3.842708 -2.024858 1.332322

 47 1 0 -2.213199 -2.668450 1.106240

 48 1 0 -3.378725 -2.668072 -1.051610

 49 1 0 -3.779509 -0.955678 -0.912467

 50 56 0 0.098362 0.090831 0.223383

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**16a**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 8 0 -0.055502 2.893191 0.096623

 2 8 0 -1.533061 0.262840 -0.311448

 3 8 0 0.055502 -2.893191 0.096623

 4 8 0 1.533061 -0.262840 -0.311448

 5 6 0 -1.434968 -0.967307 0.387210

 6 6 0 -0.862130 -2.023379 -0.567337

 7 6 0 1.434968 -2.646554 -0.136722

 8 6 0 1.968830 -1.360393 0.475089

 9 6 0 1.434968 0.967307 0.387210

 10 6 0 0.862130 2.023379 -0.567337

 11 6 0 -1.434968 2.646554 -0.136722

 12 6 0 -1.968830 1.360393 0.475089

 13 1 0 -2.418870 -1.267795 0.773858

 14 1 0 -0.762253 -0.861657 1.247055

 15 1 0 -1.657731 -2.657661 -0.965542

 16 1 0 -0.376941 -1.500954 -1.394028

 17 1 0 1.957914 -3.495785 0.309517

 18 1 0 1.644685 -2.639726 -1.215000

 19 1 0 3.068340 -1.395370 0.507118

 20 1 0 1.602850 -1.266691 1.506176

 21 1 0 2.418870 1.267795 0.773858

 22 1 0 0.762253 0.861657 1.247055

 23 1 0 1.657731 2.657661 -0.965542

 24 1 0 0.376941 1.500954 -1.394028

 25 1 0 -1.957914 3.495785 0.309517

 26 1 0 -1.644685 2.639726 -1.215000

 27 1 0 -3.068340 1.395370 0.507118

 28 1 0 -1.602850 1.266691 1.506176

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**16b**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 8 0 3.230866 -0.764654 0.391304

 2 8 0 0.150509 -1.213400 -0.140602

 3 8 0 -3.086856 -1.245829 -0.178425

 4 8 0 -2.000489 2.198378 0.442816

 5 8 0 1.501583 2.298676 -0.598505

 6 6 0 -0.855897 -1.992169 0.539592

 7 6 0 -2.033847 -2.193058 -0.419125

 8 6 0 -2.791548 0.125599 -0.524353

 9 6 0 -2.486128 0.885026 0.774381

 10 6 0 -0.578731 2.394453 0.539786

 11 6 0 0.128440 1.859938 -0.710500

 12 6 0 2.499223 1.267599 -0.660488

 13 6 0 2.582629 0.499668 0.664976

 14 6 0 2.389095 -1.925568 0.472858

 15 6 0 1.307435 -1.931257 -0.611479

 16 1 0 -0.450772 -2.938811 0.923525

 17 1 0 -1.146323 -1.338753 1.391080

 18 1 0 -2.561813 -3.149853 -0.242267

 19 1 0 -1.705791 -2.131434 -1.472342

 20 1 0 -3.729183 0.473165 -0.995604

 21 1 0 -1.966010 0.198929 -1.249850

 22 1 0 -3.407005 1.097398 1.349309

 23 1 0 -1.778511 0.326441 1.412499

 24 1 0 -0.505994 3.498886 0.602461

 25 1 0 -0.179600 1.950515 1.465029

 26 1 0 -0.250652 2.339891 -1.630251

 27 1 0 0.042747 0.761618 -0.801502

 28 1 0 3.414311 1.857193 -0.861417

 29 1 0 2.311780 0.586392 -1.508501

 30 1 0 3.257880 0.984978 1.391154

 31 1 0 1.585934 0.361219 1.117048

 32 1 0 3.128345 -2.737488 0.327979

 33 1 0 1.949763 -1.992977 1.483411

 34 1 0 1.041287 -2.946937 -0.940023

 35 1 0 1.620682 -1.327136 -1.488340

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**16c**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 1.381351 -1.927326 0.155572

 2 8 0 0.137799 -1.904565 -0.535633

 3 8 0 3.736658 -1.454777 -0.252961

 4 6 0 2.461351 -1.608218 -0.869786

 5 8 0 2.509214 0.920697 1.080786

 6 6 0 3.903139 0.690430 0.953308

 7 6 0 4.287600 -0.147306 -0.263067

 8 8 0 -0.167855 2.643570 -0.602329

 9 6 0 0.465702 1.621201 0.163004

 10 6 0 1.955723 1.906773 0.218857

 11 6 0 -0.987686 -1.967192 0.326301

 12 6 0 -2.232431 -1.955131 -0.549928

 13 8 0 -3.411754 -1.918088 0.253257

 14 6 0 -4.151568 -0.709151 0.238159

 15 6 0 -3.529545 0.414265 1.059903

 16 8 0 -2.348777 0.941308 0.464090

 17 6 0 -2.559042 2.031146 -0.422688

 18 6 0 -1.329351 2.225328 -1.294588

 19 1 0 1.398933 -1.172328 0.947116

 20 1 0 1.553983 -2.914497 0.605199

 21 1 0 2.176384 -0.698623 -1.408357

 22 1 0 2.534893 -2.420002 -1.599957

 23 1 0 4.194214 0.154295 1.859120

 24 1 0 4.455880 1.642117 0.923235

 25 1 0 5.375915 -0.267090 -0.256436

 26 1 0 4.020741 0.366382 -1.195520

 27 1 0 0.054488 1.583609 1.175291

 28 1 0 0.298999 0.645137 -0.301434

 29 1 0 2.380105 1.848329 -0.790324

 30 1 0 2.148506 2.914088 0.611008

 31 1 0 -0.998723 -1.102979 0.999853

 32 1 0 -0.963193 -2.883055 0.932652

 33 1 0 -2.269473 -2.866387 -1.153775

 34 1 0 -2.188174 -1.095051 -1.223185

 35 1 0 -4.315465 -0.375250 -0.796603

 36 1 0 -5.126893 -0.956734 0.667009

 37 1 0 -4.269814 1.211349 1.216754

 38 1 0 -3.239123 0.023274 2.038095

 39 1 0 -2.767860 2.944778 0.151035

 40 1 0 -3.415550 1.838267 -1.085635

 41 1 0 -1.545942 3.012528 -2.021782

 42 1 0 -1.126561 1.293766 -1.841309

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**16d**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 8 0 2.589853 2.558905 0.086766

 2 8 0 3.346817 -0.137810 -1.027724

 3 8 0 2.878462 -1.751762 1.368902

 4 8 0 -0.555131 -2.268125 0.291659

 5 8 0 -3.928943 -1.854001 -1.012800

 6 8 0 -3.597425 0.820928 0.345932

 7 8 0 -0.983415 2.161859 0.103650

 8 6 0 3.703019 2.217559 -0.721709

 9 6 0 4.233164 0.818481 -0.463243

 10 6 0 0.294401 2.477092 0.630367

 11 6 0 1.326310 2.161721 -0.435281

 12 6 0 -4.903715 -1.081196 -0.333983

 13 6 0 -4.698027 0.417200 -0.449133

 14 6 0 3.778303 -1.483051 -0.931936

 15 6 0 3.962466 -2.001649 0.496501

 16 6 0 -1.579579 -1.558713 -0.397107

 17 6 0 -2.853771 -2.376257 -0.239187

 18 6 0 1.668897 -2.445207 1.079322

 19 6 0 0.656660 -1.544412 0.382747

 20 6 0 -3.361608 2.216714 0.298749

 21 6 0 -2.043255 2.534464 0.964270

 22 1 0 4.491207 2.932601 -0.469133

 23 1 0 3.460883 2.334139 -1.786469

 24 1 0 5.231414 0.720803 -0.920150

 25 1 0 4.326743 0.671682 0.618592

 26 1 0 0.351257 3.541838 0.897348

 27 1 0 0.499039 1.889864 1.536256

 28 1 0 1.098506 2.725301 -1.350531

 29 1 0 1.316612 1.096957 -0.672426

 30 1 0 -5.868142 -1.322828 -0.793106

 31 1 0 -4.950691 -1.362781 0.725432

 32 1 0 -5.616548 0.924664 -0.111823

 33 1 0 -4.525307 0.685644 -1.500706

 34 1 0 4.732172 -1.622271 -1.466448

 35 1 0 3.018852 -2.066067 -1.456714

 36 1 0 4.175090 -3.080243 0.433694

 37 1 0 4.824941 -1.528087 0.969396

 38 1 0 -1.329063 -1.464034 -1.463210

 39 1 0 -1.707157 -0.554525 0.015343

 40 1 0 -2.669455 -3.394556 -0.592373

 41 1 0 -3.129066 -2.429126 0.820158

 42 1 0 1.862665 -3.338494 0.473094

 43 1 0 1.247593 -2.774115 2.032574

 44 1 0 1.008612 -1.248629 -0.612788

 45 1 0 0.520624 -0.627794 0.971766

 46 1 0 -4.171315 2.752733 0.817148

 47 1 0 -3.330566 2.566098 -0.742317

 48 1 0 -1.998031 3.614395 1.171486

 49 1 0 -1.972209 2.000400 1.922556

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**17a**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 1 0 3.984316 0.381024 -2.448522

 2 6 0 3.764462 0.214134 -1.400035

 3 6 0 3.318308 -0.217196 1.332061

 4 6 0 3.689254 -1.093072 -0.900208

 5 6 0 3.616801 1.305345 -0.533517

 6 6 0 3.393684 1.089663 0.832921

 7 6 0 3.466563 -1.308664 0.466096

 8 1 0 3.851167 -1.935972 -1.562607

 9 1 0 3.722678 2.315612 -0.912451

 10 1 0 3.324148 1.933684 1.509610

 11 1 0 3.454388 -2.318383 0.860426

 12 1 0 3.195191 -0.384856 2.396012

 13 56 0 0.439844 -0.014427 -0.522099

 14 8 0 -0.752049 -1.130605 1.628327

 15 8 0 -0.891512 1.606152 1.184695

 16 8 0 -1.727159 -1.598036 -0.924721

 17 8 0 -1.866398 1.137301 -1.370641

 18 6 0 -1.910769 -1.978921 1.478181

 19 1 0 -2.821036 -1.384317 1.598379

 20 1 0 -1.899647 -2.756854 2.246980

 21 6 0 -1.844217 -2.609619 0.100210

 22 1 0 -2.719532 -3.238388 -0.078844

 23 1 0 -0.957588 -3.240144 0.006397

 24 6 0 -0.802586 -0.208116 2.738650

 25 1 0 -1.271093 -0.677669 3.606773

 26 1 0 0.236233 0.009642 2.994682

 27 6 0 -1.536378 1.063302 2.356296

 28 1 0 -2.589414 0.862943 2.138092

 29 1 0 -1.483090 1.786519 3.175172

 30 6 0 -1.639885 2.626336 0.486110

 31 1 0 -0.901618 3.238060 -0.036639

 32 1 0 -2.163545 3.271005 1.195832

 33 6 0 -2.615870 2.007208 -0.496123

 34 1 0 -3.387959 1.431509 0.022739

 35 1 0 -3.102694 2.791063 -1.083487

 36 6 0 -2.977738 -1.035922 -1.377234

 37 1 0 -3.494290 -1.754970 -2.019481

 38 1 0 -3.615951 -0.818211 -0.515868

 39 6 0 -2.662461 0.224877 -2.159443

 40 1 0 -2.067968 -0.007882 -3.045417

 41 1 0 -3.582039 0.709855 -2.495283

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**17b**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 1 0 3.771473 -0.386524 -1.582428

 2 6 0 3.581518 -0.152503 -0.541013

 3 6 0 3.215107 0.455894 2.167391

 4 6 0 3.499605 -1.183737 0.402417

 5 6 0 3.479736 1.182568 -0.131529

 6 6 0 3.296159 1.486979 1.222807

 7 6 0 3.316139 -0.879655 1.756891

 8 1 0 3.617955 -2.215273 0.091517

 9 1 0 3.584583 1.982515 -0.855405

 10 1 0 3.262165 2.521139 1.546040

 11 1 0 3.296943 -1.675299 2.492934

 12 1 0 3.118599 0.692866 3.220918

 13 56 0 0.229373 0.030468 0.450791

 14 8 0 -2.123384 -0.974937 1.284984

 15 8 0 -1.745790 1.744325 1.175049

 16 8 0 -0.464455 -2.502586 -0.309284

 17 8 0 -0.540220 1.997294 -1.332535

 18 6 0 -2.575924 -2.294904 0.918717

 19 1 0 -3.234082 -2.219207 0.047365

 20 1 0 -3.135516 -2.745531 1.743605

 21 6 0 -1.346441 -3.140255 0.637728

 22 1 0 -1.639006 -4.130963 0.280551

 23 1 0 -0.761139 -3.271134 1.550061

 24 6 0 -3.113005 -0.091925 1.865428

 25 1 0 -4.108749 -0.532957 1.785008

 26 1 0 -2.871848 0.038603 2.922724

 27 6 0 -3.092678 1.232464 1.133226

 28 1 0 -3.409167 1.099145 0.093490

 29 1 0 -3.770505 1.936755 1.625258

 30 6 0 -1.553200 3.042927 0.579208

 31 1 0 -0.602790 3.407343 0.974864

 32 1 0 -2.336780 3.731417 0.907166

 33 6 0 -1.515923 2.980317 -0.936457

 34 1 0 -2.489630 2.700525 -1.351838

 35 1 0 -1.245088 3.964023 -1.333308

 36 6 0 -0.570127 1.720383 -2.746918

 37 1 0 -1.603628 1.515664 -3.043643

 38 1 0 -0.202464 2.585050 -3.307763

 39 6 0 0.295288 0.511721 -3.029982

 40 1 0 0.167689 0.215135 -4.074518

 41 1 0 1.357091 0.721208 -2.856316

 42 8 0 -0.144149 -0.539042 -2.150827

 43 6 0 -0.748036 -2.785041 -1.694473

 44 1 0 -1.801471 -2.580085 -1.907031

 45 1 0 -0.534892 -3.836624 -1.906963

 46 6 0 0.130617 -1.895695 -2.545057

 47 1 0 1.192343 -2.121250 -2.395508

 48 1 0 -0.116005 -2.040398 -3.600478

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**17c**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 1 0 -0.835923 2.522496 -2.947190

 2 6 0 -0.347601 1.555166 -2.969537

 3 6 0 0.920632 -0.934832 -3.124770

 4 6 0 -1.106572 0.393714 -3.153342

 5 6 0 1.045282 1.472579 -2.864711

 6 6 0 1.678924 0.227132 -2.943375

 7 6 0 -0.472865 -0.851514 -3.229364

 8 1 0 -2.181911 0.463320 -3.264781

 9 1 0 1.634677 2.375396 -2.756412

 10 1 0 2.760563 0.167459 -2.907566

 11 1 0 -1.055921 -1.747849 -3.405886

 12 1 0 1.413292 -1.895221 -3.222252

 13 56 0 -0.011414 -0.021220 0.127057

 14 8 0 -1.584447 -2.273051 0.645914

 15 8 0 2.671770 -0.255567 0.818727

 16 8 0 -2.793421 0.162735 0.005585

 17 8 0 1.452155 2.201779 0.986196

 18 6 0 -3.000707 -2.119641 0.844221

 19 1 0 -3.199748 -1.815057 1.878332

 20 1 0 -3.507759 -3.072436 0.660458

 21 6 0 -3.484579 -1.089323 -0.153025

 22 1 0 -4.563869 -0.943818 -0.059533

 23 1 0 -3.269391 -1.425988 -1.168764

 24 6 0 -0.990953 -3.324249 1.427860

 25 1 0 -1.629140 -4.213076 1.408046

 26 6 0 3.456279 0.933276 0.637007

 27 1 0 3.504447 1.188736 -0.427859

 28 1 0 4.474074 0.772755 1.005312

 29 6 0 2.809677 2.037437 1.435030

 30 1 0 2.811800 1.789124 2.501791

 31 1 0 3.364046 2.969650 1.286781

 32 6 0 0.764905 3.248566 1.693933

 33 1 0 0.650985 2.962655 2.745404

 34 1 0 1.345797 4.175139 1.643002

 35 6 0 -0.579253 3.476316 1.052263

 36 1 0 -1.114337 4.247597 1.614862

 37 1 0 -0.468997 3.812359 0.014903

 38 8 0 -1.324563 2.245689 1.079511

 39 6 0 -3.420404 1.102553 0.895170

 40 1 0 -3.362503 0.746099 1.929624

 41 1 0 -4.473136 1.226094 0.623825

 42 6 0 -2.713044 2.425496 0.747391

 43 1 0 -2.798582 2.794891 -0.280472

 44 1 0 -3.163663 3.156615 1.425805

 45 1 0 -0.887132 -2.991859 2.467223

 46 6 0 0.352139 -3.667587 0.827297

 47 1 0 0.237304 -4.121826 -0.160821

 48 1 0 0.860634 -4.377203 1.485149

 49 8 0 1.134955 -2.463953 0.691340

 50 6 0 3.287943 -1.464335 0.350199

 51 1 0 4.334415 -1.504491 0.667502

 52 1 0 3.253886 -1.493469 -0.745280

 53 6 0 2.542120 -2.633522 0.950004

 54 1 0 2.699938 -2.685522 2.031340

 55 1 0 2.902208 -3.558728 0.490578

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**17d**

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 1 0 -1.039696 -2.981625 2.580397

 2 6 0 -0.071213 -2.501277 2.528040

 3 6 0 2.462243 -1.321043 2.455111

 4 6 0 0.191776 -1.365398 3.298156

 5 6 0 0.928342 -3.040738 1.712249

 6 6 0 2.194516 -2.450874 1.676492

 7 6 0 1.461219 -0.774004 3.261898

 8 1 0 -0.568375 -0.968932 3.961755

 9 1 0 0.733537 -3.942628 1.143364

 10 1 0 2.982091 -2.891886 1.077036

 11 1 0 1.677734 0.078882 3.895144

 12 1 0 3.455707 -0.891165 2.453345

 13 56 0 0.182893 0.073831 0.033374

 14 8 0 1.243690 2.647654 0.387638

 15 8 0 1.670291 -0.800888 -2.173709

 16 8 0 -1.504823 2.329059 -0.072434

 17 8 0 -1.065720 -1.252621 -2.071620

 18 6 0 0.423363 3.791783 0.094440

 19 1 0 0.444569 3.988680 -0.983411

 20 1 0 0.811612 4.670099 0.620584

 21 6 0 -0.979253 3.512097 0.568962

 22 1 0 -1.606176 4.375667 0.337836

 23 1 0 -0.998034 3.357532 1.652306

 24 6 0 2.646449 2.904522 0.201054

 25 1 0 2.957973 3.743115 0.832489

 26 6 0 1.091235 -1.731364 -3.105118

 27 1 0 1.172438 -2.750182 -2.709086

 28 1 0 1.627129 -1.687774 -4.058679

 29 6 0 -0.347464 -1.314896 -3.315894

 30 1 0 -0.387794 -0.307467 -3.733512

 31 1 0 -0.847721 -1.995928 -4.009456

 32 6 0 -3.636134 0.405391 1.317832

 33 1 0 -2.800463 1.090239 1.495003

 34 8 0 -4.269046 0.673521 0.074661

 35 6 0 -2.817665 2.540232 -0.669682

 36 1 0 -2.681746 3.119697 -1.587831

 37 1 0 -3.437871 3.115976 0.022206

 38 6 0 -3.495434 1.220715 -0.983398

 39 1 0 -4.218128 1.396994 -1.781868

 40 1 0 -2.758798 0.503340 -1.367184

 41 1 0 2.831972 3.173017 -0.844994

 42 6 0 3.399388 1.657830 0.607482

 43 1 0 3.201513 1.428292 1.655789

 44 1 0 4.476225 1.804572 0.486053

 45 8 0 2.959843 0.512677 -0.139594

 46 6 0 3.095480 -0.935409 -2.025742

 47 1 0 3.561262 -1.071757 -3.006069

 48 1 0 3.317898 -1.809116 -1.404253

 49 6 0 3.625473 0.328331 -1.398036

 50 1 0 3.439472 1.183499 -2.056340

 51 1 0 4.704086 0.232808 -1.237361

 52 1 0 -4.379789 0.591165 2.097702

 53 6 0 -1.628508 -2.497742 -1.613958

 54 1 0 -0.851197 -3.110681 -1.142527

 55 1 0 -2.042675 -3.053063 -2.460044

 56 6 0 -2.735477 -2.182690 -0.639523

 57 1 0 -3.549987 -1.649376 -1.135723

 58 1 0 -3.126640 -3.118673 -0.228151

 59 8 0 -2.201433 -1.370174 0.420439

 60 6 0 -3.182966 -1.037516 1.432769

 61 1 0 -4.036539 -1.710858 1.336251

 62 1 0 -2.720237 -1.208545 2.408425

 ---------------------------------------------------------------------

**19** (S0) BHandH

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -1.670492 -0.250365 -0.305750

 2 6 0 -0.967460 0.798483 0.262092

 3 6 0 -0.938701 -1.234219 -0.951972

 4 6 0 0.397710 0.880428 0.178413

 5 1 0 -1.499364 1.567854 0.805680

 6 6 0 0.425578 -1.168035 -1.045969

 7 1 0 -1.466008 -2.074540 -1.382614

 8 6 0 1.140417 -0.100792 -0.487747

 9 1 0 0.891909 1.731134 0.622153

 10 1 0 0.947509 -1.974397 -1.538409

 11 6 0 7.333370 -1.295987 2.672102

 12 1 0 7.841939 -2.076783 2.099259

 13 1 0 7.565646 -1.470785 3.727748

 14 6 0 7.842167 0.052954 2.270423

 15 1 0 8.903172 0.140632 2.531592

 16 1 0 7.296221 0.818187 2.822948

 17 6 0 8.595972 -0.226863 0.069846

 18 1 0 8.812976 -1.272973 0.318291

 19 1 0 9.535546 0.332859 0.154645

 20 6 0 8.086345 -0.175843 -1.332767

 21 1 0 7.118433 -0.685769 -1.375017

 22 1 0 8.787026 -0.708824 -1.980849

 23 6 0 6.680161 1.515365 -2.172330

 24 1 0 6.234272 0.757701 -2.828224

 25 1 0 6.772687 2.436993 -2.746277

 26 6 0 5.794918 1.723234 -0.981864

 27 1 0 6.184047 2.539672 -0.361120

 28 1 0 5.803237 0.816381 -0.374292

 29 6 0 3.597603 2.174548 -0.391881

 30 1 0 2.704914 2.630677 -0.820776

 31 1 0 4.002233 2.858966 0.364638

 32 6 0 3.243509 0.865323 0.262743

 33 1 0 2.685260 1.062647 1.176897

 34 1 0 4.150181 0.342257 0.571546

 35 6 0 3.232136 -0.840056 -1.493741

 36 1 0 3.994244 -0.218302 -1.968257

 37 1 0 2.571127 -1.175126 -2.289029

 38 6 0 3.920443 -2.019976 -0.871502

 39 1 0 4.129476 -2.777704 -1.636077

 40 1 0 3.275593 -2.476183 -0.110986

 41 6 0 5.805307 -2.564090 0.397760

 42 1 0 5.567455 -3.558022 0.003604

 43 1 0 6.871913 -2.399060 0.233480

 44 6 0 5.498738 -2.520897 1.864501

 45 1 0 4.418887 -2.550343 2.015964

 46 1 0 5.926475 -3.404513 2.352158

 47 7 0 2.491832 -0.022155 -0.577768

 48 8 0 4.513556 2.028969 -1.433286

 49 8 0 7.963110 1.140547 -1.786062

 50 8 0 7.638536 0.308308 0.919714

 51 8 0 5.955875 -1.353488 2.469409

 52 8 0 5.120791 -1.581849 -0.311633

 53 6 0 -5.050258 -1.258233 -0.268138

 54 6 0 -4.024017 0.682042 0.087879

 55 7 0 -5.199792 0.041101 0.049913

 56 6 0 -6.306112 0.772734 0.275747

 57 6 0 -7.479499 0.080512 0.207806

 58 6 0 -7.413802 -1.288450 -0.096343

 59 6 0 -6.234154 -1.969362 -0.339611

 60 1 0 -8.435393 0.551772 0.372058

 61 1 0 -6.260740 -3.021042 -0.580994

 62 6 0 -4.374306 2.045337 0.369714

 63 6 0 -5.788367 2.096603 0.496703

 64 6 0 -3.640517 3.212976 0.506301

 65 6 0 -6.435480 3.286148 0.771168

 66 6 0 -5.685508 4.425750 0.912080

 67 6 0 -4.302409 4.384870 0.774878

 68 1 0 -3.734412 5.298997 0.880272

 69 1 0 -7.512304 3.316091 0.868428

 70 1 0 -2.566458 3.216145 0.392201

 71 7 0 -3.751675 -1.499086 -0.432624

 72 6 0 -3.106292 -0.339140 -0.217008

 73 1 0 -6.171975 5.366897 1.126013

 74 6 0 -8.652300 -2.077934 -0.180196

 75 8 0 -8.685961 -3.245134 -0.442209

 76 8 0 -9.726494 -1.368480 0.063849

 77 6 0 -10.952695 -2.058268 0.001911

 78 1 0 -11.720356 -1.329141 0.233937

 79 1 0 -11.107217 -2.466567 -0.994351

 80 1 0 -10.968022 -2.868578 0.727331

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**19** (S1) BHandH

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -1.670601 -0.277856 -0.340993

 2 6 0 -0.937972 0.762678 0.250155

 3 6 0 -0.943248 -1.257489 -1.037027

 4 6 0 0.439523 0.840017 0.143243

 5 1 0 -1.451792 1.520082 0.827902

 6 6 0 0.433292 -1.194834 -1.154329

 7 1 0 -1.477029 -2.083558 -1.489820

 8 6 0 1.176377 -0.135975 -0.572649

 9 1 0 0.942780 1.675535 0.607648

 10 1 0 0.937314 -1.988619 -1.686491

 11 6 0 7.227887 -1.300849 2.702754

 12 1 0 7.721928 -2.069992 2.100645

 13 1 0 7.357031 -1.578490 3.757965

 14 6 0 7.875639 0.051127 2.458460

 15 1 0 8.909963 0.028975 2.826035

 16 1 0 7.334059 0.819826 3.014030

 17 6 0 8.793775 -0.162827 0.246055

 18 1 0 8.993936 -1.195776 0.555515

 19 1 0 9.739987 0.392025 0.297126

 20 6 0 8.275218 -0.200494 -1.177424

 21 1 0 7.304038 -0.703828 -1.195298

 22 1 0 8.977780 -0.779998 -1.787260

 23 6 0 6.866120 1.466022 -2.197967

 24 1 0 6.410589 0.637572 -2.754252

 25 1 0 6.995396 2.304474 -2.885121

 26 6 0 5.965776 1.854537 -1.033628

 27 1 0 6.331217 2.774382 -0.557922

 28 1 0 5.992188 1.061285 -0.285050

 29 6 0 3.678069 2.170219 -0.482793

 30 1 0 2.788846 2.609185 -0.938583

 31 1 0 4.047032 2.858890 0.289570

 32 6 0 3.335068 0.824689 0.159894

 33 1 0 2.799358 1.000571 1.093530

 34 1 0 4.247953 0.293366 0.430989

 35 6 0 3.273993 -0.912440 -1.625646

 36 1 0 4.087908 -0.324547 -2.052337

 37 1 0 2.617092 -1.179318 -2.452377

 38 6 0 3.862865 -2.174272 -1.005143

 39 1 0 4.032879 -2.933250 -1.780820

 40 1 0 3.169388 -2.589218 -0.264567

 41 6 0 5.609808 -2.799889 0.518173

 42 1 0 5.222865 -3.798008 0.281000

 43 1 0 6.693366 -2.830840 0.381214

 44 6 0 5.260105 -2.450928 1.959254

 45 1 0 4.180094 -2.320861 2.057193

 46 1 0 5.564437 -3.273822 2.620168

 47 7 0 2.544214 -0.060686 -0.691740

 48 8 0 4.643620 2.055227 -1.529427

 49 8 0 8.169879 1.110604 -1.745822

 50 8 0 7.828351 0.449989 1.093594

 51 8 0 5.841749 -1.221082 2.384315

 52 8 0 5.107398 -1.829591 -0.396154

 53 6 0 -5.108171 -1.271110 -0.254755

 54 6 0 -4.034806 0.691823 0.090325

 55 7 0 -5.236493 0.053212 0.069342

 56 6 0 -6.351043 0.811353 0.295644

 57 6 0 -7.544926 0.120539 0.233453

 58 6 0 -7.506431 -1.268067 -0.066857

 59 6 0 -6.314110 -1.969810 -0.316753

 60 1 0 -8.489879 0.614340 0.398206

 61 1 0 -6.345826 -3.022214 -0.558109

 62 6 0 -4.374543 2.074665 0.361797

 63 6 0 -5.812009 2.144721 0.500818

 64 6 0 -3.620418 3.248193 0.480657

 65 6 0 -6.444918 3.359937 0.768407

 66 6 0 -5.669674 4.505480 0.890868

 67 6 0 -4.273375 4.446103 0.742678

 68 1 0 -3.692174 5.356189 0.833131

 69 1 0 -7.522289 3.406775 0.873736

 70 1 0 -2.545652 3.234851 0.360395

 71 7 0 -3.792865 -1.531069 -0.436535

 72 6 0 -3.117366 -0.355285 -0.229171

 73 1 0 -6.144572 5.456839 1.097333

 74 6 0 -8.768937 -2.052732 -0.143995

 75 8 0 -8.823649 -3.240447 -0.397520

 76 8 0 -9.856863 -1.304414 0.098234

 77 6 0 -11.129420 -1.982109 0.043131

 78 1 0 -11.871388 -1.218329 0.259622

 79 1 0 -11.289624 -2.402410 -0.949619

 80 1 0 -11.166356 -2.775405 0.789620

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**19·Ba(ClO4)2** (S0) BHandH

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -0.149897 2.014101 -1.763257

 2 6 0 0.200791 2.976041 -0.829467

 3 6 0 0.840142 1.527551 -2.596874

 4 6 0 1.515950 3.290819 -0.610868

 5 1 0 -0.556326 3.378939 -0.171103

 6 6 0 2.153851 1.878086 -2.416930

 7 1 0 0.589643 0.780022 -3.337758

 8 6 0 2.537214 2.670409 -1.336511

 9 1 0 1.745846 3.974865 0.190250

 10 1 0 2.889094 1.434165 -3.064461

 11 6 0 2.929161 -3.082762 1.740062

 12 1 0 3.132403 -2.761949 2.769560

 13 1 0 3.557418 -3.955880 1.529181

 14 6 0 1.503012 -3.477223 1.551046

 15 1 0 1.250075 -4.293800 2.234077

 16 1 0 1.361500 -3.813151 0.525686

 17 6 0 0.189075 -2.152401 3.035681

 18 1 0 0.177567 -3.078334 3.618423

 19 1 0 -0.827001 -1.782508 2.944108

 20 6 0 1.025033 -1.124467 3.739428

 21 1 0 1.980211 -1.530275 4.095004

 22 1 0 0.459050 -0.761368 4.603572

 23 6 0 1.791321 1.049462 3.511333

 24 1 0 2.682988 0.759825 4.082352

 25 1 0 1.038817 1.448576 4.200788

 26 6 0 2.137690 2.090245 2.496475

 27 1 0 2.607681 2.937794 3.003206

 28 1 0 1.224313 2.439961 2.016167

 29 6 0 4.232424 2.175905 1.370133

 30 1 0 4.935257 1.402645 1.073529

 31 1 0 4.559425 2.606754 2.323466

 32 6 0 4.215885 3.256239 0.315672

 33 1 0 5.219319 3.685237 0.262889

 34 1 0 3.565321 4.075654 0.617501

 35 6 0 4.873404 2.167707 -1.776090

 36 1 0 5.821865 2.520822 -1.372371

 37 1 0 4.825234 2.531473 -2.807788

 38 6 0 4.910288 0.651629 -1.829587

 39 1 0 5.929677 0.368655 -2.124567

 40 1 0 4.234492 0.225600 -2.572960

 41 6 0 5.007833 -1.223882 -0.507569

 42 1 0 4.567298 -1.816558 -1.313348

 43 1 0 6.101581 -1.279782 -0.589464

 44 6 0 4.607823 -1.799615 0.802609

 45 1 0 5.151303 -2.741652 0.926513

 46 1 0 4.894148 -1.129580 1.622828

 47 7 0 3.850909 2.796544 -0.991728

 48 8 0 2.995841 1.545989 1.532970

 49 8 0 1.278488 -0.071194 2.863654

 50 8 0 0.631695 -2.404291 1.734813

 51 8 0 3.237240 -2.055176 0.851061

 52 8 0 4.607708 0.106191 -0.590896

 53 56 0 1.089211 -0.239603 0.108641

 54 6 0 -2.676090 1.684272 -1.296407

 55 6 0 -2.508648 -0.534861 -1.341339

 56 6 0 -4.589465 0.582727 -0.702654

 57 6 0 -3.092899 -1.768330 -1.118482

 58 1 0 -2.551906 -2.694573 -1.243958

 59 6 0 -5.176134 -0.624317 -0.476992

 60 1 0 -6.190009 -0.718009 -0.122490

 61 6 0 -4.407582 -1.781391 -0.699124

 62 6 0 -4.835378 2.000354 -0.599913

 63 6 0 -3.649045 2.680883 -0.966608

 64 6 0 -5.954031 2.705617 -0.209474

 65 1 0 -6.859437 2.187980 0.076999

 66 6 0 -3.606707 4.060795 -0.938455

 67 6 0 -4.730866 4.744485 -0.546978

 68 1 0 -4.712617 5.825342 -0.518831

 69 6 0 -5.893729 4.076770 -0.185917

 70 1 0 -2.706499 4.590223 -1.219529

 71 7 0 -3.317464 0.517317 -1.134453

 72 1 0 -6.760123 4.645994 0.120044

 73 7 0 -1.301876 -0.065526 -1.656715

 74 6 0 -1.390395 1.280953 -1.634669

 75 6 0 -4.997896 -3.106935 -0.456468

 76 8 0 -4.418035 -4.138890 -0.590691

 77 8 0 -6.254954 -3.041050 -0.061325

 78 6 0 -6.866326 -4.278524 0.192306

 79 1 0 -7.881831 -4.057051 0.502577

 80 1 0 -6.866471 -4.894655 -0.704921

 81 1 0 -6.334739 -4.812196 0.977963

 82 17 0 1.952614 -2.502399 -2.283408

 83 17 0 -1.673873 0.808913 2.029232

 84 8 0 3.040705 -3.401182 -2.008885

 85 8 0 2.433322 -1.113991 -2.161787

 86 8 0 0.925090 -2.637089 -1.248380

 87 8 0 1.403067 -2.721789 -3.578429

 88 8 0 -1.459410 -0.460218 1.334304

 89 8 0 -0.668081 1.720122 1.476393

 90 8 0 -1.448203 0.635123 3.440957

 91 8 0 -2.990076 1.300872 1.766184

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**19·Ba(ClO4)2** (S1) BHandH

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -0.368426 2.475186 -1.322086

 2 6 0 0.007083 3.208431 -0.187168

 3 6 0 0.587005 2.292291 -2.327565

 4 6 0 1.332887 3.551111 0.025808

 5 1 0 -0.718324 3.387760 0.595399

 6 6 0 1.905101 2.683499 -2.143247

 7 1 0 0.317807 1.756979 -3.229236

 8 6 0 2.338264 3.185391 -0.898411

 9 1 0 1.589477 4.017927 0.964546

 10 1 0 2.606258 2.494443 -2.939017

 11 6 0 3.516740 -3.323247 0.977044

 12 1 0 3.855573 -3.195775 2.013850

 13 1 0 4.148334 -4.087376 0.504955

 14 6 0 2.079447 -3.795503 0.902631

 15 1 0 1.977693 -4.748327 1.434557

 16 1 0 1.800208 -3.935651 -0.141146

 17 6 0 0.866924 -2.880523 2.819296

 18 1 0 0.993658 -3.898410 3.204028

 19 1 0 -0.176652 -2.588473 2.909043

 20 6 0 1.729843 -1.918875 3.620258

 21 1 0 2.771885 -2.257306 3.697130

 22 1 0 1.315194 -1.845492 4.633826

 23 6 0 2.262081 0.397521 3.764418

 24 1 0 3.304264 0.149590 4.012255

 25 1 0 1.694057 0.518451 4.695660

 26 6 0 2.187237 1.676462 2.955573

 27 1 0 2.611583 2.505268 3.530733

 28 1 0 1.145020 1.900331 2.729439

 29 6 0 4.163797 2.134724 1.610213

 30 1 0 4.819690 1.419633 1.119946

 31 1 0 4.553646 2.350954 2.612403

 32 6 0 4.122286 3.430723 0.793512

 33 1 0 5.134644 3.846883 0.784747

 34 1 0 3.496713 4.173981 1.288576

 35 6 0 4.699953 2.821544 -1.545685

 36 1 0 5.667803 3.084888 -1.115774

 37 1 0 4.604288 3.401388 -2.471972

 38 6 0 4.742387 1.342782 -1.956631

 39 1 0 5.674091 1.208594 -2.526214

 40 1 0 3.914408 1.054433 -2.605036

 41 6 0 5.136778 -0.838204 -1.172796

 42 1 0 4.525351 -1.217013 -1.994984

 43 1 0 6.190471 -0.831098 -1.489065

 44 6 0 5.008316 -1.756066 0.016156

 45 1 0 5.563035 -2.672984 -0.215357

 46 1 0 5.453091 -1.301133 0.911453

 47 7 0 3.690326 3.266287 -0.589369

 48 8 0 2.877575 1.512828 1.711205

 49 8 0 1.694542 -0.647551 2.984131

 50 8 0 1.153735 -2.842178 1.419565

 51 8 0 3.643379 -2.092889 0.268697

 52 8 0 4.745021 0.485576 -0.821853

 53 56 0 1.157387 -0.358529 0.155087

 54 6 0 -2.919030 1.922261 -1.028762

 55 6 0 -2.579515 -0.308866 -1.209843

 56 6 0 -4.803868 0.622642 -0.627794

 57 6 0 -3.082611 -1.603549 -1.089246

 58 1 0 -2.453006 -2.471005 -1.223522

 59 6 0 -5.306034 -0.654156 -0.506281

 60 1 0 -6.326929 -0.836403 -0.208671

 61 6 0 -4.433012 -1.752252 -0.747529

 62 6 0 -5.162811 2.020662 -0.426225

 63 6 0 -3.991216 2.823834 -0.671977

 64 6 0 -6.360100 2.623408 -0.044090

 65 1 0 -7.242428 2.023611 0.146205

 66 6 0 -4.054873 4.210533 -0.526707

 67 6 0 -5.260045 4.787955 -0.145947

 68 1 0 -5.321801 5.863753 -0.029545

 69 6 0 -6.400991 4.005629 0.093637

 70 1 0 -3.179479 4.822333 -0.708262

 71 7 0 -3.491748 0.684811 -1.000587

 72 1 0 -7.324281 4.487617 0.391897

 73 7 0 -1.372540 0.278298 -1.402050

 74 6 0 -1.569903 1.637069 -1.302241

 75 6 0 -4.926981 -3.149285 -0.601598

 76 8 0 -4.250614 -4.139999 -0.753656

 77 8 0 -6.238199 -3.199459 -0.272753

 78 6 0 -6.784196 -4.517769 -0.104180

 79 1 0 -7.829933 -4.367763 0.154709

 80 1 0 -6.693616 -5.088302 -1.029387

 81 1 0 -6.261397 -5.046311 0.693955

 82 17 0 1.732565 -1.977750 -2.852297

 83 17 0 -1.632866 0.117351 2.289092

 84 8 0 2.929309 -2.842321 -2.991287

 85 8 0 2.176615 -0.574609 -2.444474

 86 8 0 0.878311 -2.465667 -1.697289

 87 8 0 0.952136 -1.922026 -4.094278

 88 8 0 -1.240104 -1.134499 1.534580

 89 8 0 -0.686211 1.197084 1.787130

 90 8 0 -1.434920 -0.086913 3.743253

 91 8 0 -3.023865 0.488427 1.974072

 ---------------------------------------------------------------------

**19** (S0) BHandHLYP

---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -1.740312 -0.251948 -0.107915

 2 6 0 -1.061080 0.709329 0.634134

 3 6 0 -0.965857 -1.139894 -0.852073

 4 6 0 0.313342 0.800380 0.626246

 5 1 0 -1.611082 1.394340 1.254983

 6 6 0 0.408008 -1.063923 -0.871180

 7 1 0 -1.454922 -1.906244 -1.426871

 8 6 0 1.099612 -0.082081 -0.136084

 9 1 0 0.770447 1.571794 1.215026

 10 1 0 0.945073 -1.786734 -1.454547

 11 6 0 8.231418 -2.024162 1.372134

 12 1 0 8.037370 -2.477395 0.400883

 13 1 0 8.797382 -2.740718 1.970196

 14 6 0 9.043965 -0.764204 1.198798

 15 1 0 10.056082 -1.023418 0.893924

 16 1 0 9.103575 -0.247510 2.151370

 17 6 0 8.942098 0.027580 -1.040895

 18 1 0 9.121277 -1.011804 -1.314729

 19 1 0 9.885586 0.566352 -1.131961

 20 6 0 7.922141 0.583874 -1.995613

 21 1 0 6.989184 0.042514 -1.862772

 22 1 0 8.263281 0.419812 -3.017340

 23 6 0 6.398932 2.402486 -1.930399

 24 1 0 5.911613 1.885871 -2.755659

 25 1 0 6.434504 3.458139 -2.173882

 26 6 0 5.611730 2.178204 -0.653538

 27 1 0 5.938199 2.876871 0.116779

 28 1 0 5.804024 1.172594 -0.286049

 29 6 0 3.394242 2.310979 0.184051

 30 1 0 2.450831 2.734576 -0.140157

 31 1 0 3.792317 2.939388 0.981981

 32 6 0 3.184335 0.904014 0.728658

 33 1 0 2.663482 0.977464 1.677255

 34 1 0 4.137430 0.444208 0.954477

 35 6 0 3.265161 -0.785318 -1.073870

 36 1 0 4.137907 -0.202312 -1.339579

 37 1 0 2.717965 -0.943896 -1.996076

 38 6 0 3.730737 -2.126362 -0.542167

 39 1 0 4.256869 -2.648020 -1.343303

 40 1 0 2.888514 -2.746087 -0.233858

 41 6 0 5.311642 -3.056674 0.937370

 42 1 0 4.631396 -3.877856 1.170442

 43 1 0 5.955305 -3.386054 0.121106

 44 6 0 6.111418 -2.744195 2.180648

 45 1 0 5.432488 -2.434497 2.967662

 46 1 0 6.618650 -3.651947 2.509370

 47 7 0 2.466624 0.005770 -0.157577

 48 8 0 4.247366 2.367435 -0.938344

 49 8 0 7.728700 1.964977 -1.778862

 50 8 0 8.456939 0.124855 0.276126

 51 8 0 7.031480 -1.692410 2.026111

 52 8 0 4.594685 -1.914910 0.546948

 53 6 0 -5.137749 -1.272564 -0.323714

 54 6 0 -4.137787 0.654236 0.211404

 55 7 0 -5.313080 0.010625 0.065222

 56 6 0 -6.443752 0.729269 0.260813

 57 6 0 -7.610284 0.036470 0.074109

 58 6 0 -7.523523 -1.322627 -0.308618

 59 6 0 -6.317577 -1.984209 -0.514583

 60 1 0 -8.567783 0.500656 0.202964

 61 1 0 -6.310396 -3.012968 -0.819555

 62 6 0 -4.517438 2.007897 0.549016

 63 6 0 -5.944498 2.049284 0.590179

 64 6 0 -3.795674 3.172286 0.799000

 65 6 0 -6.614551 3.227928 0.891676

 66 6 0 -5.876670 4.364345 1.143659

 67 6 0 -4.480731 4.332736 1.091975

 68 1 0 -3.927052 5.235549 1.284022

 69 1 0 -7.689961 3.253465 0.923820

 70 1 0 -2.722145 3.179924 0.757037

 71 7 0 -3.822803 -1.503014 -0.425354

 72 6 0 -3.192353 -0.347484 -0.101608

 73 1 0 -6.378032 5.286909 1.378023

 74 6 0 -8.761458 -2.114605 -0.525198

 75 8 0 -8.769424 -3.270314 -0.853370

 76 8 0 -9.863074 -1.413036 -0.319157

 77 6 0 -11.107142 -2.086949 -0.504531

 78 1 0 -11.869306 -1.354530 -0.286827

 79 1 0 -11.196851 -2.433575 -1.525854

 80 1 0 -11.183834 -2.925911 0.174732

 ---------------------------------------------------------------------

**19** (S1) BHandHLYP

---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -1.670601 -0.277856 -0.340993

 2 6 0 -0.937972 0.762678 0.250155

 3 6 0 -0.943248 -1.257489 -1.037027

 4 6 0 0.439523 0.840017 0.143243

 5 1 0 -1.451792 1.520082 0.827902

 6 6 0 0.433292 -1.194834 -1.154329

 7 1 0 -1.477029 -2.083558 -1.489820

 8 6 0 1.176377 -0.135975 -0.572649

 9 1 0 0.942780 1.675535 0.607648

 10 1 0 0.937314 -1.988619 -1.686491

 11 6 0 7.227887 -1.300849 2.702754

 12 1 0 7.721928 -2.069992 2.100645

 13 1 0 7.357031 -1.578490 3.757965

 14 6 0 7.875639 0.051127 2.458460

 15 1 0 8.909963 0.028975 2.826035

 16 1 0 7.334059 0.819826 3.014030

 17 6 0 8.793775 -0.162827 0.246055

 18 1 0 8.993936 -1.195776 0.555515

 19 1 0 9.739987 0.392025 0.297126

 20 6 0 8.275218 -0.200494 -1.177424

 21 1 0 7.304038 -0.703828 -1.195298

 22 1 0 8.977780 -0.779998 -1.787260

 23 6 0 6.866120 1.466022 -2.197967

 24 1 0 6.410589 0.637572 -2.754252

 25 1 0 6.995396 2.304474 -2.885121

 26 6 0 5.965776 1.854537 -1.033628

 27 1 0 6.331217 2.774382 -0.557922

 28 1 0 5.992188 1.061285 -0.285050

 29 6 0 3.678069 2.170219 -0.482793

 30 1 0 2.788846 2.609185 -0.938583

 31 1 0 4.047032 2.858890 0.289570

 32 6 0 3.335068 0.824689 0.159894

 33 1 0 2.799358 1.000571 1.093530

 34 1 0 4.247953 0.293366 0.430989

 35 6 0 3.273993 -0.912440 -1.625646

 36 1 0 4.087908 -0.324547 -2.052337

 37 1 0 2.617092 -1.179318 -2.452377

 38 6 0 3.862865 -2.174272 -1.005143

 39 1 0 4.032879 -2.933250 -1.780820

 40 1 0 3.169388 -2.589218 -0.264567

 41 6 0 5.609808 -2.799889 0.518173

 42 1 0 5.222865 -3.798008 0.281000

 43 1 0 6.693366 -2.830840 0.381214

 44 6 0 5.260105 -2.450928 1.959254

 45 1 0 4.180094 -2.320861 2.057193

 46 1 0 5.564437 -3.273822 2.620168

 47 7 0 2.544214 -0.060686 -0.691740

 48 8 0 4.643620 2.055227 -1.529427

 49 8 0 8.169879 1.110604 -1.745822

 50 8 0 7.828351 0.449989 1.093594

 51 8 0 5.841749 -1.221082 2.384315

 52 8 0 5.107398 -1.829591 -0.396154

 53 6 0 -5.108171 -1.271110 -0.254755

 54 6 0 -4.034806 0.691823 0.090325

 55 7 0 -5.236493 0.053212 0.069342

 56 6 0 -6.351043 0.811353 0.295644

 57 6 0 -7.544926 0.120539 0.233453

 58 6 0 -7.506431 -1.268067 -0.066857

 59 6 0 -6.314110 -1.969810 -0.316753

 60 1 0 -8.489879 0.614340 0.398206

 61 1 0 -6.345826 -3.022214 -0.558109

 62 6 0 -4.374543 2.074665 0.361797

 63 6 0 -5.812009 2.144721 0.500818

 64 6 0 -3.620418 3.248193 0.480657

 65 6 0 -6.444918 3.359937 0.768407

 66 6 0 -5.669674 4.505480 0.890868

 67 6 0 -4.273375 4.446103 0.742678

 68 1 0 -3.692174 5.356189 0.833131

 69 1 0 -7.522289 3.406775 0.873736

 70 1 0 -2.545652 3.234851 0.360395

 71 7 0 -3.792865 -1.531069 -0.436535

 72 6 0 -3.117366 -0.355285 -0.229171

 73 1 0 -6.144572 5.456839 1.097333

 74 6 0 -8.768937 -2.052732 -0.143995

 75 8 0 -8.823649 -3.240447 -0.397520

 76 8 0 -9.856863 -1.304414 0.098234

 77 6 0 -11.129420 -1.982109 0.043131

 78 1 0 -11.871388 -1.218329 0.259622

 79 1 0 -11.289624 -2.402410 -0.949619

 80 1 0 -11.166356 -2.775405 0.789620

 ---------------------------------------------------------------------

**19·Ba(ClO4)2** (S0) BHandHLYP

---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -0.544642 2.401384 -0.985180

 2 6 0 -0.100200 3.086593 0.141253

 3 6 0 0.329842 2.285293 -2.055736

 4 6 0 1.214767 3.479064 0.256139

 5 1 0 -0.759209 3.212102 0.981655

 6 6 0 1.638417 2.712906 -1.962380

 7 1 0 0.010666 1.785339 -2.953125

 8 6 0 2.148669 3.202403 -0.755200

 9 1 0 1.524731 3.922542 1.181364

 10 1 0 2.273488 2.565121 -2.810526

 11 6 0 3.975807 -3.181724 0.530325

 12 1 0 4.395114 -3.085724 1.532960

 13 1 0 4.599154 -3.884271 -0.024218

 14 6 0 2.576455 -3.742922 0.559417

 15 1 0 2.591861 -4.725767 1.026801

 16 1 0 2.211618 -3.843348 -0.454226

 17 6 0 1.455762 -3.090175 2.612327

 18 1 0 1.687061 -4.115011 2.894715

 19 1 0 0.406356 -2.904110 2.792139

 20 6 0 2.283647 -2.133360 3.438580

 21 1 0 3.345601 -2.380035 3.408064

 22 1 0 1.950733 -2.192668 4.475019

 23 6 0 2.691358 0.171597 3.717477

 24 1 0 3.762077 -0.022678 3.807429

 25 1 0 2.255155 0.182002 4.716511

 26 6 0 2.441694 1.498181 3.047380

 27 1 0 2.879606 2.296766 3.641855

 28 1 0 1.374265 1.665552 2.975816

 29 6 0 4.207260 2.162169 1.535839

 30 1 0 4.842861 1.499173 0.967240

 31 1 0 4.678356 2.363080 2.497401

 32 6 0 4.046720 3.476722 0.782160

 33 1 0 5.032067 3.928416 0.706760

 34 1 0 3.448226 4.170876 1.360562

 35 6 0 4.452271 3.107352 -1.632147

 36 1 0 5.413450 3.469693 -1.285510

 37 1 0 4.188673 3.719701 -2.493665

 38 6 0 4.641461 1.682840 -2.150499

 39 1 0 5.514140 1.710476 -2.808197

 40 1 0 3.801078 1.337461 -2.741482

 41 6 0 5.240590 -0.496861 -1.587543

 42 1 0 4.557330 -0.834228 -2.360636

 43 1 0 6.243837 -0.431122 -2.014424

 44 6 0 5.272354 -1.509612 -0.478416

 45 1 0 5.834453 -2.368517 -0.842829

 46 1 0 5.794198 -1.109466 0.391962

 47 7 0 3.508616 3.355896 -0.558541

 48 8 0 2.969206 1.499022 1.734297

 49 8 0 2.090807 -0.833262 2.938204

 50 8 0 1.653413 -2.905365 1.224101

 51 8 0 3.974505 -1.931338 -0.116200

 52 8 0 4.858972 0.770324 -1.104748

 53 56 0 1.141479 -0.376685 0.159731

 54 6 0 -3.095291 1.887673 -0.721745

 55 6 0 -2.800948 -0.321420 -0.914192

 56 6 0 -5.021181 0.643594 -0.492201

 57 6 0 -3.348650 -1.600970 -0.895476

 58 1 0 -2.745828 -2.477569 -1.036062

 59 6 0 -5.570242 -0.607240 -0.470936

 60 1 0 -6.615815 -0.766042 -0.296410

 61 6 0 -4.712805 -1.716589 -0.677006

 62 6 0 -5.366348 2.047880 -0.339550

 63 6 0 -4.174745 2.815490 -0.482398

 64 6 0 -6.579542 2.673281 -0.094298

 65 1 0 -7.481589 2.096651 0.017413

 66 6 0 -4.225873 4.199126 -0.379125

 67 6 0 -5.443076 4.801003 -0.136736

 68 1 0 -5.495826 5.873060 -0.054913

 69 6 0 -6.609697 4.048480 0.005852

 70 1 0 -3.333268 4.789939 -0.487331

 71 7 0 -3.687906 0.675016 -0.718955

 72 1 0 -7.542787 4.549178 0.196680

 73 7 0 -1.586247 0.232575 -1.051950

 74 6 0 -1.755970 1.577822 -0.943488

 75 6 0 -5.263147 -3.096854 -0.656695

 76 8 0 -4.612224 -4.085131 -0.821988

 77 8 0 -6.575797 -3.122715 -0.432875

 78 6 0 -7.178575 -4.409281 -0.391207

 79 1 0 -8.227763 -4.235193 -0.201800

 80 1 0 -7.042464 -4.921490 -1.335617

 81 1 0 -6.743137 -5.004803 0.401541

 82 17 0 1.681502 -1.769142 -2.990116

 83 17 0 -1.419470 -0.247299 2.566290

 84 8 0 2.883230 -2.520188 -3.301988

 85 8 0 2.058098 -0.402602 -2.527810

 86 8 0 0.990171 -2.380296 -1.828526

 87 8 0 0.798907 -1.684598 -4.124881

 88 8 0 -0.987972 -1.404857 1.745930

 89 8 0 -0.566091 0.884493 2.115354

 90 8 0 -1.176787 -0.518466 3.968888

 91 8 0 -2.808929 0.056394 2.312958

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**19·Ba(ClO4)2** (S1) BHandHLYP

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -0.368426 2.475186 -1.322086

 2 6 0 0.007083 3.208431 -0.187168

 3 6 0 0.587005 2.292291 -2.327565

 4 6 0 1.332887 3.551111 0.025808

 5 1 0 -0.718324 3.387760 0.595399

 6 6 0 1.905101 2.683499 -2.143247

 7 1 0 0.317807 1.756979 -3.229236

 8 6 0 2.338264 3.185391 -0.898411

 9 1 0 1.589477 4.017927 0.964546

 10 1 0 2.606258 2.494443 -2.939017

 11 6 0 3.516740 -3.323247 0.977044

 12 1 0 3.855573 -3.195775 2.013850

 13 1 0 4.148334 -4.087376 0.504955

 14 6 0 2.079447 -3.795503 0.902631

 15 1 0 1.977693 -4.748327 1.434557

 16 1 0 1.800208 -3.935651 -0.141146

 17 6 0 0.866924 -2.880523 2.819296

 18 1 0 0.993658 -3.898410 3.204028

 19 1 0 -0.176652 -2.588473 2.909043

 20 6 0 1.729843 -1.918875 3.620258

 21 1 0 2.771885 -2.257306 3.697130

 22 1 0 1.315194 -1.845492 4.633826

 23 6 0 2.262081 0.397521 3.764418

 24 1 0 3.304264 0.149590 4.012255

 25 1 0 1.694057 0.518451 4.695660

 26 6 0 2.187237 1.676462 2.955573

 27 1 0 2.611583 2.505268 3.530733

 28 1 0 1.145020 1.900331 2.729439

 29 6 0 4.163797 2.134724 1.610213

 30 1 0 4.819690 1.419633 1.119946

 31 1 0 4.553646 2.350954 2.612403

 32 6 0 4.122286 3.430723 0.793512

 33 1 0 5.134644 3.846883 0.784747

 34 1 0 3.496713 4.173981 1.288576

 35 6 0 4.699953 2.821544 -1.545685

 36 1 0 5.667803 3.084888 -1.115774

 37 1 0 4.604288 3.401388 -2.471972

 38 6 0 4.742387 1.342782 -1.956631

 39 1 0 5.674091 1.208594 -2.526214

 40 1 0 3.914408 1.054433 -2.605036

 41 6 0 5.136778 -0.838204 -1.172796

 42 1 0 4.525351 -1.217013 -1.994984

 43 1 0 6.190471 -0.831098 -1.489065

 44 6 0 5.008316 -1.756066 0.016156

 45 1 0 5.563035 -2.672984 -0.215357

 46 1 0 5.453091 -1.301133 0.911453

 47 7 0 3.690326 3.266287 -0.589369

 48 8 0 2.877575 1.512828 1.711205

 49 8 0 1.694542 -0.647551 2.984131

 50 8 0 1.153735 -2.842178 1.419565

 51 8 0 3.643379 -2.092889 0.268697

 52 8 0 4.745021 0.485576 -0.821853

 53 56 0 1.157387 -0.358529 0.155087

 54 6 0 -2.919030 1.922261 -1.028762

 55 6 0 -2.579515 -0.308866 -1.209843

 56 6 0 -4.803868 0.622642 -0.627794

 57 6 0 -3.082611 -1.603549 -1.089246

 58 1 0 -2.453006 -2.471005 -1.223522

 59 6 0 -5.306034 -0.654156 -0.506281

 60 1 0 -6.326929 -0.836403 -0.208671

 61 6 0 -4.433012 -1.752252 -0.747529

 62 6 0 -5.162811 2.020662 -0.426225

 63 6 0 -3.991216 2.823834 -0.671977

 64 6 0 -6.360100 2.623408 -0.044090

 65 1 0 -7.242428 2.023611 0.146205

 66 6 0 -4.054873 4.210533 -0.526707

 67 6 0 -5.260045 4.787955 -0.145947

 68 1 0 -5.321801 5.863753 -0.029545

 69 6 0 -6.400991 4.005629 0.093637

 70 1 0 -3.179479 4.822333 -0.708262

 71 7 0 -3.491748 0.684811 -1.000587

 72 1 0 -7.324281 4.487617 0.391897

 73 7 0 -1.372540 0.278298 -1.402050

 74 6 0 -1.569903 1.637069 -1.302241

 75 6 0 -4.926981 -3.149285 -0.601598

 76 8 0 -4.250614 -4.139999 -0.753656

 77 8 0 -6.238199 -3.199459 -0.272753

 78 6 0 -6.784196 -4.517769 -0.104180

 79 1 0 -7.829933 -4.367763 0.154709

 80 1 0 -6.693616 -5.088302 -1.029387

 81 1 0 -6.261397 -5.046311 0.693955

 82 17 0 1.732565 -1.977750 -2.852297

 83 17 0 -1.632866 0.117351 2.289092

 84 8 0 2.929309 -2.842321 -2.991287

 85 8 0 2.176615 -0.574609 -2.444474

 86 8 0 0.878311 -2.465667 -1.697289

 87 8 0 0.952136 -1.922026 -4.094278

 88 8 0 -1.240104 -1.134499 1.534580

 89 8 0 -0.686211 1.197084 1.787130

 90 8 0 -1.434920 -0.086913 3.743253

 91 8 0 -3.023865 0.488427 1.974072

 ---------------------------------------------------------------------

**19** (S0) B3LYP

---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -1.568331 -0.256182 -0.395187

 2 6 0 -0.825695 0.799472 0.149469

 3 6 0 -0.856799 -1.267242 -1.058554

 4 6 0 0.552113 0.862001 0.029936

 5 1 0 -1.332291 1.580364 0.702110

 6 6 0 0.518902 -1.218361 -1.186985

 7 1 0 -1.408439 -2.103554 -1.468740

 8 6 0 1.273958 -0.147219 -0.649105

 9 1 0 1.067421 1.710328 0.456559

 10 1 0 1.013865 -2.033519 -1.695529

 11 6 0 6.634488 -1.063442 2.895739

 12 1 0 7.200463 -1.895954 2.461344

 13 1 0 6.589561 -1.229165 3.982687

 14 6 0 7.345792 0.250258 2.613423

 15 1 0 8.313966 0.261173 3.134305

 16 1 0 6.742823 1.074968 2.999606

 17 6 0 8.569865 -0.190489 0.589452

 18 1 0 8.725477 -1.179789 1.041537

 19 1 0 9.500812 0.382152 0.694769

 20 6 0 8.244572 -0.401667 -0.878856

 21 1 0 7.272122 -0.898615 -0.961262

 22 1 0 9.010005 -1.063649 -1.303478

 23 6 0 7.016438 1.179442 -2.212682

 24 1 0 6.514678 0.301609 -2.639183

 25 1 0 7.253191 1.862162 -3.030571

 26 6 0 6.093356 1.837715 -1.195519

 27 1 0 6.465847 2.835385 -0.926067

 28 1 0 6.088364 1.232796 -0.288433

 29 6 0 3.786096 2.136551 -0.761377

 30 1 0 2.902824 2.507201 -1.285285

 31 1 0 4.114057 2.907319 -0.048289

 32 6 0 3.451367 0.846529 -0.005525

 33 1 0 2.929031 1.086750 0.921391

 34 1 0 4.368462 0.340431 0.297904

 35 6 0 3.345174 -0.973728 -1.704854

 36 1 0 4.198240 -0.427007 -2.108138

 37 1 0 2.690510 -1.195810 -2.549340

 38 6 0 3.842493 -2.273292 -1.082601

 39 1 0 4.037769 -3.021503 -1.864328

 40 1 0 3.081141 -2.674800 -0.404655

 41 6 0 5.308250 -2.842489 0.736271

 42 1 0 4.891205 -3.846485 0.580364

 43 1 0 6.394110 -2.950433 0.800572

 44 6 0 4.749605 -2.255682 2.029563

 45 1 0 3.678312 -2.071528 1.920630

 46 1 0 4.886922 -2.975849 2.850160

 47 7 0 2.646676 -0.098842 -0.773344

 48 8 0 4.786218 1.939639 -1.756439

 49 8 0 8.259908 0.811005 -1.625984

 50 8 0 7.505071 0.499288 1.228885

 51 8 0 5.325084 -0.999268 2.354263

 52 8 0 5.053853 -2.002498 -0.377893

 53 6 0 -4.997945 -1.246355 -0.263458

 54 6 0 -3.929698 0.724983 0.047640

 55 7 0 -5.129499 0.083387 0.048488

 56 6 0 -6.243560 0.839803 0.280917

 57 6 0 -7.435029 0.142635 0.240659

 58 6 0 -7.393930 -1.248458 -0.046186

 59 6 0 -6.202499 -1.948690 -0.303413

 60 1 0 -8.383000 0.628888 0.411435

 61 1 0 -6.237714 -3.003743 -0.532801

 62 6 0 -4.270175 2.108117 0.306538

 63 6 0 -5.706110 2.176420 0.464533

 64 6 0 -3.520026 3.286762 0.397477

 65 6 0 -6.336484 3.393555 0.726441

 66 6 0 -5.564790 4.542796 0.823353

 67 6 0 -4.171408 4.485408 0.653673

 68 1 0 -3.592104 5.398962 0.721028

 69 1 0 -7.412735 3.438931 0.846708

 70 1 0 -2.447803 3.273151 0.254817

 71 7 0 -3.686353 -1.502987 -0.457136

 72 6 0 -3.014373 -0.327899 -0.269487

 73 1 0 -6.039730 5.495377 1.024718

 74 6 0 -8.650978 -2.042250 -0.101197

 75 8 0 -8.709123 -3.226655 -0.342577

 76 8 0 -9.747421 -1.291368 0.151021

 77 6 0 -11.001663 -1.992452 0.113939

 78 1 0 -11.758814 -1.243934 0.336246

 79 1 0 -11.166007 -2.425993 -0.873286

 80 1 0 -11.014901 -2.787956 0.859980

 ---------------------------------------------------------------------

**19** (S1) B3LYP

---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -1.670948 -0.378697 -0.302234

 2 6 0 -0.920991 0.814243 -0.359748

 3 6 0 -0.945632 -1.591469 -0.365833

 4 6 0 0.430462 0.805522 -0.454104

 5 1 0 -1.436045 1.761681 -0.359211

 6 6 0 0.404222 -1.608349 -0.464788

 7 1 0 -1.501089 -2.516469 -0.314024

 8 6 0 1.153629 -0.408517 -0.507661

 9 1 0 0.949167 1.748567 -0.529431

 10 1 0 0.909106 -2.561889 -0.470942

 11 6 0 7.098074 0.481832 2.861987

 12 1 0 7.617288 -0.481043 2.874303

 13 1 0 7.219599 0.923790 3.856764

 14 6 0 7.713206 1.381660 1.837444

 15 1 0 8.751322 1.599291 2.113584

 16 1 0 7.167446 2.325249 1.814673

 17 6 0 8.604366 -0.104257 0.253402

 18 1 0 8.779909 -0.784275 1.095339

 19 1 0 9.557210 0.387215 0.022846

 20 6 0 8.143116 -0.917795 -0.911368

 21 1 0 7.174654 -1.367927 -0.670128

 22 1 0 8.863621 -1.721328 -1.084888

 23 6 0 6.767236 -0.079801 -2.626681

 24 1 0 6.321236 -1.079519 -2.695341

 25 1 0 6.876019 0.304800 -3.640347

 26 6 0 5.870160 0.808763 -1.820462

 27 1 0 6.256182 1.834855 -1.818557

 28 1 0 5.863291 0.459713 -0.786366

 29 6 0 3.663831 1.484705 -1.628451

 30 1 0 2.787320 1.632533 -2.259733

 31 1 0 4.066024 2.470216 -1.364532

 32 6 0 3.270906 0.768105 -0.359432

 33 1 0 2.719830 1.446277 0.287564

 34 1 0 4.161947 0.466683 0.195139

 35 6 0 3.224989 -1.606220 -0.932390

 36 1 0 3.993052 -1.322687 -1.654858

 37 1 0 2.565717 -2.308045 -1.433300

 38 6 0 3.894118 -2.264880 0.239407

 39 1 0 4.106156 -3.312650 -0.001147

 40 1 0 3.228864 -2.246331 1.110250

 41 6 0 5.667444 -1.931562 1.723731

 42 1 0 5.398543 -2.953949 2.008033

 43 1 0 6.749724 -1.909816 1.582319

 44 6 0 5.266893 -0.977251 2.807927

 45 1 0 4.178986 -0.905803 2.851131

 46 1 0 5.613440 -1.352020 3.777563

 47 7 0 2.490789 -0.416969 -0.593403

 48 8 0 4.594267 0.775868 -2.381323

 49 8 0 8.041119 -0.145514 -2.072057

 50 8 0 7.636679 0.843013 0.558956

 51 8 0 5.746776 0.307744 2.571320

 52 8 0 5.083877 -1.590671 0.504540

 53 6 0 -5.042632 -1.263696 -0.120475

 54 6 0 -3.978284 0.700656 -0.054233

 55 7 0 -5.163203 0.082190 -0.022302

 56 6 0 -6.258203 0.874194 0.116498

 57 6 0 -7.457671 0.194820 0.150708

 58 6 0 -7.422381 -1.200377 0.047424

 59 6 0 -6.262950 -1.955651 -0.086379

 60 1 0 -8.401407 0.704905 0.255521

 61 1 0 -6.316137 -3.029460 -0.157453

 62 6 0 -4.287284 2.087532 0.087278

 63 6 0 -5.717987 2.181179 0.187007

 64 6 0 -3.528720 3.249036 0.155798

 65 6 0 -6.329357 3.418973 0.335839

 66 6 0 -5.548958 4.542227 0.391273

 67 6 0 -4.156586 4.458895 0.304214

 68 1 0 -3.564866 5.361637 0.357609

 69 1 0 -7.406242 3.491953 0.409673

 70 1 0 -2.450398 3.224974 0.105213

 71 7 0 -3.772572 -1.574595 -0.223877

 72 6 0 -3.061375 -0.396508 -0.196225

 73 1 0 -6.014999 5.511014 0.508333

 74 6 0 -8.686569 -1.949815 0.082838

 75 8 0 -8.760766 -3.142954 0.000311

 76 8 0 -9.744703 -1.182708 0.215952

 77 6 0 -10.985603 -1.843413 0.257885

 78 1 0 -11.735810 -1.069509 0.374359

 79 1 0 -11.153742 -2.396307 -0.663955

 80 1 0 -11.021130 -2.533451 1.098321

 ---------------------------------------------------------------------

**19·Ba(ClO4)2** (S0) B3LYP

---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -0.353552 2.431930 -1.417442

 2 6 0 0.014407 3.221840 -0.318007

 3 6 0 0.614826 2.185729 -2.397477

 4 6 0 1.339929 3.566584 -0.107037

 5 1 0 -0.718430 3.446547 0.445921

 6 6 0 1.933010 2.577065 -2.217764

 7 1 0 0.353390 1.602466 -3.271188

 8 6 0 2.354226 3.145162 -0.997555

 9 1 0 1.588687 4.081002 0.808798

 10 1 0 2.642416 2.337651 -2.992059

 11 6 0 3.487101 -3.292399 1.118429

 12 1 0 3.809799 -3.127316 2.155042

 13 1 0 4.124491 -4.074402 0.684958

 14 6 0 2.050380 -3.765558 1.038835

 15 1 0 1.939232 -4.698448 1.603212

 16 1 0 1.787045 -3.943196 -0.003323

 17 6 0 0.809727 -2.781609 2.902665

 18 1 0 0.926193 -3.785859 3.324676

 19 1 0 -0.233801 -2.482961 2.965903

 20 6 0 1.664354 -1.795687 3.682995

 21 1 0 2.702043 -2.138098 3.793562

 22 1 0 1.230318 -1.680622 4.684381

 23 6 0 2.206205 0.521627 3.752887

 24 1 0 3.243365 0.281175 4.027674

 25 1 0 1.621284 0.674456 4.668725

 26 6 0 2.147211 1.772550 2.900141

 27 1 0 2.567912 2.618676 3.452290

 28 1 0 1.109344 1.993008 2.652585

 29 6 0 4.143805 2.175166 1.567593

 30 1 0 4.802978 1.440969 1.111322

 31 1 0 4.520259 2.423923 2.567309

 32 6 0 4.119235 3.441988 0.706122

 33 1 0 5.133415 3.853527 0.694830

 34 1 0 3.490903 4.204342 1.167347

 35 6 0 4.722917 2.755911 -1.605750

 36 1 0 5.685155 3.042144 -1.177847

 37 1 0 4.630439 3.300304 -2.553549

 38 6 0 4.779913 1.262584 -1.961522

 39 1 0 5.725298 1.111243 -2.503683

 40 1 0 3.968676 0.947486 -2.618701

 41 6 0 5.149793 -0.890136 -1.092916

 42 1 0 4.550818 -1.296371 -1.911186

 43 1 0 6.208737 -0.898153 -1.391103

 44 6 0 4.997791 -1.764182 0.126030

 45 1 0 5.553871 -2.690023 -0.062811

 46 1 0 5.428468 -1.278427 1.011975

 47 7 0 3.702664 3.228788 -0.674769

 48 8 0 2.852629 1.563931 1.670972

 49 8 0 1.651597 -0.549231 2.998444

 50 8 0 1.117785 -2.793661 1.506885

 51 8 0 3.627905 -2.089228 0.367182

 52 8 0 4.757537 0.446822 -0.797012

 53 56 0 1.148274 -0.356373 0.159304

 54 6 0 -2.899719 1.895519 -1.076194

 55 6 0 -2.577402 -0.338820 -1.250991

 56 6 0 -4.787291 0.611009 -0.642054

 57 6 0 -3.087305 -1.629228 -1.115299

 58 1 0 -2.465308 -2.501646 -1.253421

 59 6 0 -5.296364 -0.661822 -0.507114

 60 1 0 -6.314427 -0.835497 -0.195060

 61 6 0 -4.434067 -1.766956 -0.753804

 62 6 0 -5.133820 2.012233 -0.442834

 63 6 0 -3.960348 2.806067 -0.709387

 64 6 0 -6.321150 2.625083 -0.046041

 65 1 0 -7.204621 2.032310 0.160285

 66 6 0 -4.012445 4.193898 -0.569895

 67 6 0 -5.207842 4.781424 -0.174320

 68 1 0 -5.260516 5.858166 -0.062189

 69 6 0 -6.350536 4.008136 0.085672

 70 1 0 -3.135794 4.798951 -0.767367

 71 7 0 -3.479858 0.662185 -1.032712

 72 1 0 -7.265962 4.497914 0.395272

 73 7 0 -1.369687 0.238947 -1.466315

 74 6 0 -1.556277 1.599374 -1.368165

 75 6 0 -4.935331 -3.159685 -0.593137

 76 8 0 -4.267299 -4.155825 -0.746918

 77 8 0 -6.242960 -3.199271 -0.248771

 78 6 0 -6.795556 -4.512880 -0.065809

 79 1 0 -7.837165 -4.354390 0.204435

 80 1 0 -6.719664 -5.089553 -0.988529

 81 1 0 -6.266881 -5.040155 0.729293

 82 17 0 1.768408 -2.082016 -2.780226

 83 17 0 -1.652564 0.212951 2.260626

 84 8 0 2.963156 -2.955629 -2.870566

 85 8 0 2.212073 -0.667479 -2.413194

 86 8 0 0.893580 -2.526552 -1.623075

 87 8 0 1.008106 -2.065432 -4.035715

 88 8 0 -1.275708 -1.062792 1.538667

 89 8 0 -0.706655 1.271315 1.714240

 90 8 0 -1.436229 0.051104 3.718006

 91 8 0 -3.045695 0.581792 1.954084

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**19·Ba(ClO4)2** (S1) B3LYP

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -0.128717 1.793809 -1.927706

 2 6 0 0.221319 2.914295 -1.163325

 3 6 0 0.876584 1.193148 -2.692979

 4 6 0 1.531649 3.237201 -0.975827

 5 1 0 -0.538243 3.424491 -0.586742

 6 6 0 2.183030 1.559209 -2.550187

 7 1 0 0.619149 0.363201 -3.337087

 8 6 0 2.561505 2.498084 -1.585375

 9 1 0 1.762560 4.041627 -0.295564

 10 1 0 2.923049 1.033069 -3.127097

 11 6 0 2.888856 -2.935069 2.023993

 12 1 0 3.083868 -2.513046 3.017881

 13 1 0 3.516298 -3.826094 1.906968

 14 6 0 1.462709 -3.342885 1.865389

 15 1 0 1.201804 -4.079451 2.631071

 16 1 0 1.326106 -3.786954 0.881615

 17 6 0 0.138157 -1.862777 3.188741

 18 1 0 0.103428 -2.724289 3.861982

 19 1 0 -0.870558 -1.489382 3.044318

 20 6 0 0.982303 -0.782181 3.797168

 21 1 0 1.925299 -1.164961 4.206024

 22 1 0 0.410298 -0.323783 4.609878

 23 6 0 1.771492 1.352115 3.371234

 24 1 0 2.657487 1.118868 3.975781

 25 1 0 1.009342 1.810086 4.011320

 26 6 0 2.126540 2.295116 2.268253

 27 1 0 2.591049 3.186115 2.699576

 28 1 0 1.218961 2.596982 1.746498

 29 6 0 4.232133 2.278846 1.165980

 30 1 0 4.943738 1.486180 0.954852

 31 1 0 4.543898 2.804842 2.075733

 32 6 0 4.221774 3.253303 0.011919

 33 1 0 5.222559 3.681841 -0.077312

 34 1 0 3.558875 4.089181 0.227224

 35 6 0 4.903269 1.958450 -1.949024

 36 1 0 5.843746 2.366857 -1.580925

 37 1 0 4.852585 2.209320 -3.013429

 38 6 0 4.960672 0.444634 -1.838804

 39 1 0 5.991266 0.148839 -2.076768

 40 1 0 4.310246 -0.066763 -2.550313

 41 6 0 5.027390 -1.284586 -0.329390

 42 1 0 4.615752 -1.955083 -1.087554

 43 1 0 6.123422 -1.344100 -0.366161

 44 6 0 4.580449 -1.731169 1.015946

 45 1 0 5.128628 -2.648001 1.254697

 46 1 0 4.827509 -0.978309 1.774796

 47 7 0 3.867978 2.655959 -1.241633

 48 8 0 2.996633 1.663635 1.369572

 49 8 0 1.267229 0.175313 2.824188

 50 8 0 0.593912 -2.252940 1.926605

 51 8 0 3.211710 -2.001357 1.040515

 52 8 0 4.631453 0.029916 -0.558378

 53 56 0 1.069255 -0.275473 0.114331

 54 6 0 -2.623028 1.579464 -1.293831

 55 6 0 -2.575713 -0.649452 -1.360517

 56 6 0 -4.586720 0.590503 -0.676997

 57 6 0 -3.223161 -1.861693 -1.138765

 58 1 0 -2.747235 -2.816431 -1.288794

 59 6 0 -5.246464 -0.604342 -0.448403

 60 1 0 -6.261253 -0.648182 -0.090320

 61 6 0 -4.541157 -1.786121 -0.686282

 62 6 0 -4.750606 2.001450 -0.595756

 63 6 0 -3.516376 2.624464 -0.992676

 64 6 0 -5.810474 2.795622 -0.211157

 65 1 0 -6.746628 2.354930 0.103110

 66 6 0 -3.390719 4.002131 -1.000781

 67 6 0 -4.464220 4.769408 -0.615421

 68 1 0 -4.385411 5.846717 -0.614154

 69 6 0 -5.657077 4.165671 -0.225479

 70 1 0 -2.464141 4.466578 -1.311721

 71 7 0 -3.317295 0.440553 -1.113918

 72 1 0 -6.486783 4.789909 0.077086

 73 7 0 -1.352049 -0.249504 -1.733234

 74 6 0 -1.337739 1.096530 -1.709516

 75 6 0 -5.208587 -3.076577 -0.444451

 76 8 0 -4.689913 -4.138484 -0.597883

 77 8 0 -6.456942 -2.947627 -0.034396

 78 6 0 -7.129983 -4.152918 0.211519

 79 1 0 -8.129086 -3.881855 0.535796

 80 1 0 -7.172789 -4.758119 -0.692343

 81 1 0 -6.619646 -4.724581 0.984727

 82 17 0 2.022878 -2.746003 -2.018601

 83 17 0 -1.662734 1.039341 1.952640

 84 8 0 3.100065 -3.614628 -1.628345

 85 8 0 2.501957 -1.351265 -2.012036

 86 8 0 0.963659 -2.781457 -1.008217

 87 8 0 1.514035 -3.084371 -3.304435

 88 8 0 -1.457099 -0.266390 1.318688

 89 8 0 -0.700018 1.933333 1.304282

 90 8 0 -1.372586 0.947282 3.360965

 91 8 0 -2.998450 1.491334 1.725213

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**19**(S0)CAM-B3LYP

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -1.742338 -0.261580 -0.106584

 2 6 0 -1.063162 0.695902 0.647273

 3 6 0 -0.966508 -1.143510 -0.862756

 4 6 0 0.315192 0.789403 0.638792

 5 1 0 -1.619033 1.377424 1.279216

 6 6 0 0.411378 -1.065717 -0.881892

 7 1 0 -1.460350 -1.908889 -1.448138

 8 6 0 1.103228 -0.087058 -0.135674

 9 1 0 0.775890 1.560584 1.238068

 10 1 0 0.953618 -1.786979 -1.475514

 11 6 0 8.252466 -2.032883 1.362801

 12 1 0 8.044503 -2.469760 0.379141

 13 1 0 8.818632 -2.770134 1.948306

 14 6 0 9.074889 -0.773219 1.205113

 15 1 0 10.092488 -1.033951 0.895149

 16 1 0 9.135387 -0.264217 2.169342

 17 6 0 8.958212 0.023111 -1.042738

 18 1 0 9.127595 -1.026731 -1.309878

 19 1 0 9.909592 0.558660 -1.152385

 20 6 0 7.925059 0.578003 -1.988752

 21 1 0 6.983158 0.044913 -1.831331

 22 1 0 8.248063 0.399550 -3.021422

 23 6 0 6.411372 2.417054 -1.932051

 24 1 0 5.919022 1.899072 -2.762791

 25 1 0 6.453716 3.478973 -2.176488

 26 6 0 5.621110 2.193219 -0.651991

 27 1 0 5.942486 2.900648 0.122313

 28 1 0 5.818005 1.182670 -0.278452

 29 6 0 3.394216 2.316088 0.189441

 30 1 0 2.442006 2.736475 -0.136009

 31 1 0 3.795003 2.951888 0.989720

 32 6 0 3.194371 0.903447 0.732903

 33 1 0 2.674490 0.969539 1.690363

 34 1 0 4.156403 0.443279 0.954016

 35 6 0 3.277157 -0.780265 -1.084964

 36 1 0 4.152205 -0.187495 -1.349902

 37 1 0 2.725498 -0.934948 -2.013201

 38 6 0 3.748501 -2.125304 -0.559485

 39 1 0 4.283408 -2.645381 -1.365369

 40 1 0 2.903606 -2.754073 -0.251549

 41 6 0 5.331258 -3.063616 0.928337

 42 1 0 4.643347 -3.889588 1.154810

 43 1 0 5.981409 -3.391135 0.106956

 44 6 0 6.126573 -2.757267 2.180245

 45 1 0 5.440571 -2.447067 2.970132

 46 1 0 6.635989 -3.672162 2.509344

 47 7 0 2.475092 0.003676 -0.158107

 48 8 0 4.248011 2.376863 -0.944272

 49 8 0 7.748391 1.972215 -1.780245

 50 8 0 8.489249 0.137964 0.288960

 51 8 0 7.053176 -1.697585 2.035967

 52 8 0 4.614404 -1.910161 0.539521

 53 6 0 -5.154620 -1.283447 -0.320273

 54 6 0 -4.143897 0.650571 0.213027

 55 7 0 -5.326160 0.007526 0.068385

 56 6 0 -6.459814 0.733543 0.262646

 57 6 0 -7.630455 0.041141 0.075789

 58 6 0 -7.548038 -1.323028 -0.305137

 59 6 0 -6.341739 -1.991083 -0.509940

 60 1 0 -8.593473 0.510956 0.203389

 61 1 0 -6.340303 -3.027430 -0.815121

 62 6 0 -4.522694 2.010939 0.548568

 63 6 0 -5.953094 2.057260 0.589833

 64 6 0 -3.795047 3.176015 0.796392

 65 6 0 -6.620763 3.241722 0.889338

 66 6 0 -5.876695 4.379672 1.139323

 67 6 0 -4.477719 4.343334 1.087540

 68 1 0 -3.917142 5.250451 1.278709

 69 1 0 -7.703120 3.270877 0.921740

 70 1 0 -2.714347 3.178514 0.754156

 71 7 0 -3.833621 -1.518111 -0.422506

 72 6 0 -3.199269 -0.356950 -0.099887

 73 1 0 -6.378438 5.310369 1.373089

 74 6 0 -8.791850 -2.114240 -0.521704

 75 8 0 -8.807171 -3.278374 -0.849969

 76 8 0 -9.898691 -1.401241 -0.315476

 77 6 0 -11.147823 -2.083621 -0.503920

 78 1 0 -11.916532 -1.347797 -0.287626

 79 1 0 -11.233394 -2.434707 -1.531300

 80 1 0 -11.222837 -2.927307 0.180549

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**19** (S1)CAM-B3LYP

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -1.670601 -0.277856 -0.340993

 2 6 0 -0.937972 0.762678 0.250155

 3 6 0 -0.943248 -1.257489 -1.037027

 4 6 0 0.439523 0.840017 0.143243

 5 1 0 -1.451792 1.520082 0.827902

 6 6 0 0.433292 -1.194834 -1.154329

 7 1 0 -1.477029 -2.083558 -1.489820

 8 6 0 1.176377 -0.135975 -0.572649

 9 1 0 0.942780 1.675535 0.607648

 10 1 0 0.937314 -1.988619 -1.686491

 11 6 0 7.227887 -1.300849 2.702754

 12 1 0 7.721928 -2.069992 2.100645

 13 1 0 7.357031 -1.578490 3.757965

 14 6 0 7.875639 0.051127 2.458460

 15 1 0 8.909963 0.028975 2.826035

 16 1 0 7.334059 0.819826 3.014030

 17 6 0 8.793775 -0.162827 0.246055

 18 1 0 8.993936 -1.195776 0.555515

 19 1 0 9.739987 0.392025 0.297126

 20 6 0 8.275218 -0.200494 -1.177424

 21 1 0 7.304038 -0.703828 -1.195298

 22 1 0 8.977780 -0.779998 -1.787260

 23 6 0 6.866120 1.466022 -2.197967

 24 1 0 6.410589 0.637572 -2.754252

 25 1 0 6.995396 2.304474 -2.885121

 26 6 0 5.965776 1.854537 -1.033628

 27 1 0 6.331217 2.774382 -0.557922

 28 1 0 5.992188 1.061285 -0.285050

 29 6 0 3.678069 2.170219 -0.482793

 30 1 0 2.788846 2.609185 -0.938583

 31 1 0 4.047032 2.858890 0.289570

 32 6 0 3.335068 0.824689 0.159894

 33 1 0 2.799358 1.000571 1.093530

 34 1 0 4.247953 0.293366 0.430989

 35 6 0 3.273993 -0.912440 -1.625646

 36 1 0 4.087908 -0.324547 -2.052337

 37 1 0 2.617092 -1.179318 -2.452377

 38 6 0 3.862865 -2.174272 -1.005143

 39 1 0 4.032879 -2.933250 -1.780820

 40 1 0 3.169388 -2.589218 -0.264567

 41 6 0 5.609808 -2.799889 0.518173

 42 1 0 5.222865 -3.798008 0.281000

 43 1 0 6.693366 -2.830840 0.381214

 44 6 0 5.260105 -2.450928 1.959254

 45 1 0 4.180094 -2.320861 2.057193

 46 1 0 5.564437 -3.273822 2.620168

 47 7 0 2.544214 -0.060686 -0.691740

 48 8 0 4.643620 2.055227 -1.529427

 49 8 0 8.169879 1.110604 -1.745822

 50 8 0 7.828351 0.449989 1.093594

 51 8 0 5.841749 -1.221082 2.384315

 52 8 0 5.107398 -1.829591 -0.396154

 53 6 0 -5.108171 -1.271110 -0.254755

 54 6 0 -4.034806 0.691823 0.090325

 55 7 0 -5.236493 0.053212 0.069342

 56 6 0 -6.351043 0.811353 0.295644

 57 6 0 -7.544926 0.120539 0.233453

 58 6 0 -7.506431 -1.268067 -0.066857

 59 6 0 -6.314110 -1.969810 -0.316753

 60 1 0 -8.489879 0.614340 0.398206

 61 1 0 -6.345826 -3.022214 -0.558109

 62 6 0 -4.374543 2.074665 0.361797

 63 6 0 -5.812009 2.144721 0.500818

 64 6 0 -3.620418 3.248193 0.480657

 65 6 0 -6.444918 3.359937 0.768407

 66 6 0 -5.669674 4.505480 0.890868

 67 6 0 -4.273375 4.446103 0.742678

 68 1 0 -3.692174 5.356189 0.833131

 69 1 0 -7.522289 3.406775 0.873736

 70 1 0 -2.545652 3.234851 0.360395

 71 7 0 -3.792865 -1.531069 -0.436535

 72 6 0 -3.117366 -0.355285 -0.229171

 73 1 0 -6.144572 5.456839 1.097333

 74 6 0 -8.768937 -2.052732 -0.143995

 75 8 0 -8.823649 -3.240447 -0.397520

 76 8 0 -9.856863 -1.304414 0.098234

 77 6 0 -11.129420 -1.982109 0.043131

 78 1 0 -11.871388 -1.218329 0.259622

 79 1 0 -11.289624 -2.402410 -0.949619

 80 1 0 -11.166356 -2.775405 0.789620

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**19·Ba(ClO4)2** (S0) CAM-B3LYP

---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -0.514913 2.423466 -0.981545

 2 6 0 -0.072595 3.097436 0.157194

 3 6 0 0.364647 2.316321 -2.053738

 4 6 0 1.247758 3.481773 0.282972

 5 1 0 -0.740493 3.217630 1.000333

 6 6 0 1.678257 2.738770 -1.950027

 7 1 0 0.044062 1.823778 -2.963158

 8 6 0 2.186842 3.208945 -0.729957

 9 1 0 1.558467 3.917283 1.220027

 10 1 0 2.320694 2.599396 -2.803167

 11 6 0 3.911764 -3.220547 0.540582

 12 1 0 4.321813 -3.129774 1.555073

 13 1 0 4.540928 -3.929758 -0.012932

 14 6 0 2.503456 -3.768948 0.546907

 15 1 0 2.499618 -4.761367 1.010490

 16 1 0 2.147853 -3.855194 -0.479064

 17 6 0 1.368762 -3.111202 2.602348

 18 1 0 1.582713 -4.148474 2.879633

 19 1 0 0.314850 -2.905259 2.777026

 20 6 0 2.210103 -2.169583 3.439542

 21 1 0 3.275536 -2.433072 3.416600

 22 1 0 1.865358 -2.224450 4.479857

 23 6 0 2.651674 0.138744 3.731610

 24 1 0 3.725012 -0.075102 3.831536

 25 1 0 2.201036 0.151439 4.731990

 26 6 0 2.427297 1.472645 3.058981

 27 1 0 2.872143 2.271377 3.660393

 28 1 0 1.355712 1.653933 2.972347

 29 6 0 4.227647 2.121079 1.564317

 30 1 0 4.860657 1.455019 0.982761

 31 1 0 4.696847 2.299568 2.538802

 32 6 0 4.084183 3.450943 0.826396

 33 1 0 5.079796 3.898391 0.762177

 34 1 0 3.483373 4.147968 1.411548

 35 6 0 4.501302 3.092201 -1.596530

 36 1 0 5.471891 3.439278 -1.239264

 37 1 0 4.250670 3.718778 -2.460311

 38 6 0 4.669341 1.664642 -2.123841

 39 1 0 5.549498 1.678641 -2.783616

 40 1 0 3.818346 1.329480 -2.719022

 41 6 0 5.231778 -0.537517 -1.568128

 42 1 0 4.535553 -0.858537 -2.346854

 43 1 0 6.241791 -0.486512 -1.999163

 44 6 0 5.243225 -1.556904 -0.461221

 45 1 0 5.794900 -2.430452 -0.827758

 46 1 0 5.769513 -1.166300 0.419648

 47 7 0 3.551743 3.347242 -0.523165

 48 8 0 2.973484 1.462952 1.743620

 49 8 0 2.039139 -0.858352 2.935810

 50 8 0 1.574219 -2.920383 1.207180

 51 8 0 3.927401 -1.960296 -0.106684

 52 8 0 4.871749 0.741005 -1.072142

 53 56 0 1.148677 -0.371929 0.160269

 54 6 0 -3.075624 1.906390 -0.738692

 55 6 0 -2.774372 -0.312892 -0.928150

 56 6 0 -5.007036 0.652412 -0.508149

 57 6 0 -3.322160 -1.596275 -0.903357

 58 1 0 -2.713519 -2.478747 -1.037953

 59 6 0 -5.552117 -0.603960 -0.481084

 60 1 0 -6.603485 -0.767646 -0.301437

 61 6 0 -4.689580 -1.714721 -0.684551

 62 6 0 -5.354855 2.060933 -0.351329

 63 6 0 -4.161748 2.833062 -0.493543

 64 6 0 -6.571877 2.684858 -0.101700

 65 1 0 -7.478409 2.102081 0.009694

 66 6 0 -4.215336 4.219646 -0.384689

 67 6 0 -5.436627 4.820677 -0.137446

 68 1 0 -5.491156 5.899284 -0.050784

 69 6 0 -6.604447 4.063713 0.004039

 70 1 0 -3.317615 4.815594 -0.492650

 71 7 0 -3.668607 0.687638 -0.740380

 72 1 0 -7.544367 4.565043 0.199276

 73 7 0 -1.554455 0.246891 -1.058487

 74 6 0 -1.729998 1.597891 -0.951002

 75 6 0 -5.236700 -3.100690 -0.657321

 76 8 0 -4.581317 -4.097113 -0.816532

 77 8 0 -6.560496 -3.127243 -0.433975

 78 6 0 -7.154241 -4.427559 -0.387867

 79 1 0 -8.211723 -4.260495 -0.200661

 80 1 0 -7.008336 -4.945517 -1.335529

 81 1 0 -6.710806 -5.018701 0.413048

 82 17 0 1.682071 -1.744427 -2.998127

 83 17 0 -1.443983 -0.225610 2.537831

 84 8 0 2.891479 -2.509953 -3.316973

 85 8 0 2.074189 -0.369366 -2.514666

 86 8 0 0.974379 -2.367154 -1.830710

 87 8 0 0.794530 -1.639087 -4.145764

 88 8 0 -1.010828 -1.397618 1.708481

 89 8 0 -0.562797 0.911603 2.094961

 90 8 0 -1.218566 -0.506998 3.956963

 91 8 0 -2.841033 0.098399 2.265322

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**19·Ba(ClO4)2** (S1) CAM-B3LYP

---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -0.368426 2.475186 -1.322086

 2 6 0 0.007083 3.208431 -0.187168

 3 6 0 0.587005 2.292291 -2.327565

 4 6 0 1.332887 3.551111 0.025808

 5 1 0 -0.718324 3.387760 0.595399

 6 6 0 1.905101 2.683499 -2.143247

 7 1 0 0.317807 1.756979 -3.229236

 8 6 0 2.338264 3.185391 -0.898411

 9 1 0 1.589477 4.017927 0.964546

 10 1 0 2.606258 2.494443 -2.939017

 11 6 0 3.516740 -3.323247 0.977044

 12 1 0 3.855573 -3.195775 2.013850

 13 1 0 4.148334 -4.087376 0.504955

 14 6 0 2.079447 -3.795503 0.902631

 15 1 0 1.977693 -4.748327 1.434557

 16 1 0 1.800208 -3.935651 -0.141146

 17 6 0 0.866924 -2.880523 2.819296

 18 1 0 0.993658 -3.898410 3.204028

 19 1 0 -0.176652 -2.588473 2.909043

 20 6 0 1.729843 -1.918875 3.620258

 21 1 0 2.771885 -2.257306 3.697130

 22 1 0 1.315194 -1.845492 4.633826

 23 6 0 2.262081 0.397521 3.764418

 24 1 0 3.304264 0.149590 4.012255

 25 1 0 1.694057 0.518451 4.695660

 26 6 0 2.187237 1.676462 2.955573

 27 1 0 2.611583 2.505268 3.530733

 28 1 0 1.145020 1.900331 2.729439

 29 6 0 4.163797 2.134724 1.610213

 30 1 0 4.819690 1.419633 1.119946

 31 1 0 4.553646 2.350954 2.612403

 32 6 0 4.122286 3.430723 0.793512

 33 1 0 5.134644 3.846883 0.784747

 34 1 0 3.496713 4.173981 1.288576

 35 6 0 4.699953 2.821544 -1.545685

 36 1 0 5.667803 3.084888 -1.115774

 37 1 0 4.604288 3.401388 -2.471972

 38 6 0 4.742387 1.342782 -1.956631

 39 1 0 5.674091 1.208594 -2.526214

 40 1 0 3.914408 1.054433 -2.605036

 41 6 0 5.136778 -0.838204 -1.172796

 42 1 0 4.525351 -1.217013 -1.994984

 43 1 0 6.190471 -0.831098 -1.489065

 44 6 0 5.008316 -1.756066 0.016156

 45 1 0 5.563035 -2.672984 -0.215357

 46 1 0 5.453091 -1.301133 0.911453

 47 7 0 3.690326 3.266287 -0.589369

 48 8 0 2.877575 1.512828 1.711205

 49 8 0 1.694542 -0.647551 2.984131

 50 8 0 1.153735 -2.842178 1.419565

 51 8 0 3.643379 -2.092889 0.268697

 52 8 0 4.745021 0.485576 -0.821853

 53 56 0 1.157387 -0.358529 0.155087

 54 6 0 -2.919030 1.922261 -1.028762

 55 6 0 -2.579515 -0.308866 -1.209843

 56 6 0 -4.803868 0.622642 -0.627794

 57 6 0 -3.082611 -1.603549 -1.089246

 58 1 0 -2.453006 -2.471005 -1.223522

 59 6 0 -5.306034 -0.654156 -0.506281

 60 1 0 -6.326929 -0.836403 -0.208671

 61 6 0 -4.433012 -1.752252 -0.747529

 62 6 0 -5.162811 2.020662 -0.426225

 63 6 0 -3.991216 2.823834 -0.671977

 64 6 0 -6.360100 2.623408 -0.044090

 65 1 0 -7.242428 2.023611 0.146205

 66 6 0 -4.054873 4.210533 -0.526707

 67 6 0 -5.260045 4.787955 -0.145947

 68 1 0 -5.321801 5.863753 -0.029545

 69 6 0 -6.400991 4.005629 0.093637

 70 1 0 -3.179479 4.822333 -0.708262

 71 7 0 -3.491748 0.684811 -1.000587

 72 1 0 -7.324281 4.487617 0.391897

 73 7 0 -1.372540 0.278298 -1.402050

 74 6 0 -1.569903 1.637069 -1.302241

 75 6 0 -4.926981 -3.149285 -0.601598

 76 8 0 -4.250614 -4.139999 -0.753656

 77 8 0 -6.238199 -3.199459 -0.272753

 78 6 0 -6.784196 -4.517769 -0.104180

 79 1 0 -7.829933 -4.367763 0.154709

 80 1 0 -6.693616 -5.088302 -1.029387

 81 1 0 -6.261397 -5.046311 0.693955

 82 17 0 1.732565 -1.977750 -2.852297

 83 17 0 -1.632866 0.117351 2.289092

 84 8 0 2.929309 -2.842321 -2.991287

 85 8 0 2.176615 -0.574609 -2.444474

 86 8 0 0.878311 -2.465667 -1.697289

 87 8 0 0.952136 -1.922026 -4.094278

 88 8 0 -1.240104 -1.134499 1.534580

 89 8 0 -0.686211 1.197084 1.787130

 90 8 0 -1.434920 -0.086913 3.743253

 91 8 0 -3.023865 0.488427 1.974072

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**19** (S0) M06

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -1.699911 -0.272689 -0.322824

 2 6 0 -0.979479 0.778731 0.249547

 3 6 0 -0.967506 -1.257946 -0.992075

 4 6 0 0.393794 0.863294 0.145700

 5 1 0 -1.504357 1.543512 0.815269

 6 6 0 0.405504 -1.189363 -1.104018

 7 1 0 -1.496549 -2.099133 -1.429536

 8 6 0 1.135172 -0.117281 -0.546204

 9 1 0 0.893229 1.713660 0.595499

 10 1 0 0.919594 -1.994889 -1.615894

 11 6 0 7.345356 -1.294471 2.626152

 12 1 0 7.813471 -2.074926 2.008197

 13 1 0 7.485488 -1.594663 3.677155

 14 6 0 8.025288 0.030284 2.383872

 15 1 0 9.073994 -0.030559 2.714819

 16 1 0 7.532460 0.806529 2.979199

 17 6 0 8.844377 -0.177896 0.157905

 18 1 0 9.049681 -1.217855 0.457073

 19 1 0 9.805828 0.360765 0.162580

 20 6 0 8.259802 -0.206046 -1.229277

 21 1 0 7.290955 -0.726089 -1.200827

 22 1 0 8.932982 -0.778258 -1.883323

 23 6 0 6.800421 1.430947 -2.168887

 24 1 0 6.343512 0.603499 -2.736183

 25 1 0 6.882939 2.287260 -2.846694

 26 6 0 5.922117 1.774410 -0.986975

 27 1 0 6.315034 2.662093 -0.463369

 28 1 0 5.940797 0.940930 -0.272354

 29 6 0 3.674765 2.156742 -0.413072

 30 1 0 2.792129 2.638402 -0.848592

 31 1 0 4.075098 2.824171 0.367908

 32 6 0 3.286277 0.826702 0.210086

 33 1 0 2.729887 1.012514 1.133660

 34 1 0 4.183663 0.272066 0.510318

 35 6 0 3.237362 -0.895321 -1.573046

 36 1 0 4.049109 -0.310518 -2.021362

 37 1 0 2.583627 -1.188401 -2.397230

 38 6 0 3.841234 -2.123646 -0.921009

 39 1 0 3.952380 -2.938308 -1.654914

 40 1 0 3.177517 -2.485817 -0.118623

 41 6 0 5.658220 -2.723413 0.483727

 42 1 0 5.285423 -3.733558 0.257702

 43 1 0 6.742549 -2.736886 0.311865

 44 6 0 5.356819 -2.375227 1.925289

 45 1 0 4.277004 -2.228754 2.050803

 46 1 0 5.657991 -3.206975 2.581938

 47 7 0 2.501842 -0.029839 -0.666902

 48 8 0 4.615840 2.022236 -1.460438

 49 8 0 8.107889 1.100572 -1.757973

 50 8 0 7.937241 0.443192 1.039656

 51 8 0 5.972998 -1.169816 2.325888

 52 8 0 5.111471 -1.773445 -0.405759

 53 6 0 -5.112481 -1.271282 -0.237229

 54 6 0 -4.058234 0.689307 0.088834

 55 7 0 -5.252560 0.048397 0.071388

 56 6 0 -6.364723 0.802398 0.286740

 57 6 0 -7.551829 0.109487 0.228482

 58 6 0 -7.503656 -1.276638 -0.057502

 59 6 0 -6.314413 -1.972928 -0.295552

 60 1 0 -8.501953 0.602988 0.385977

 61 1 0 -6.344234 -3.030609 -0.526886

 62 6 0 -4.404551 2.068965 0.345466

 63 6 0 -5.831887 2.133101 0.479262

 64 6 0 -3.660148 3.245193 0.454461

 65 6 0 -6.473506 3.342149 0.733278

 66 6 0 -5.710182 4.488925 0.847557

 67 6 0 -4.318224 4.436155 0.703269

 68 1 0 -3.741813 5.352264 0.786838

 69 1 0 -7.554257 3.379012 0.834841

 70 1 0 -2.582089 3.238921 0.334536

 71 7 0 -3.804976 -1.529554 -0.412113

 72 6 0 -3.144758 -0.354660 -0.215288

 73 1 0 -6.191618 5.441097 1.044878

 74 6 0 -8.756806 -2.070686 -0.132931

 75 8 0 -8.800135 -3.252880 -0.379881

 76 8 0 -9.842184 -1.332224 0.103613

 77 6 0 -11.095114 -2.015255 0.049593

 78 1 0 -11.853871 -1.266059 0.266606

 79 1 0 -11.256854 -2.440209 -0.943369

 80 1 0 -11.128449 -2.813588 0.794055

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**19** (S1) M06

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -1.670601 -0.277856 -0.340993

 2 6 0 -0.937972 0.762678 0.250155

 3 6 0 -0.943248 -1.257489 -1.037027

 4 6 0 0.439523 0.840017 0.143243

 5 1 0 -1.451792 1.520082 0.827902

 6 6 0 0.433292 -1.194834 -1.154329

 7 1 0 -1.477029 -2.083558 -1.489820

 8 6 0 1.176377 -0.135975 -0.572649

 9 1 0 0.942780 1.675535 0.607648

 10 1 0 0.937314 -1.988619 -1.686491

 11 6 0 7.227887 -1.300849 2.702754

 12 1 0 7.721928 -2.069992 2.100645

 13 1 0 7.357031 -1.578490 3.757965

 14 6 0 7.875639 0.051127 2.458460

 15 1 0 8.909963 0.028975 2.826035

 16 1 0 7.334059 0.819826 3.014030

 17 6 0 8.793775 -0.162827 0.246055

 18 1 0 8.993936 -1.195776 0.555515

 19 1 0 9.739987 0.392025 0.297126

 20 6 0 8.275218 -0.200494 -1.177424

 21 1 0 7.304038 -0.703828 -1.195298

 22 1 0 8.977780 -0.779998 -1.787260

 23 6 0 6.866120 1.466022 -2.197967

 24 1 0 6.410589 0.637572 -2.754252

 25 1 0 6.995396 2.304474 -2.885121

 26 6 0 5.965776 1.854537 -1.033628

 27 1 0 6.331217 2.774382 -0.557922

 28 1 0 5.992188 1.061285 -0.285050

 29 6 0 3.678069 2.170219 -0.482793

 30 1 0 2.788846 2.609185 -0.938583

 31 1 0 4.047032 2.858890 0.289570

 32 6 0 3.335068 0.824689 0.159894

 33 1 0 2.799358 1.000571 1.093530

 34 1 0 4.247953 0.293366 0.430989

 35 6 0 3.273993 -0.912440 -1.625646

 36 1 0 4.087908 -0.324547 -2.052337

 37 1 0 2.617092 -1.179318 -2.452377

 38 6 0 3.862865 -2.174272 -1.005143

 39 1 0 4.032879 -2.933250 -1.780820

 40 1 0 3.169388 -2.589218 -0.264567

 41 6 0 5.609808 -2.799889 0.518173

 42 1 0 5.222865 -3.798008 0.281000

 43 1 0 6.693366 -2.830840 0.381214

 44 6 0 5.260105 -2.450928 1.959254

 45 1 0 4.180094 -2.320861 2.057193

 46 1 0 5.564437 -3.273822 2.620168

 47 7 0 2.544214 -0.060686 -0.691740

 48 8 0 4.643620 2.055227 -1.529427

 49 8 0 8.169879 1.110604 -1.745822

 50 8 0 7.828351 0.449989 1.093594

 51 8 0 5.841749 -1.221082 2.384315

 52 8 0 5.107398 -1.829591 -0.396154

 53 6 0 -5.108171 -1.271110 -0.254755

 54 6 0 -4.034806 0.691823 0.090325

 55 7 0 -5.236493 0.053212 0.069342

 56 6 0 -6.351043 0.811353 0.295644

 57 6 0 -7.544926 0.120539 0.233453

 58 6 0 -7.506431 -1.268067 -0.066857

 59 6 0 -6.314110 -1.969810 -0.316753

 60 1 0 -8.489879 0.614340 0.398206

 61 1 0 -6.345826 -3.022214 -0.558109

 62 6 0 -4.374543 2.074665 0.361797

 63 6 0 -5.812009 2.144721 0.500818

 64 6 0 -3.620418 3.248193 0.480657

 65 6 0 -6.444918 3.359937 0.768407

 66 6 0 -5.669674 4.505480 0.890868

 67 6 0 -4.273375 4.446103 0.742678

 68 1 0 -3.692174 5.356189 0.833131

 69 1 0 -7.522289 3.406775 0.873736

 70 1 0 -2.545652 3.234851 0.360395

 71 7 0 -3.792865 -1.531069 -0.436535

 72 6 0 -3.117366 -0.355285 -0.229171

 73 1 0 -6.144572 5.456839 1.097333

 74 6 0 -8.768937 -2.052732 -0.143995

 75 8 0 -8.823649 -3.240447 -0.397520

 76 8 0 -9.856863 -1.304414 0.098234

 77 6 0 -11.129420 -1.982109 0.043131

 78 1 0 -11.871388 -1.218329 0.259622

 79 1 0 -11.289624 -2.402410 -0.949619

 80 1 0 -11.166356 -2.775405 0.789620

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**19·Ba(ClO4)2** (S0) M06

---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -0.335517 2.279349 -1.393611

 2 6 0 0.034963 3.120145 -0.341491

 3 6 0 0.624813 1.979976 -2.356679

 4 6 0 1.354337 3.484329 -0.160358

 5 1 0 -0.701310 3.387735 0.411604

 6 6 0 1.937086 2.386106 -2.207997

 7 1 0 0.357208 1.350514 -3.200798

 8 6 0 2.361344 3.030498 -1.034648

 9 1 0 1.605722 4.059394 0.722689

 10 1 0 2.642484 2.107244 -2.977092

 11 6 0 3.524380 -3.220287 1.156532

 12 1 0 3.847601 -3.010687 2.190926

 13 1 0 4.176595 -4.015400 0.760033

 14 6 0 2.103275 -3.708100 1.095314

 15 1 0 2.001898 -4.631855 1.682672

 16 1 0 1.846554 -3.924629 0.054016

 17 6 0 0.873056 -2.702641 2.919999

 18 1 0 1.005408 -3.698013 3.367031

 19 1 0 -0.180600 -2.424788 2.989779

 20 6 0 1.707977 -1.693313 3.674669

 21 1 0 2.752509 -2.024233 3.806622

 22 1 0 1.268450 -1.558257 4.676119

 23 6 0 2.239544 0.600706 3.692468

 24 1 0 3.269776 0.351801 4.005093

 25 1 0 1.636091 0.795533 4.593624

 26 6 0 2.236938 1.813006 2.800048

 27 1 0 2.652416 2.676257 3.337441

 28 1 0 1.205260 2.050215 2.516419

 29 6 0 4.230498 2.198676 1.499090

 30 1 0 4.927016 1.483057 1.056635

 31 1 0 4.607251 2.481220 2.494522

 32 6 0 4.143555 3.435487 0.616583

 33 1 0 5.139744 3.894285 0.575749

 34 1 0 3.493945 4.186808 1.076398

 35 6 0 4.722526 2.713379 -1.679678

 36 1 0 5.683450 3.041498 -1.269220

 37 1 0 4.603979 3.242425 -2.637281

 38 6 0 4.829151 1.224462 -2.005013

 39 1 0 5.812729 1.080158 -2.486547

 40 1 0 4.073193 0.878543 -2.721811

 41 6 0 5.162587 -0.886795 -1.092239

 42 1 0 4.583242 -1.329485 -1.914847

 43 1 0 6.228529 -0.886397 -1.378483

 44 6 0 5.003323 -1.719783 0.141961

 45 1 0 5.588364 -2.641256 0.000399

 46 1 0 5.410730 -1.193278 1.022378

 47 7 0 3.708329 3.165457 -0.742327

 48 8 0 2.980867 1.539108 1.621443

 49 8 0 1.690672 -0.474652 2.966698

 50 8 0 1.174303 -2.738702 1.536321

 51 8 0 3.649266 -2.059810 0.362330

 52 8 0 4.744847 0.437749 -0.842431

 53 56 0 1.142369 -0.323512 0.121783

 54 6 0 -2.882734 1.856113 -1.035527

 55 6 0 -2.655190 -0.377158 -1.186994

 56 6 0 -4.820084 0.671089 -0.603453

 57 6 0 -3.227206 -1.639303 -1.047031

 58 1 0 -2.647481 -2.545266 -1.179532

 59 6 0 -5.388065 -0.570858 -0.467092

 60 1 0 -6.421215 -0.695136 -0.170054

 61 6 0 -4.575444 -1.710378 -0.697620

 62 6 0 -5.104503 2.083870 -0.437278

 63 6 0 -3.904296 2.816244 -0.703395

 64 6 0 -6.270317 2.750392 -0.078579

 65 1 0 -7.180668 2.194444 0.127038

 66 6 0 -3.903095 4.204885 -0.606302

 67 6 0 -5.075246 4.847375 -0.249691

 68 1 0 -5.087735 5.930310 -0.171559

 69 6 0 -6.247701 4.130476 0.013090

 70 1 0 -2.999045 4.770640 -0.811217

 71 7 0 -3.511800 0.655734 -0.973552

 72 1 0 -7.149119 4.666390 0.292669

 73 7 0 -1.431285 0.137544 -1.420329

 74 6 0 -1.562955 1.494681 -1.329902

 75 6 0 -5.140789 -3.076428 -0.548840

 76 8 0 -4.522746 -4.095734 -0.706192

 77 8 0 -6.442444 -3.053384 -0.215508

 78 6 0 -7.051579 -4.328087 -0.051504

 79 1 0 -8.089804 -4.134101 0.214905

 80 1 0 -6.998182 -4.904207 -0.978776

 81 1 0 -6.555334 -4.894129 0.740826

 82 17 0 1.769836 -2.178021 -2.706991

 83 17 0 -1.620877 0.178206 2.265554

 84 8 0 2.909354 -3.093968 -2.733847

 85 8 0 2.261634 -0.785368 -2.412824

 86 8 0 0.872304 -2.523691 -1.561382

 87 8 0 1.035481 -2.190065 -3.956277

 88 8 0 -1.255522 -1.055270 1.508590

 89 8 0 -0.684404 1.240282 1.769832

 90 8 0 -1.410701 -0.034282 3.697076

 91 8 0 -2.995306 0.557327 1.972504

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**19·Ba(ClO4)2 (S1)** M06

 ---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -0.368426 2.475186 -1.322086

 2 6 0 0.007083 3.208431 -0.187168

 3 6 0 0.587005 2.292291 -2.327565

 4 6 0 1.332887 3.551111 0.025808

 5 1 0 -0.718324 3.387760 0.595399

 6 6 0 1.905101 2.683499 -2.143247

 7 1 0 0.317807 1.756979 -3.229236

 8 6 0 2.338264 3.185391 -0.898411

 9 1 0 1.589477 4.017927 0.964546

 10 1 0 2.606258 2.494443 -2.939017

 11 6 0 3.516740 -3.323247 0.977044

 12 1 0 3.855573 -3.195775 2.013850

 13 1 0 4.148334 -4.087376 0.504955

 14 6 0 2.079447 -3.795503 0.902631

 15 1 0 1.977693 -4.748327 1.434557

 16 1 0 1.800208 -3.935651 -0.141146

 17 6 0 0.866924 -2.880523 2.819296

 18 1 0 0.993658 -3.898410 3.204028

 19 1 0 -0.176652 -2.588473 2.909043

 20 6 0 1.729843 -1.918875 3.620258

 21 1 0 2.771885 -2.257306 3.697130

 22 1 0 1.315194 -1.845492 4.633826

 23 6 0 2.262081 0.397521 3.764418

 24 1 0 3.304264 0.149590 4.012255

 25 1 0 1.694057 0.518451 4.695660

 26 6 0 2.187237 1.676462 2.955573

 27 1 0 2.611583 2.505268 3.530733

 28 1 0 1.145020 1.900331 2.729439

 29 6 0 4.163797 2.134724 1.610213

 30 1 0 4.819690 1.419633 1.119946

 31 1 0 4.553646 2.350954 2.612403

 32 6 0 4.122286 3.430723 0.793512

 33 1 0 5.134644 3.846883 0.784747

 34 1 0 3.496713 4.173981 1.288576

 35 6 0 4.699953 2.821544 -1.545685

 36 1 0 5.667803 3.084888 -1.115774

 37 1 0 4.604288 3.401388 -2.471972

 38 6 0 4.742387 1.342782 -1.956631

 39 1 0 5.674091 1.208594 -2.526214

 40 1 0 3.914408 1.054433 -2.605036

 41 6 0 5.136778 -0.838204 -1.172796

 42 1 0 4.525351 -1.217013 -1.994984

 43 1 0 6.190471 -0.831098 -1.489065

 44 6 0 5.008316 -1.756066 0.016156

 45 1 0 5.563035 -2.672984 -0.215357

 46 1 0 5.453091 -1.301133 0.911453

 47 7 0 3.690326 3.266287 -0.589369

 48 8 0 2.877575 1.512828 1.711205

 49 8 0 1.694542 -0.647551 2.984131

 50 8 0 1.153735 -2.842178 1.419565

 51 8 0 3.643379 -2.092889 0.268697

 52 8 0 4.745021 0.485576 -0.821853

 53 56 0 1.157387 -0.358529 0.155087

 54 6 0 -2.919030 1.922261 -1.028762

 55 6 0 -2.579515 -0.308866 -1.209843

 56 6 0 -4.803868 0.622642 -0.627794

 57 6 0 -3.082611 -1.603549 -1.089246

 58 1 0 -2.453006 -2.471005 -1.223522

 59 6 0 -5.306034 -0.654156 -0.506281

 60 1 0 -6.326929 -0.836403 -0.208671

 61 6 0 -4.433012 -1.752252 -0.747529

 62 6 0 -5.162811 2.020662 -0.426225

 63 6 0 -3.991216 2.823834 -0.671977

 64 6 0 -6.360100 2.623408 -0.044090

 65 1 0 -7.242428 2.023611 0.146205

 66 6 0 -4.054873 4.210533 -0.526707

 67 6 0 -5.260045 4.787955 -0.145947

 68 1 0 -5.321801 5.863753 -0.029545

 69 6 0 -6.400991 4.005629 0.093637

 70 1 0 -3.179479 4.822333 -0.708262

 71 7 0 -3.491748 0.684811 -1.000587

 72 1 0 -7.324281 4.487617 0.391897

 73 7 0 -1.372540 0.278298 -1.402050

 74 6 0 -1.569903 1.637069 -1.302241

 75 6 0 -4.926981 -3.149285 -0.601598

 76 8 0 -4.250614 -4.139999 -0.753656

 77 8 0 -6.238199 -3.199459 -0.272753

 78 6 0 -6.784196 -4.517769 -0.104180

 79 1 0 -7.829933 -4.367763 0.154709

 80 1 0 -6.693616 -5.088302 -1.029387

 81 1 0 -6.261397 -5.046311 0.693955

 82 17 0 1.732565 -1.977750 -2.852297

 83 17 0 -1.632866 0.117351 2.289092

 84 8 0 2.929309 -2.842321 -2.991287

 85 8 0 2.176615 -0.574609 -2.444474

 86 8 0 0.878311 -2.465667 -1.697289

 87 8 0 0.952136 -1.922026 -4.094278

 88 8 0 -1.240104 -1.134499 1.534580

 89 8 0 -0.686211 1.197084 1.787130

 90 8 0 -1.434920 -0.086913 3.743253

 91 8 0 -3.023865 0.488427 1.974072

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**19** (S0) M06-L

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -1.689697 -0.175691 -0.401018

 2 6 0 -0.978576 0.902888 0.145232

 3 6 0 -0.939161 -1.170575 -1.047673

 4 6 0 0.395644 0.998360 0.047202

 5 1 0 -1.512790 1.678856 0.683215

 6 6 0 0.434502 -1.090136 -1.157298

 7 1 0 -1.458323 -2.027339 -1.463949

 8 6 0 1.152513 0.003321 -0.615143

 9 1 0 0.885477 1.864621 0.474157

 10 1 0 0.960158 -1.899528 -1.648669

 11 6 0 7.272874 -1.392469 2.732408

 12 1 0 7.724522 -2.195531 2.135276

 13 1 0 7.439741 -1.651675 3.788546

 14 6 0 7.938213 -0.072576 2.418502

 15 1 0 8.991838 -0.105177 2.732252

 16 1 0 7.449168 0.728088 2.981212

 17 6 0 8.746885 -0.362999 0.197475

 18 1 0 8.861346 -1.426588 0.457342

 19 1 0 9.740028 0.103148 0.294311

 20 6 0 8.248673 -0.278291 -1.222688

 21 1 0 7.252561 -0.733761 -1.285326

 22 1 0 8.924586 -0.852231 -1.870328

 23 6 0 6.939421 1.492501 -2.150164

 24 1 0 6.508167 0.752476 -2.841982

 25 1 0 7.107039 2.412794 -2.716505

 26 6 0 5.986574 1.730998 -0.997638

 27 1 0 6.364504 2.533657 -0.345220

 28 1 0 5.928139 0.819786 -0.389457

 29 6 0 3.746246 2.269432 -0.502157

 30 1 0 2.898453 2.770399 -0.978283

 31 1 0 4.145474 2.940813 0.274271

 32 6 0 3.294651 0.969352 0.147972

 33 1 0 2.709539 1.200526 1.040479

 34 1 0 4.162564 0.401715 0.499480

 35 6 0 3.270231 -0.809778 -1.580221

 36 1 0 4.110622 -0.253250 -2.006006

 37 1 0 2.641183 -1.103756 -2.421072

 38 6 0 3.822767 -2.039750 -0.879910

 39 1 0 3.924880 -2.876365 -1.588511

 40 1 0 3.139622 -2.366389 -0.081002

 41 6 0 5.641023 -2.707154 0.495285

 42 1 0 5.297983 -3.704236 0.185808

 43 1 0 6.726931 -2.683649 0.349785

 44 6 0 5.298114 -2.472521 1.953040

 45 1 0 4.216339 -2.349505 2.068938

 46 1 0 5.595831 -3.347736 2.549555

 47 7 0 2.519334 0.098743 -0.726968

 48 8 0 4.716113 2.084458 -1.524271

 49 8 0 8.209775 1.071343 -1.683803

 50 8 0 7.820529 0.281831 1.051745

 51 8 0 5.881873 -1.285529 2.466542

 52 8 0 5.099801 -1.705405 -0.352962

 53 6 0 -5.080745 -1.246925 -0.318906

 54 6 0 -4.067688 0.732636 0.066723

 55 7 0 -5.246855 0.062001 0.038249

 56 6 0 -6.377066 0.777188 0.306686

 57 6 0 -7.550090 0.049974 0.244955

 58 6 0 -7.474256 -1.323739 -0.094649

 59 6 0 -6.264430 -1.978794 -0.381931

 60 1 0 -8.508451 0.509686 0.442117

 61 1 0 -6.272132 -3.027202 -0.649838

 62 6 0 -4.444194 2.089473 0.386713

 63 6 0 -5.877030 2.110349 0.546429

 64 6 0 -3.729932 3.283891 0.533343

 65 6 0 -6.544354 3.293948 0.862571

 66 6 0 -5.807872 4.458031 1.012997

 67 6 0 -4.415518 4.448625 0.843476

 68 1 0 -3.861288 5.374684 0.955094

 69 1 0 -7.622938 3.299216 0.983033

 70 1 0 -2.655425 3.313761 0.395710

 71 7 0 -3.766689 -1.470088 -0.521090

 72 6 0 -3.128385 -0.282670 -0.287075

 73 1 0 -6.310967 5.387061 1.257693

 74 6 0 -8.702988 -2.147535 -0.173768

 75 8 0 -8.726365 -3.326048 -0.467987

 76 8 0 -9.809696 -1.442465 0.120214

 77 6 0 -11.038845 -2.176971 0.064130

 78 1 0 -11.818924 -1.469154 0.332061

 79 1 0 -11.206998 -2.564831 -0.941506

 80 1 0 -11.020263 -3.007818 0.770749

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**19** (S1)M06-L

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -1.670601 -0.277856 -0.340993

 2 6 0 -0.937972 0.762678 0.250155

 3 6 0 -0.943248 -1.257489 -1.037027

 4 6 0 0.439523 0.840017 0.143243

 5 1 0 -1.451792 1.520082 0.827902

 6 6 0 0.433292 -1.194834 -1.154329

 7 1 0 -1.477029 -2.083558 -1.489820

 8 6 0 1.176377 -0.135975 -0.572649

 9 1 0 0.942780 1.675535 0.607648

 10 1 0 0.937314 -1.988619 -1.686491

 11 6 0 7.227887 -1.300849 2.702754

 12 1 0 7.721928 -2.069992 2.100645

 13 1 0 7.357031 -1.578490 3.757965

 14 6 0 7.875639 0.051127 2.458460

 15 1 0 8.909963 0.028975 2.826035

 16 1 0 7.334059 0.819826 3.014030

 17 6 0 8.793775 -0.162827 0.246055

 18 1 0 8.993936 -1.195776 0.555515

 19 1 0 9.739987 0.392025 0.297126

 20 6 0 8.275218 -0.200494 -1.177424

 21 1 0 7.304038 -0.703828 -1.195298

 22 1 0 8.977780 -0.779998 -1.787260

 23 6 0 6.866120 1.466022 -2.197967

 24 1 0 6.410589 0.637572 -2.754252

 25 1 0 6.995396 2.304474 -2.885121

 26 6 0 5.965776 1.854537 -1.033628

 27 1 0 6.331217 2.774382 -0.557922

 28 1 0 5.992188 1.061285 -0.285050

 29 6 0 3.678069 2.170219 -0.482793

 30 1 0 2.788846 2.609185 -0.938583

 31 1 0 4.047032 2.858890 0.289570

 32 6 0 3.335068 0.824689 0.159894

 33 1 0 2.799358 1.000571 1.093530

 34 1 0 4.247953 0.293366 0.430989

 35 6 0 3.273993 -0.912440 -1.625646

 36 1 0 4.087908 -0.324547 -2.052337

 37 1 0 2.617092 -1.179318 -2.452377

 38 6 0 3.862865 -2.174272 -1.005143

 39 1 0 4.032879 -2.933250 -1.780820

 40 1 0 3.169388 -2.589218 -0.264567

 41 6 0 5.609808 -2.799889 0.518173

 42 1 0 5.222865 -3.798008 0.281000

 43 1 0 6.693366 -2.830840 0.381214

 44 6 0 5.260105 -2.450928 1.959254

 45 1 0 4.180094 -2.320861 2.057193

 46 1 0 5.564437 -3.273822 2.620168

 47 7 0 2.544214 -0.060686 -0.691740

 48 8 0 4.643620 2.055227 -1.529427

 49 8 0 8.169879 1.110604 -1.745822

 50 8 0 7.828351 0.449989 1.093594

 51 8 0 5.841749 -1.221082 2.384315

 52 8 0 5.107398 -1.829591 -0.396154

 53 6 0 -5.108171 -1.271110 -0.254755

 54 6 0 -4.034806 0.691823 0.090325

 55 7 0 -5.236493 0.053212 0.069342

 56 6 0 -6.351043 0.811353 0.295644

 57 6 0 -7.544926 0.120539 0.233453

 58 6 0 -7.506431 -1.268067 -0.066857

 59 6 0 -6.314110 -1.969810 -0.316753

 60 1 0 -8.489879 0.614340 0.398206

 61 1 0 -6.345826 -3.022214 -0.558109

 62 6 0 -4.374543 2.074665 0.361797

 63 6 0 -5.812009 2.144721 0.500818

 64 6 0 -3.620418 3.248193 0.480657

 65 6 0 -6.444918 3.359937 0.768407

 66 6 0 -5.669674 4.505480 0.890868

 67 6 0 -4.273375 4.446103 0.742678

 68 1 0 -3.692174 5.356189 0.833131

 69 1 0 -7.522289 3.406775 0.873736

 70 1 0 -2.545652 3.234851 0.360395

 71 7 0 -3.792865 -1.531069 -0.436535

 72 6 0 -3.117366 -0.355285 -0.229171

 73 1 0 -6.144572 5.456839 1.097333

 74 6 0 -8.768937 -2.052732 -0.143995

 75 8 0 -8.823649 -3.240447 -0.397520

 76 8 0 -9.856863 -1.304414 0.098234

 77 6 0 -11.129420 -1.982109 0.043131

 78 1 0 -11.871388 -1.218329 0.259622

 79 1 0 -11.289624 -2.402410 -0.949619

 80 1 0 -11.166356 -2.775405 0.789620

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**19·Ba(ClO4)2** (S0) M06-L

---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -0.322763 2.219036 -1.449290

 2 6 0 0.072646 3.088244 -0.423256

 3 6 0 0.641452 1.845954 -2.391434

 4 6 0 1.404087 3.416090 -0.246613

 5 1 0 -0.653967 3.408510 0.315969

 6 6 0 1.967958 2.217916 -2.253312

 7 1 0 0.361918 1.184340 -3.205231

 8 6 0 2.404717 2.916004 -1.110693

 9 1 0 1.669647 4.018278 0.612536

 10 1 0 2.671018 1.879804 -2.999621

 11 6 0 3.391046 -3.225384 1.260765

 12 1 0 3.721795 -3.028586 2.293592

 13 1 0 4.032093 -4.023567 0.856293

 14 6 0 1.958753 -3.684322 1.201977

 15 1 0 1.834983 -4.586535 1.815552

 16 1 0 1.693825 -3.921277 0.169969

 17 6 0 0.771989 -2.592412 3.006679

 18 1 0 0.906199 -3.573059 3.481343

 19 1 0 -0.275759 -2.303111 3.086673

 20 6 0 1.629646 -1.563570 3.710458

 21 1 0 2.668061 -1.900728 3.860328

 22 1 0 1.195808 -1.364399 4.701464

 23 6 0 2.161217 0.732870 3.644048

 24 1 0 3.152247 0.474954 4.052762

 25 1 0 1.494915 0.991286 4.480460

 26 6 0 2.264724 1.891670 2.686723

 27 1 0 2.669609 2.769616 3.203838

 28 1 0 1.267993 2.146881 2.311197

 29 6 0 4.311110 2.242868 1.446269

 30 1 0 5.044934 1.534297 1.061460

 31 1 0 4.649700 2.593241 2.431954

 32 6 0 4.200062 3.428879 0.492630

 33 1 0 5.189586 3.892838 0.412480

 34 1 0 3.547878 4.199505 0.910636

 35 6 0 4.760174 2.603619 -1.780574

 36 1 0 5.715322 2.981963 -1.406944

 37 1 0 4.603796 3.078362 -2.758743

 38 6 0 4.889007 1.096470 -2.020720

 39 1 0 5.898525 0.916589 -2.426379

 40 1 0 4.180058 0.713639 -2.764023

 41 6 0 5.151710 -0.962306 -0.963983

 42 1 0 4.628610 -1.448288 -1.796123

 43 1 0 6.232560 -0.972774 -1.181441

 44 6 0 4.915055 -1.727780 0.303179

 45 1 0 5.495561 -2.658444 0.241636

 46 1 0 5.277769 -1.166169 1.179197

 47 7 0 3.752260 3.080275 -0.845224

 48 8 0 3.089598 1.522560 1.578222

 49 8 0 1.636175 -0.375715 2.934794

 50 8 0 1.042331 -2.678900 1.611211

 51 8 0 3.539843 -2.052692 0.471413

 52 8 0 4.718551 0.380772 -0.815039

 53 56 0 1.151157 -0.269497 0.108547

 54 6 0 -2.886832 1.841881 -1.067778

 55 6 0 -2.682078 -0.401246 -1.211066

 56 6 0 -4.839424 0.675540 -0.631271

 57 6 0 -3.263203 -1.657011 -1.061374

 58 1 0 -2.692136 -2.568447 -1.184935

 59 6 0 -5.418854 -0.567056 -0.487429

 60 1 0 -6.451582 -0.680469 -0.188142

 61 6 0 -4.618436 -1.717689 -0.709374

 62 6 0 -5.110144 2.089033 -0.469192

 63 6 0 -3.897245 2.812077 -0.739267

 64 6 0 -6.269770 2.771493 -0.108317

 65 1 0 -7.185532 2.227239 0.100340

 66 6 0 -3.883843 4.203852 -0.642571

 67 6 0 -5.051380 4.860560 -0.283537

 68 1 0 -5.051888 5.942987 -0.206007

 69 6 0 -6.232604 4.154708 -0.017445

 70 1 0 -2.976160 4.761822 -0.848569

 71 7 0 -3.528785 0.646861 -1.004398

 72 1 0 -7.127623 4.699173 0.263682

 73 7 0 -1.448031 0.099567 -1.449080

 74 6 0 -1.565372 1.462378 -1.364620

 75 6 0 -5.191527 -3.075491 -0.547050

 76 8 0 -4.582020 -4.108549 -0.696845

 77 8 0 -6.501109 -3.036577 -0.205656

 78 6 0 -7.106077 -4.317955 -0.028867

 79 1 0 -8.142493 -4.123783 0.238927

 80 1 0 -7.051885 -4.900697 -0.950386

 81 1 0 -6.604467 -4.874787 0.764837

 82 17 0 1.864214 -2.279457 -2.600631

 83 17 0 -1.606570 0.264658 2.239570

 84 8 0 3.008534 -3.195352 -2.504701

 85 8 0 2.340712 -0.860006 -2.374497

 86 8 0 0.900220 -2.552723 -1.480754

 87 8 0 1.196683 -2.378619 -3.889311

 88 8 0 -1.236571 -0.990210 1.508206

 89 8 0 -0.698825 1.334622 1.683196

 90 8 0 -1.354409 0.098349 3.676924

 91 8 0 -2.999531 0.613386 1.972534

 ---------------------------------------------------------------------

**19·Ba(ClO4)2** (S1) M06-L

 ---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -0.368426 2.475186 -1.322086

 2 6 0 0.007083 3.208431 -0.187168

 3 6 0 0.587005 2.292291 -2.327565

 4 6 0 1.332887 3.551111 0.025808

 5 1 0 -0.718324 3.387760 0.595399

 6 6 0 1.905101 2.683499 -2.143247

 7 1 0 0.317807 1.756979 -3.229236

 8 6 0 2.338264 3.185391 -0.898411

 9 1 0 1.589477 4.017927 0.964546

 10 1 0 2.606258 2.494443 -2.939017

 11 6 0 3.516740 -3.323247 0.977044

 12 1 0 3.855573 -3.195775 2.013850

 13 1 0 4.148334 -4.087376 0.504955

 14 6 0 2.079447 -3.795503 0.902631

 15 1 0 1.977693 -4.748327 1.434557

 16 1 0 1.800208 -3.935651 -0.141146

 17 6 0 0.866924 -2.880523 2.819296

 18 1 0 0.993658 -3.898410 3.204028

 19 1 0 -0.176652 -2.588473 2.909043

 20 6 0 1.729843 -1.918875 3.620258

 21 1 0 2.771885 -2.257306 3.697130

 22 1 0 1.315194 -1.845492 4.633826

 23 6 0 2.262081 0.397521 3.764418

 24 1 0 3.304264 0.149590 4.012255

 25 1 0 1.694057 0.518451 4.695660

 26 6 0 2.187237 1.676462 2.955573

 27 1 0 2.611583 2.505268 3.530733

 28 1 0 1.145020 1.900331 2.729439

 29 6 0 4.163797 2.134724 1.610213

 30 1 0 4.819690 1.419633 1.119946

 31 1 0 4.553646 2.350954 2.612403

 32 6 0 4.122286 3.430723 0.793512

 33 1 0 5.134644 3.846883 0.784747

 34 1 0 3.496713 4.173981 1.288576

 35 6 0 4.699953 2.821544 -1.545685

 36 1 0 5.667803 3.084888 -1.115774

 37 1 0 4.604288 3.401388 -2.471972

 38 6 0 4.742387 1.342782 -1.956631

 39 1 0 5.674091 1.208594 -2.526214

 40 1 0 3.914408 1.054433 -2.605036

 41 6 0 5.136778 -0.838204 -1.172796

 42 1 0 4.525351 -1.217013 -1.994984

 43 1 0 6.190471 -0.831098 -1.489065

 44 6 0 5.008316 -1.756066 0.016156

 45 1 0 5.563035 -2.672984 -0.215357

 46 1 0 5.453091 -1.301133 0.911453

 47 7 0 3.690326 3.266287 -0.589369

 48 8 0 2.877575 1.512828 1.711205

 49 8 0 1.694542 -0.647551 2.984131

 50 8 0 1.153735 -2.842178 1.419565

 51 8 0 3.643379 -2.092889 0.268697

 52 8 0 4.745021 0.485576 -0.821853

 53 56 0 1.157387 -0.358529 0.155087

 54 6 0 -2.919030 1.922261 -1.028762

 55 6 0 -2.579515 -0.308866 -1.209843

 56 6 0 -4.803868 0.622642 -0.627794

 57 6 0 -3.082611 -1.603549 -1.089246

 58 1 0 -2.453006 -2.471005 -1.223522

 59 6 0 -5.306034 -0.654156 -0.506281

 60 1 0 -6.326929 -0.836403 -0.208671

 61 6 0 -4.433012 -1.752252 -0.747529

 62 6 0 -5.162811 2.020662 -0.426225

 63 6 0 -3.991216 2.823834 -0.671977

 64 6 0 -6.360100 2.623408 -0.044090

 65 1 0 -7.242428 2.023611 0.146205

 66 6 0 -4.054873 4.210533 -0.526707

 67 6 0 -5.260045 4.787955 -0.145947

 68 1 0 -5.321801 5.863753 -0.029545

 69 6 0 -6.400991 4.005629 0.093637

 70 1 0 -3.179479 4.822333 -0.708262

 71 7 0 -3.491748 0.684811 -1.000587

 72 1 0 -7.324281 4.487617 0.391897

 73 7 0 -1.372540 0.278298 -1.402050

 74 6 0 -1.569903 1.637069 -1.302241

 75 6 0 -4.926981 -3.149285 -0.601598

 76 8 0 -4.250614 -4.139999 -0.753656

 77 8 0 -6.238199 -3.199459 -0.272753

 78 6 0 -6.784196 -4.517769 -0.104180

 79 1 0 -7.829933 -4.367763 0.154709

 80 1 0 -6.693616 -5.088302 -1.029387

 81 1 0 -6.261397 -5.046311 0.693955

 82 17 0 1.732565 -1.977750 -2.852297

 83 17 0 -1.632866 0.117351 2.289092

 84 8 0 2.929309 -2.842321 -2.991287

 85 8 0 2.176615 -0.574609 -2.444474

 86 8 0 0.878311 -2.465667 -1.697289

 87 8 0 0.952136 -1.922026 -4.094278

 88 8 0 -1.240104 -1.134499 1.534580

 89 8 0 -0.686211 1.197084 1.787130

 90 8 0 -1.434920 -0.086913 3.743253

 91 8 0 -3.023865 0.488427 1.974072

 ---------------------------------------------------------------------

**19** (S0) M06-2X

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -1.695557 -0.185657 -0.298252

 2 6 0 -1.018040 0.825519 0.390458

 3 6 0 -0.932704 -1.074418 -1.062254

 4 6 0 0.356052 0.963864 0.308923

 5 1 0 -1.574311 1.507586 1.024226

 6 6 0 0.442686 -0.951691 -1.153028

 7 1 0 -1.432242 -1.878538 -1.589833

 8 6 0 1.132009 0.079977 -0.474822

 9 1 0 0.826545 1.778945 0.842289

 10 1 0 0.985682 -1.680718 -1.739124

 11 6 0 7.470722 -1.861114 2.434299

 12 1 0 7.928644 -2.546467 1.713561

 13 1 0 7.708303 -2.232906 3.437976

 14 6 0 8.037679 -0.463646 2.266604

 15 1 0 9.110123 -0.466785 2.499091

 16 1 0 7.536943 0.211169 2.964180

 17 6 0 8.750014 -0.337775 -0.001223

 18 1 0 8.941320 -1.418540 0.035744

 19 1 0 9.702477 0.180439 0.171752

 20 6 0 8.203489 0.006865 -1.369497

 21 1 0 7.221244 -0.463517 -1.489021

 22 1 0 8.879439 -0.390009 -2.133718

 23 6 0 6.811868 1.895297 -1.848970

 24 1 0 6.363557 1.304865 -2.658628

 25 1 0 6.933923 2.920430 -2.202734

 26 6 0 5.906935 1.861005 -0.629190

 27 1 0 6.323567 2.493654 0.165303

 28 1 0 5.849485 0.835685 -0.253608

 29 6 0 3.692918 2.334751 0.044702

 30 1 0 2.830093 2.903963 -0.307228

 31 1 0 4.119104 2.847177 0.918080

 32 6 0 3.257557 0.929640 0.453233

 33 1 0 2.663115 0.995762 1.365315

 34 1 0 4.130676 0.321477 0.702658

 35 6 0 3.258655 -0.499437 -1.578458

 36 1 0 4.080243 0.141040 -1.908187

 37 1 0 2.623653 -0.665385 -2.447912

 38 6 0 3.862324 -1.818316 -1.106027

 39 1 0 3.993695 -2.499447 -1.956751

 40 1 0 3.202353 -2.302356 -0.374362

 41 6 0 5.797405 -2.664046 -0.010607

 42 1 0 5.506597 -3.568930 -0.558327

 43 1 0 6.865549 -2.503026 -0.179369

 44 6 0 5.526054 -2.858698 1.472726

 45 1 0 4.449175 -2.858080 1.656581

 46 1 0 5.924901 -3.829811 1.792660

 47 7 0 2.497496 0.226376 -0.573283

 48 8 0 4.630888 2.341818 -1.019099

 49 8 0 8.106951 1.415863 -1.536980

 50 8 0 7.802471 0.051016 0.971159

 51 8 0 6.063504 -1.814403 2.263738

 52 8 0 5.130461 -1.531595 -0.535871

 53 6 0 -5.090185 -1.288017 -0.261925

 54 6 0 -4.090538 0.694803 0.098080

 55 7 0 -5.266788 0.024174 0.062214

 56 6 0 -6.402702 0.744718 0.279576

 57 6 0 -7.572005 0.022300 0.205285

 58 6 0 -7.480269 -1.362005 -0.098341

 59 6 0 -6.275712 -2.026112 -0.337515

 60 1 0 -8.535503 0.484483 0.362131

 61 1 0 -6.273134 -3.079602 -0.580904

 62 6 0 -4.474452 2.069624 0.368731

 63 6 0 -5.902632 2.095932 0.493775

 64 6 0 -3.753444 3.261974 0.491279

 65 6 0 -6.578182 3.287619 0.756793

 66 6 0 -5.840635 4.453105 0.886014

 67 6 0 -4.443730 4.436326 0.747769

 68 1 0 -3.891971 5.364051 0.841650

 69 1 0 -7.657553 3.298754 0.852335

 70 1 0 -2.677531 3.278830 0.375498

 71 7 0 -3.771456 -1.508643 -0.429317

 72 6 0 -3.146833 -0.319424 -0.210959

 73 1 0 -6.345306 5.389478 1.089182

 74 6 0 -8.721357 -2.188300 -0.189671

 75 8 0 -8.731494 -3.366925 -0.452952

 76 8 0 -9.825795 -1.483103 0.052373

 77 6 0 -11.061361 -2.207056 -0.016700

 78 1 0 -11.837983 -1.482366 0.208044

 79 1 0 -11.197822 -2.618789 -1.015997

 80 1 0 -11.063893 -3.012870 0.716357

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**19** (S1) M06-2X

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -1.670601 -0.277856 -0.340993

 2 6 0 -0.937972 0.762678 0.250155

 3 6 0 -0.943248 -1.257489 -1.037027

 4 6 0 0.439523 0.840017 0.143243

 5 1 0 -1.451792 1.520082 0.827902

 6 6 0 0.433292 -1.194834 -1.154329

 7 1 0 -1.477029 -2.083558 -1.489820

 8 6 0 1.176377 -0.135975 -0.572649

 9 1 0 0.942780 1.675535 0.607648

 10 1 0 0.937314 -1.988619 -1.686491

 11 6 0 7.227887 -1.300849 2.702754

 12 1 0 7.721928 -2.069992 2.100645

 13 1 0 7.357031 -1.578490 3.757965

 14 6 0 7.875639 0.051127 2.458460

 15 1 0 8.909963 0.028975 2.826035

 16 1 0 7.334059 0.819826 3.014030

 17 6 0 8.793775 -0.162827 0.246055

 18 1 0 8.993936 -1.195776 0.555515

 19 1 0 9.739987 0.392025 0.297126

 20 6 0 8.275218 -0.200494 -1.177424

 21 1 0 7.304038 -0.703828 -1.195298

 22 1 0 8.977780 -0.779998 -1.787260

 23 6 0 6.866120 1.466022 -2.197967

 24 1 0 6.410589 0.637572 -2.754252

 25 1 0 6.995396 2.304474 -2.885121

 26 6 0 5.965776 1.854537 -1.033628

 27 1 0 6.331217 2.774382 -0.557922

 28 1 0 5.992188 1.061285 -0.285050

 29 6 0 3.678069 2.170219 -0.482793

 30 1 0 2.788846 2.609185 -0.938583

 31 1 0 4.047032 2.858890 0.289570

 32 6 0 3.335068 0.824689 0.159894

 33 1 0 2.799358 1.000571 1.093530

 34 1 0 4.247953 0.293366 0.430989

 35 6 0 3.273993 -0.912440 -1.625646

 36 1 0 4.087908 -0.324547 -2.052337

 37 1 0 2.617092 -1.179318 -2.452377

 38 6 0 3.862865 -2.174272 -1.005143

 39 1 0 4.032879 -2.933250 -1.780820

 40 1 0 3.169388 -2.589218 -0.264567

 41 6 0 5.609808 -2.799889 0.518173

 42 1 0 5.222865 -3.798008 0.281000

 43 1 0 6.693366 -2.830840 0.381214

 44 6 0 5.260105 -2.450928 1.959254

 45 1 0 4.180094 -2.320861 2.057193

 46 1 0 5.564437 -3.273822 2.620168

 47 7 0 2.544214 -0.060686 -0.691740

 48 8 0 4.643620 2.055227 -1.529427

 49 8 0 8.169879 1.110604 -1.745822

 50 8 0 7.828351 0.449989 1.093594

 51 8 0 5.841749 -1.221082 2.384315

 52 8 0 5.107398 -1.829591 -0.396154

 53 6 0 -5.108171 -1.271110 -0.254755

 54 6 0 -4.034806 0.691823 0.090325

 55 7 0 -5.236493 0.053212 0.069342

 56 6 0 -6.351043 0.811353 0.295644

 57 6 0 -7.544926 0.120539 0.233453

 58 6 0 -7.506431 -1.268067 -0.066857

 59 6 0 -6.314110 -1.969810 -0.316753

 60 1 0 -8.489879 0.614340 0.398206

 61 1 0 -6.345826 -3.022214 -0.558109

 62 6 0 -4.374543 2.074665 0.361797

 63 6 0 -5.812009 2.144721 0.500818

 64 6 0 -3.620418 3.248193 0.480657

 65 6 0 -6.444918 3.359937 0.768407

 66 6 0 -5.669674 4.505480 0.890868

 67 6 0 -4.273375 4.446103 0.742678

 68 1 0 -3.692174 5.356189 0.833131

 69 1 0 -7.522289 3.406775 0.873736

 70 1 0 -2.545652 3.234851 0.360395

 71 7 0 -3.792865 -1.531069 -0.436535

 72 6 0 -3.117366 -0.355285 -0.229171

 73 1 0 -6.144572 5.456839 1.097333

 74 6 0 -8.768937 -2.052732 -0.143995

 75 8 0 -8.823649 -3.240447 -0.397520

 76 8 0 -9.856863 -1.304414 0.098234

 77 6 0 -11.129420 -1.982109 0.043131

 78 1 0 -11.871388 -1.218329 0.259622

 79 1 0 -11.289624 -2.402410 -0.949619

 80 1 0 -11.166356 -2.775405 0.789620

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**19·Ba(ClO4)2** (S0) M06-2X

---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -0.263463 2.216085 -1.469542

 2 6 0 0.084225 3.069925 -0.417542

 3 6 0 0.729456 1.859349 -2.381960

 4 6 0 1.406209 3.408228 -0.190106

 5 1 0 -0.673564 3.370581 0.296479

 6 6 0 2.050704 2.231823 -2.185333

 7 1 0 0.484133 1.206085 -3.211889

 8 6 0 2.439924 2.916743 -1.018463

 9 1 0 1.630607 4.007342 0.680147

 10 1 0 2.778744 1.904619 -2.909020

 11 6 0 3.239699 -3.303481 1.244500

 12 1 0 3.516423 -3.157398 2.297858

 13 1 0 3.875206 -4.093943 0.825906

 14 6 0 1.794369 -3.717304 1.097467

 15 1 0 1.609376 -4.630794 1.673112

 16 1 0 1.577930 -3.905925 0.047113

 17 6 0 0.567802 -2.634100 2.882019

 18 1 0 0.715160 -3.614905 3.347509

 19 1 0 -0.486749 -2.374289 2.925444

 20 6 0 1.374072 -1.595364 3.644940

 21 1 0 2.400536 -1.929080 3.847561

 22 1 0 0.870854 -1.408437 4.601678

 23 6 0 1.875415 0.705609 3.653746

 24 1 0 2.806827 0.434195 4.170208

 25 1 0 1.110408 0.972332 4.393282

 26 6 0 2.118470 1.874168 2.721191

 27 1 0 2.528798 2.713753 3.292164

 28 1 0 1.174047 2.186008 2.272637

 29 6 0 4.241621 2.184358 1.601701

 30 1 0 4.976710 1.480764 1.218301

 31 1 0 4.552467 2.515906 2.600757

 32 6 0 4.168929 3.395848 0.668356

 33 1 0 5.162393 3.852846 0.640214

 34 1 0 3.504977 4.156987 1.078763

 35 6 0 4.813519 2.593763 -1.593876

 36 1 0 5.759806 2.939038 -1.174751

 37 1 0 4.706422 3.081447 -2.570006

 38 6 0 4.922370 1.078430 -1.843904

 39 1 0 5.957135 0.886636 -2.161904

 40 1 0 4.267391 0.718687 -2.639990

 41 6 0 5.147381 -0.968347 -0.755204

 42 1 0 4.724712 -1.486567 -1.621349

 43 1 0 6.241395 -0.928978 -0.857775

 44 6 0 4.815149 -1.729905 0.500278

 45 1 0 5.431492 -2.635783 0.510613

 46 1 0 5.054491 -1.134723 1.391594

 47 7 0 3.775779 3.078286 -0.696033

 48 8 0 3.015324 1.472398 1.688131

 49 8 0 1.426707 -0.397890 2.888276

 50 8 0 0.911604 -2.685442 1.503864

 51 8 0 3.444023 -2.097521 0.523930

 52 8 0 4.643008 0.352241 -0.665396

 53 56 0 1.185201 -0.261818 0.096774

 54 6 0 -2.833034 1.836045 -1.149048

 55 6 0 -2.632367 -0.403073 -1.264095

 56 6 0 -4.780186 0.675751 -0.678481

 57 6 0 -3.213601 -1.662537 -1.087497

 58 1 0 -2.639314 -2.572371 -1.197097

 59 6 0 -5.359603 -0.556853 -0.503479

 60 1 0 -6.383832 -0.665727 -0.179203

 61 6 0 -4.556755 -1.710073 -0.723526

 62 6 0 -5.046126 2.101620 -0.513004

 63 6 0 -3.841412 2.816285 -0.801587

 64 6 0 -6.199536 2.784226 -0.134242

 65 1 0 -7.111751 2.243139 0.088230

 66 6 0 -3.816087 4.207816 -0.707657

 67 6 0 -4.974678 4.868434 -0.329569

 68 1 0 -4.970411 5.949283 -0.252740

 69 6 0 -6.155033 4.166779 -0.044389

 70 1 0 -2.909657 4.757980 -0.930271

 71 7 0 -3.478994 0.644824 -1.078963

 72 1 0 -7.041903 4.714332 0.250058

 73 7 0 -1.398831 0.093247 -1.493154

 74 6 0 -1.512620 1.452186 -1.424415

 75 6 0 -5.137554 -3.071442 -0.526124

 76 8 0 -4.529952 -4.099815 -0.665286

 77 8 0 -6.432235 -3.030491 -0.170935

 78 6 0 -7.043714 -4.303689 0.040132

 79 1 0 -8.072959 -4.093974 0.318858

 80 1 0 -7.004342 -4.897867 -0.873069

 81 1 0 -6.529985 -4.841644 0.837107

 82 17 0 2.001261 -2.211552 -2.621255

 83 17 0 -1.666077 0.261342 2.118008

 84 8 0 3.116767 -3.146606 -2.472651

 85 8 0 2.482845 -0.816284 -2.338954

 86 8 0 0.972172 -2.483259 -1.575976

 87 8 0 1.420777 -2.278097 -3.947340

 88 8 0 -1.286173 -0.972201 1.379208

 89 8 0 -0.734549 1.324092 1.625476

 90 8 0 -1.470317 0.060819 3.555777

 91 8 0 -3.041287 0.630239 1.811704

 ---------------------------------------------------------------------

**19·Ba(ClO4)2** (S1) M06-2X

 ---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -0.368426 2.475186 -1.322086

 2 6 0 0.007083 3.208431 -0.187168

 3 6 0 0.587005 2.292291 -2.327565

 4 6 0 1.332887 3.551111 0.025808

 5 1 0 -0.718324 3.387760 0.595399

 6 6 0 1.905101 2.683499 -2.143247

 7 1 0 0.317807 1.756979 -3.229236

 8 6 0 2.338264 3.185391 -0.898411

 9 1 0 1.589477 4.017927 0.964546

 10 1 0 2.606258 2.494443 -2.939017

 11 6 0 3.516740 -3.323247 0.977044

 12 1 0 3.855573 -3.195775 2.013850

 13 1 0 4.148334 -4.087376 0.504955

 14 6 0 2.079447 -3.795503 0.902631

 15 1 0 1.977693 -4.748327 1.434557

 16 1 0 1.800208 -3.935651 -0.141146

 17 6 0 0.866924 -2.880523 2.819296

 18 1 0 0.993658 -3.898410 3.204028

 19 1 0 -0.176652 -2.588473 2.909043

 20 6 0 1.729843 -1.918875 3.620258

 21 1 0 2.771885 -2.257306 3.697130

 22 1 0 1.315194 -1.845492 4.633826

 23 6 0 2.262081 0.397521 3.764418

 24 1 0 3.304264 0.149590 4.012255

 25 1 0 1.694057 0.518451 4.695660

 26 6 0 2.187237 1.676462 2.955573

 27 1 0 2.611583 2.505268 3.530733

 28 1 0 1.145020 1.900331 2.729439

 29 6 0 4.163797 2.134724 1.610213

 30 1 0 4.819690 1.419633 1.119946

 31 1 0 4.553646 2.350954 2.612403

 32 6 0 4.122286 3.430723 0.793512

 33 1 0 5.134644 3.846883 0.784747

 34 1 0 3.496713 4.173981 1.288576

 35 6 0 4.699953 2.821544 -1.545685

 36 1 0 5.667803 3.084888 -1.115774

 37 1 0 4.604288 3.401388 -2.471972

 38 6 0 4.742387 1.342782 -1.956631

 39 1 0 5.674091 1.208594 -2.526214

 40 1 0 3.914408 1.054433 -2.605036

 41 6 0 5.136778 -0.838204 -1.172796

 42 1 0 4.525351 -1.217013 -1.994984

 43 1 0 6.190471 -0.831098 -1.489065

 44 6 0 5.008316 -1.756066 0.016156

 45 1 0 5.563035 -2.672984 -0.215357

 46 1 0 5.453091 -1.301133 0.911453

 47 7 0 3.690326 3.266287 -0.589369

 48 8 0 2.877575 1.512828 1.711205

 49 8 0 1.694542 -0.647551 2.984131

 50 8 0 1.153735 -2.842178 1.419565

 51 8 0 3.643379 -2.092889 0.268697

 52 8 0 4.745021 0.485576 -0.821853

 53 56 0 1.157387 -0.358529 0.155087

 54 6 0 -2.919030 1.922261 -1.028762

 55 6 0 -2.579515 -0.308866 -1.209843

 56 6 0 -4.803868 0.622642 -0.627794

 57 6 0 -3.082611 -1.603549 -1.089246

 58 1 0 -2.453006 -2.471005 -1.223522

 59 6 0 -5.306034 -0.654156 -0.506281

 60 1 0 -6.326929 -0.836403 -0.208671

 61 6 0 -4.433012 -1.752252 -0.747529

 62 6 0 -5.162811 2.020662 -0.426225

 63 6 0 -3.991216 2.823834 -0.671977

 64 6 0 -6.360100 2.623408 -0.044090

 65 1 0 -7.242428 2.023611 0.146205

 66 6 0 -4.054873 4.210533 -0.526707

 67 6 0 -5.260045 4.787955 -0.145947

 68 1 0 -5.321801 5.863753 -0.029545

 69 6 0 -6.400991 4.005629 0.093637

 70 1 0 -3.179479 4.822333 -0.708262

 71 7 0 -3.491748 0.684811 -1.000587

 72 1 0 -7.324281 4.487617 0.391897

 73 7 0 -1.372540 0.278298 -1.402050

 74 6 0 -1.569903 1.637069 -1.302241

 75 6 0 -4.926981 -3.149285 -0.601598

 76 8 0 -4.250614 -4.139999 -0.753656

 77 8 0 -6.238199 -3.199459 -0.272753

 78 6 0 -6.784196 -4.517769 -0.104180

 79 1 0 -7.829933 -4.367763 0.154709

 80 1 0 -6.693616 -5.088302 -1.029387

 81 1 0 -6.261397 -5.046311 0.693955

 82 17 0 1.732565 -1.977750 -2.852297

 83 17 0 -1.632866 0.117351 2.289092

 84 8 0 2.929309 -2.842321 -2.991287

 85 8 0 2.176615 -0.574609 -2.444474

 86 8 0 0.878311 -2.465667 -1.697289

 87 8 0 0.952136 -1.922026 -4.094278

 88 8 0 -1.240104 -1.134499 1.534580

 89 8 0 -0.686211 1.197084 1.787130

 90 8 0 -1.434920 -0.086913 3.743253

 91 8 0 -3.023865 0.488427 1.974072

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**19** (S0) PBE

---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -1.739112 -0.251673 -0.310519

 2 6 0 -1.005575 0.752025 0.331707

 3 6 0 -1.013477 -1.202228 -1.040633

 4 6 0 0.371640 0.822682 0.240977

 5 1 0 -1.518264 1.488329 0.941433

 6 6 0 0.362330 -1.145544 -1.143428

 7 1 0 -1.549642 -2.005358 -1.534662

 8 6 0 1.107310 -0.122433 -0.510377

 9 1 0 0.876208 1.633296 0.750923

 10 1 0 0.864170 -1.921874 -1.707008

 11 6 0 7.641569 -1.761316 2.313258

 12 1 0 8.052508 -2.344574 1.479413

 13 1 0 7.950132 -2.259350 3.244753

 14 6 0 8.203544 -0.356639 2.285128

 15 1 0 9.275295 -0.386689 2.525295

 16 1 0 7.705095 0.245468 3.050517

 17 6 0 8.945122 0.013102 0.058835

 18 1 0 9.235595 -1.046758 0.076608

 19 1 0 9.852129 0.610778 0.232732

 20 6 0 8.375434 0.305173 -1.307306

 21 1 0 7.445718 -0.261656 -1.433534

 22 1 0 9.090567 -0.042285 -2.064549

 23 6 0 6.843486 2.018633 -1.948263

 24 1 0 6.504829 1.312123 -2.718384

 25 1 0 6.907635 3.008231 -2.408157

 26 6 0 5.857717 2.028166 -0.793959

 27 1 0 6.091322 2.854926 -0.106775

 28 1 0 5.960550 1.092711 -0.231845

 29 6 0 3.557898 2.192648 -0.302973

 30 1 0 2.662130 2.620472 -0.760906

 31 1 0 3.870835 2.854063 0.518777

 32 6 0 3.250283 0.808622 0.262284

 33 1 0 2.728931 0.921057 1.216440

 34 1 0 4.182644 0.286856 0.491948

 35 6 0 3.205714 -0.869902 -1.560656

 36 1 0 4.025644 -0.267868 -1.963053

 37 1 0 2.556559 -1.104585 -2.405517

 38 6 0 3.797915 -2.154192 -0.998051

 39 1 0 3.928653 -2.884787 -1.810262

 40 1 0 3.121017 -2.592974 -0.251740

 41 6 0 5.693262 -2.942591 0.211611

 42 1 0 5.257940 -3.895681 -0.115829

 43 1 0 6.739781 -2.939516 -0.111772

 44 6 0 5.607163 -2.850003 1.723533

 45 1 0 4.559287 -2.791633 2.031979

 46 1 0 6.038405 -3.759315 2.167967

 47 7 0 2.472579 -0.051920 -0.612126

 48 8 0 4.551805 2.183067 -1.313115

 49 8 0 8.143783 1.692703 -1.499227

 50 8 0 7.980040 0.296008 1.050583

 51 8 0 6.231947 -1.691092 2.240091

 52 8 0 5.056780 -1.849702 -0.425301

 53 6 0 -5.156107 -1.250149 -0.280980

 54 6 0 -4.109692 0.698697 0.122684

 55 7 0 -5.299304 0.056727 0.073878

 56 6 0 -6.415690 0.795038 0.314423

 57 6 0 -7.602310 0.098060 0.228015

 58 6 0 -7.547669 -1.277111 -0.108406

 59 6 0 -6.352325 -1.959276 -0.369109

 60 1 0 -8.554913 0.578417 0.402076

 61 1 0 -6.374331 -3.007342 -0.637738

 62 6 0 -4.459795 2.067426 0.431178

 63 6 0 -5.890477 2.122092 0.561574

 64 6 0 -3.716059 3.240621 0.589391

 65 6 0 -6.536066 3.321263 0.860637

 66 6 0 -5.773424 4.465745 1.021927

 67 6 0 -4.378791 4.421822 0.881464

 68 1 0 -3.804708 5.334600 1.002651

 69 1 0 -7.615860 3.356229 0.960528

 70 1 0 -2.638592 3.240261 0.475774

 71 7 0 -3.845332 -1.499083 -0.457790

 72 6 0 -3.186561 -0.332239 -0.214047

 73 1 0 -6.258095 5.407940 1.253731

 74 6 0 -8.799144 -2.073262 -0.213501

 75 8 0 -8.835360 -3.258168 -0.502082

 76 8 0 -9.890066 -1.347674 0.044064

 77 6 0 -11.140374 -2.038208 -0.035603

 78 1 0 -11.899759 -1.296005 0.200120

 79 1 0 -11.293089 -2.433274 -1.041171

 80 1 0 -11.169774 -2.855721 0.686493

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**19** (S1) PBE

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -1.670601 -0.277856 -0.340993

 2 6 0 -0.937972 0.762678 0.250155

 3 6 0 -0.943248 -1.257489 -1.037027

 4 6 0 0.439523 0.840017 0.143243

 5 1 0 -1.451792 1.520082 0.827902

 6 6 0 0.433292 -1.194834 -1.154329

 7 1 0 -1.477029 -2.083558 -1.489820

 8 6 0 1.176377 -0.135975 -0.572649

 9 1 0 0.942780 1.675535 0.607648

 10 1 0 0.937314 -1.988619 -1.686491

 11 6 0 7.227887 -1.300849 2.702754

 12 1 0 7.721928 -2.069992 2.100645

 13 1 0 7.357031 -1.578490 3.757965

 14 6 0 7.875639 0.051127 2.458460

 15 1 0 8.909963 0.028975 2.826035

 16 1 0 7.334059 0.819826 3.014030

 17 6 0 8.793775 -0.162827 0.246055

 18 1 0 8.993936 -1.195776 0.555515

 19 1 0 9.739987 0.392025 0.297126

 20 6 0 8.275218 -0.200494 -1.177424

 21 1 0 7.304038 -0.703828 -1.195298

 22 1 0 8.977780 -0.779998 -1.787260

 23 6 0 6.866120 1.466022 -2.197967

 24 1 0 6.410589 0.637572 -2.754252

 25 1 0 6.995396 2.304474 -2.885121

 26 6 0 5.965776 1.854537 -1.033628

 27 1 0 6.331217 2.774382 -0.557922

 28 1 0 5.992188 1.061285 -0.285050

 29 6 0 3.678069 2.170219 -0.482793

 30 1 0 2.788846 2.609185 -0.938583

 31 1 0 4.047032 2.858890 0.289570

 32 6 0 3.335068 0.824689 0.159894

 33 1 0 2.799358 1.000571 1.093530

 34 1 0 4.247953 0.293366 0.430989

 35 6 0 3.273993 -0.912440 -1.625646

 36 1 0 4.087908 -0.324547 -2.052337

 37 1 0 2.617092 -1.179318 -2.452377

 38 6 0 3.862865 -2.174272 -1.005143

 39 1 0 4.032879 -2.933250 -1.780820

 40 1 0 3.169388 -2.589218 -0.264567

 41 6 0 5.609808 -2.799889 0.518173

 42 1 0 5.222865 -3.798008 0.281000

 43 1 0 6.693366 -2.830840 0.381214

 44 6 0 5.260105 -2.450928 1.959254

 45 1 0 4.180094 -2.320861 2.057193

 46 1 0 5.564437 -3.273822 2.620168

 47 7 0 2.544214 -0.060686 -0.691740

 48 8 0 4.643620 2.055227 -1.529427

 49 8 0 8.169879 1.110604 -1.745822

 50 8 0 7.828351 0.449989 1.093594

 51 8 0 5.841749 -1.221082 2.384315

 52 8 0 5.107398 -1.829591 -0.396154

 53 6 0 -5.108171 -1.271110 -0.254755

 54 6 0 -4.034806 0.691823 0.090325

 55 7 0 -5.236493 0.053212 0.069342

 56 6 0 -6.351043 0.811353 0.295644

 57 6 0 -7.544926 0.120539 0.233453

 58 6 0 -7.506431 -1.268067 -0.066857

 59 6 0 -6.314110 -1.969810 -0.316753

 60 1 0 -8.489879 0.614340 0.398206

 61 1 0 -6.345826 -3.022214 -0.558109

 62 6 0 -4.374543 2.074665 0.361797

 63 6 0 -5.812009 2.144721 0.500818

 64 6 0 -3.620418 3.248193 0.480657

 65 6 0 -6.444918 3.359937 0.768407

 66 6 0 -5.669674 4.505480 0.890868

 67 6 0 -4.273375 4.446103 0.742678

 68 1 0 -3.692174 5.356189 0.833131

 69 1 0 -7.522289 3.406775 0.873736

 70 1 0 -2.545652 3.234851 0.360395

 71 7 0 -3.792865 -1.531069 -0.436535

 72 6 0 -3.117366 -0.355285 -0.229171

 73 1 0 -6.144572 5.456839 1.097333

 74 6 0 -8.768937 -2.052732 -0.143995

 75 8 0 -8.823649 -3.240447 -0.397520

 76 8 0 -9.856863 -1.304414 0.098234

 77 6 0 -11.129420 -1.982109 0.043131

 78 1 0 -11.871388 -1.218329 0.259622

 79 1 0 -11.289624 -2.402410 -0.949619

 80 1 0 -11.166356 -2.775405 0.789620

 ---------------------------------------------------------------------

**19·Ba(ClO4)2** (S0) PBE

---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -0.499092 2.346653 -1.111516

 2 6 0 -0.061884 3.107079 -0.021732

 3 6 0 0.392546 2.152563 -2.166863

 4 6 0 1.261523 3.492088 0.085746

 5 1 0 -0.738369 3.297340 0.804250

 6 6 0 1.707454 2.579771 -2.085945

 7 1 0 0.074409 1.595506 -3.041350

 8 6 0 2.210282 3.139980 -0.898116

 9 1 0 1.568288 3.998085 0.991020

 10 1 0 2.357016 2.377375 -2.924210

 11 6 0 3.952487 -3.159138 0.759763

 12 1 0 4.346068 -3.002407 1.775666

 13 1 0 4.593012 -3.907352 0.268235

 14 6 0 2.546599 -3.712421 0.775355

 15 1 0 2.541865 -4.678891 1.295983

 16 1 0 2.212625 -3.864289 -0.252964

 17 6 0 1.381255 -2.946927 2.760575

 18 1 0 1.598778 -3.965579 3.105010

 19 1 0 0.321690 -2.738791 2.914735

 20 6 0 2.203788 -1.950972 3.549505

 21 1 0 3.275269 -2.201406 3.548991

 22 1 0 1.852660 -1.956989 4.591767

 23 6 0 2.616301 0.364293 3.714458

 24 1 0 3.691863 0.162014 3.839631

 25 1 0 2.156656 0.437367 4.710859

 26 6 0 2.394440 1.653052 2.960149

 27 1 0 2.823768 2.491880 3.521310

 28 1 0 1.319827 1.820799 2.849922

 29 6 0 4.212381 2.202694 1.466424

 30 1 0 4.855836 1.498510 0.938020

 31 1 0 4.668101 2.440089 2.437529

 32 6 0 4.091085 3.483678 0.644821

 33 1 0 5.093161 3.917938 0.559026

 34 1 0 3.490973 4.225572 1.178413

 35 6 0 4.522498 2.982847 -1.745600

 36 1 0 5.488460 3.369455 -1.409827

 37 1 0 4.263745 3.549511 -2.650373

 38 6 0 4.713433 1.529270 -2.180865

 39 1 0 5.584626 1.522291 -2.857116

 40 1 0 3.859825 1.141655 -2.745778

 41 6 0 5.283826 -0.624709 -1.506873

 42 1 0 4.573171 -0.979824 -2.261677

 43 1 0 6.291145 -0.614964 -1.952800

 44 6 0 5.290825 -1.586075 -0.349863

 45 1 0 5.831951 -2.484761 -0.677771

 46 1 0 5.834050 -1.158958 0.506863

 47 7 0 3.568892 3.295294 -0.695664

 48 8 0 2.953568 1.568938 1.657871

 49 8 0 2.015871 -0.676259 2.974356

 50 8 0 1.594935 -2.840564 1.361531

 51 8 0 3.976160 -1.950972 0.029845

 52 8 0 4.946784 0.681196 -1.079512

 53 56 0 1.103041 -0.360177 0.160599

 54 6 0 -3.057692 1.872700 -0.788151

 55 6 0 -2.790929 -0.353260 -0.974204

 56 6 0 -5.000026 0.651745 -0.509511

 57 6 0 -3.353979 -1.626725 -0.932548

 58 1 0 -2.762234 -2.520974 -1.079110

 59 6 0 -5.564826 -0.602296 -0.466886

 60 1 0 -6.617008 -0.748682 -0.266849

 61 6 0 -4.724716 -1.724820 -0.681873

 62 6 0 -5.324676 2.059899 -0.358375

 63 6 0 -4.118920 2.815854 -0.532650

 64 6 0 -6.528248 2.706296 -0.089186

 65 1 0 -7.442567 2.138045 0.047060

 66 6 0 -4.149968 4.206242 -0.436109

 67 6 0 -5.359312 4.827843 -0.169915

 68 1 0 -5.396659 5.909665 -0.093085

 69 6 0 -6.536672 4.088632 0.003590

 70 1 0 -3.244737 4.788808 -0.569164

 71 7 0 -3.666147 0.663460 -0.766269

 72 1 0 -7.466067 4.607060 0.213618

 73 7 0 -1.564300 0.186479 -1.142793

 74 6 0 -1.717358 1.539204 -1.039323

 75 6 0 -5.286332 -3.101108 -0.638973

 76 8 0 -4.645353 -4.107104 -0.811061

 77 8 0 -6.604716 -3.107672 -0.384471

 78 6 0 -7.204213 -4.399734 -0.322685

 79 1 0 -8.257757 -4.225853 -0.110523

 80 1 0 -7.085423 -4.923175 -1.273497

 81 1 0 -6.746973 -4.996105 0.469351

 82 17 0 1.696229 -1.928960 -2.871380

 83 17 0 -1.471439 -0.124890 2.507758

 84 8 0 2.901052 -2.719677 -3.122600

 85 8 0 2.089191 -0.530319 -2.472193

 86 8 0 0.967240 -2.471658 -1.680654

 87 8 0 0.827049 -1.890825 -4.033800

 88 8 0 -1.037633 -1.325891 1.724823

 89 8 0 -0.606008 0.998618 2.010133

 90 8 0 -1.230678 -0.345101 3.931774

 91 8 0 -2.870357 0.175241 2.236983

 ---------------------------------------------------------------------

**19·Ba(ClO4)2** (S1) PBE

 ---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

 ---------------------------------------------------------------------

 1 6 0 -0.368426 2.475186 -1.322086

 2 6 0 0.007083 3.208431 -0.187168

 3 6 0 0.587005 2.292291 -2.327565

 4 6 0 1.332887 3.551111 0.025808

 5 1 0 -0.718324 3.387760 0.595399

 6 6 0 1.905101 2.683499 -2.143247

 7 1 0 0.317807 1.756979 -3.229236

 8 6 0 2.338264 3.185391 -0.898411

 9 1 0 1.589477 4.017927 0.964546

 10 1 0 2.606258 2.494443 -2.939017

 11 6 0 3.516740 -3.323247 0.977044

 12 1 0 3.855573 -3.195775 2.013850

 13 1 0 4.148334 -4.087376 0.504955

 14 6 0 2.079447 -3.795503 0.902631

 15 1 0 1.977693 -4.748327 1.434557

 16 1 0 1.800208 -3.935651 -0.141146

 17 6 0 0.866924 -2.880523 2.819296

 18 1 0 0.993658 -3.898410 3.204028

 19 1 0 -0.176652 -2.588473 2.909043

 20 6 0 1.729843 -1.918875 3.620258

 21 1 0 2.771885 -2.257306 3.697130

 22 1 0 1.315194 -1.845492 4.633826

 23 6 0 2.262081 0.397521 3.764418

 24 1 0 3.304264 0.149590 4.012255

 25 1 0 1.694057 0.518451 4.695660

 26 6 0 2.187237 1.676462 2.955573

 27 1 0 2.611583 2.505268 3.530733

 28 1 0 1.145020 1.900331 2.729439

 29 6 0 4.163797 2.134724 1.610213

 30 1 0 4.819690 1.419633 1.119946

 31 1 0 4.553646 2.350954 2.612403

 32 6 0 4.122286 3.430723 0.793512

 33 1 0 5.134644 3.846883 0.784747

 34 1 0 3.496713 4.173981 1.288576

 35 6 0 4.699953 2.821544 -1.545685

 36 1 0 5.667803 3.084888 -1.115774

 37 1 0 4.604288 3.401388 -2.471972

 38 6 0 4.742387 1.342782 -1.956631

 39 1 0 5.674091 1.208594 -2.526214

 40 1 0 3.914408 1.054433 -2.605036

 41 6 0 5.136778 -0.838204 -1.172796

 42 1 0 4.525351 -1.217013 -1.994984

 43 1 0 6.190471 -0.831098 -1.489065

 44 6 0 5.008316 -1.756066 0.016156

 45 1 0 5.563035 -2.672984 -0.215357

 46 1 0 5.453091 -1.301133 0.911453

 47 7 0 3.690326 3.266287 -0.589369

 48 8 0 2.877575 1.512828 1.711205

 49 8 0 1.694542 -0.647551 2.984131

 50 8 0 1.153735 -2.842178 1.419565

 51 8 0 3.643379 -2.092889 0.268697

 52 8 0 4.745021 0.485576 -0.821853

 53 56 0 1.157387 -0.358529 0.155087

 54 6 0 -2.919030 1.922261 -1.028762

 55 6 0 -2.579515 -0.308866 -1.209843

 56 6 0 -4.803868 0.622642 -0.627794

 57 6 0 -3.082611 -1.603549 -1.089246

 58 1 0 -2.453006 -2.471005 -1.223522

 59 6 0 -5.306034 -0.654156 -0.506281

 60 1 0 -6.326929 -0.836403 -0.208671

 61 6 0 -4.433012 -1.752252 -0.747529

 62 6 0 -5.162811 2.020662 -0.426225

 63 6 0 -3.991216 2.823834 -0.671977

 64 6 0 -6.360100 2.623408 -0.044090

 65 1 0 -7.242428 2.023611 0.146205

 66 6 0 -4.054873 4.210533 -0.526707

 67 6 0 -5.260045 4.787955 -0.145947

 68 1 0 -5.321801 5.863753 -0.029545

 69 6 0 -6.400991 4.005629 0.093637

 70 1 0 -3.179479 4.822333 -0.708262

 71 7 0 -3.491748 0.684811 -1.000587

 72 1 0 -7.324281 4.487617 0.391897

 73 7 0 -1.372540 0.278298 -1.402050

 74 6 0 -1.569903 1.637069 -1.302241

 75 6 0 -4.926981 -3.149285 -0.601598

 76 8 0 -4.250614 -4.139999 -0.753656

 77 8 0 -6.238199 -3.199459 -0.272753

 78 6 0 -6.784196 -4.517769 -0.104180

 79 1 0 -7.829933 -4.367763 0.154709

 80 1 0 -6.693616 -5.088302 -1.029387

 81 1 0 -6.261397 -5.046311 0.693955

 82 17 0 1.732565 -1.977750 -2.852297

 83 17 0 -1.632866 0.117351 2.289092

 84 8 0 2.929309 -2.842321 -2.991287

 85 8 0 2.176615 -0.574609 -2.444474

 86 8 0 0.878311 -2.465667 -1.697289

 87 8 0 0.952136 -1.922026 -4.094278

 88 8 0 -1.240104 -1.134499 1.534580

 89 8 0 -0.686211 1.197084 1.787130

 90 8 0 -1.434920 -0.086913 3.743253

 91 8 0 -3.023865 0.488427 1.974072

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**19** (S0) wB97XD

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -1.683357 -0.240507 -0.304224

 2 6 0 -0.977134 0.747933 0.385299

 3 6 0 -0.945056 -1.131547 -1.087379

 4 6 0 0.397648 0.861617 0.287703

 5 1 0 -1.507894 1.437469 1.032850

 6 6 0 0.430156 -1.034218 -1.193152

 7 1 0 -1.462775 -1.920370 -1.621141

 8 6 0 1.148667 -0.025671 -0.513375

 9 1 0 0.885652 1.661472 0.828427

 10 1 0 0.948680 -1.766849 -1.797034

 11 6 0 7.353967 -1.679164 2.481047

 12 1 0 7.824744 -2.373424 1.775840

 13 1 0 7.520044 -2.081804 3.489696

 14 6 0 8.005337 -0.311955 2.381217

 15 1 0 9.057504 -0.392607 2.686940

 16 1 0 7.506401 0.377558 3.066153

 17 6 0 8.787805 -0.237499 0.125240

 18 1 0 8.973741 -1.310069 0.267321

 19 1 0 9.753297 0.281119 0.202571

 20 6 0 8.196255 -0.055433 -1.255756

 21 1 0 7.214405 -0.540654 -1.291063

 22 1 0 8.852244 -0.549085 -1.982386

 23 6 0 6.787285 1.749061 -1.954335

 24 1 0 6.308122 1.034729 -2.637401

 25 1 0 6.903303 2.696531 -2.484966

 26 6 0 5.920106 1.929889 -0.719341

 27 1 0 6.333016 2.720891 -0.078104

 28 1 0 5.926952 0.999134 -0.146147

 29 6 0 3.672237 2.243434 -0.071166

 30 1 0 2.788517 2.774100 -0.432515

 31 1 0 4.072876 2.789758 0.794768

 32 6 0 3.292630 0.828715 0.361066

 33 1 0 2.736187 0.884389 1.298581

 34 1 0 4.191059 0.247951 0.582378

 35 6 0 3.253984 -0.636508 -1.642502

 36 1 0 4.069679 0.001497 -1.990040

 37 1 0 2.605573 -0.801195 -2.503112

 38 6 0 3.853025 -1.959204 -1.181824

 39 1 0 3.984727 -2.635546 -2.037791

 40 1 0 3.182122 -2.445530 -0.461572

 41 6 0 5.679045 -2.771119 0.117981

 42 1 0 5.314985 -3.729162 -0.274091

 43 1 0 6.758018 -2.737552 -0.058916

 44 6 0 5.381011 -2.691514 1.608023

 45 1 0 4.303176 -2.597384 1.763075

 46 1 0 5.712181 -3.618700 2.095810

 47 7 0 2.515341 0.090445 -0.623423

 48 8 0 4.610314 2.269930 -1.134508

 49 8 0 8.089382 1.318041 -1.608357

 50 8 0 7.891990 0.263364 1.096389

 51 8 0 5.967319 -1.561491 2.226003

 52 8 0 5.115231 -1.688063 -0.595353

 53 6 0 -5.097239 -1.283530 -0.232773

 54 6 0 -4.060551 0.681048 0.091586

 55 7 0 -5.247807 0.033159 0.069962

 56 6 0 -6.367187 0.776530 0.278911

 57 6 0 -7.548104 0.076870 0.217823

 58 6 0 -7.487226 -1.313670 -0.064336

 59 6 0 -6.294210 -2.000439 -0.294613

 60 1 0 -8.500676 0.562368 0.370015

 61 1 0 -6.308502 -3.057572 -0.521406

 62 6 0 -4.416454 2.064240 0.344748

 63 6 0 -5.841414 2.120099 0.472295

 64 6 0 -3.670293 3.239899 0.453721

 65 6 0 -6.490213 3.328181 0.721129

 66 6 0 -5.728529 4.478767 0.834895

 67 6 0 -4.333898 4.431325 0.696872

 68 1 0 -3.762078 5.348484 0.780772

 69 1 0 -7.569069 3.364777 0.818930

 70 1 0 -2.593566 3.229544 0.340148

 71 7 0 -3.783458 -1.531114 -0.400273

 72 6 0 -3.137152 -0.348142 -0.203927

 73 1 0 -6.213785 5.428356 1.027243

 74 6 0 -8.743620 -2.116803 -0.140800

 75 8 0 -8.776889 -3.301965 -0.381874

 76 8 0 -9.831634 -1.384377 0.086281

 77 6 0 -11.089708 -2.068627 0.032554

 78 1 0 -11.841182 -1.311209 0.239340

 79 1 0 -11.244221 -2.498720 -0.957401

 80 1 0 -11.124556 -2.855981 0.786058

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**19** (S1) wB97XDYP

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -1.670601 -0.277856 -0.340993

 2 6 0 -0.937972 0.762678 0.250155

 3 6 0 -0.943248 -1.257489 -1.037027

 4 6 0 0.439523 0.840017 0.143243

 5 1 0 -1.451792 1.520082 0.827902

 6 6 0 0.433292 -1.194834 -1.154329

 7 1 0 -1.477029 -2.083558 -1.489820

 8 6 0 1.176377 -0.135975 -0.572649

 9 1 0 0.942780 1.675535 0.607648

 10 1 0 0.937314 -1.988619 -1.686491

 11 6 0 7.227887 -1.300849 2.702754

 12 1 0 7.721928 -2.069992 2.100645

 13 1 0 7.357031 -1.578490 3.757965

 14 6 0 7.875639 0.051127 2.458460

 15 1 0 8.909963 0.028975 2.826035

 16 1 0 7.334059 0.819826 3.014030

 17 6 0 8.793775 -0.162827 0.246055

 18 1 0 8.993936 -1.195776 0.555515

 19 1 0 9.739987 0.392025 0.297126

 20 6 0 8.275218 -0.200494 -1.177424

 21 1 0 7.304038 -0.703828 -1.195298

 22 1 0 8.977780 -0.779998 -1.787260

 23 6 0 6.866120 1.466022 -2.197967

 24 1 0 6.410589 0.637572 -2.754252

 25 1 0 6.995396 2.304474 -2.885121

 26 6 0 5.965776 1.854537 -1.033628

 27 1 0 6.331217 2.774382 -0.557922

 28 1 0 5.992188 1.061285 -0.285050

 29 6 0 3.678069 2.170219 -0.482793

 30 1 0 2.788846 2.609185 -0.938583

 31 1 0 4.047032 2.858890 0.289570

 32 6 0 3.335068 0.824689 0.159894

 33 1 0 2.799358 1.000571 1.093530

 34 1 0 4.247953 0.293366 0.430989

 35 6 0 3.273993 -0.912440 -1.625646

 36 1 0 4.087908 -0.324547 -2.052337

 37 1 0 2.617092 -1.179318 -2.452377

 38 6 0 3.862865 -2.174272 -1.005143

 39 1 0 4.032879 -2.933250 -1.780820

 40 1 0 3.169388 -2.589218 -0.264567

 41 6 0 5.609808 -2.799889 0.518173

 42 1 0 5.222865 -3.798008 0.281000

 43 1 0 6.693366 -2.830840 0.381214

 44 6 0 5.260105 -2.450928 1.959254

 45 1 0 4.180094 -2.320861 2.057193

 46 1 0 5.564437 -3.273822 2.620168

 47 7 0 2.544214 -0.060686 -0.691740

 48 8 0 4.643620 2.055227 -1.529427

 49 8 0 8.169879 1.110604 -1.745822

 50 8 0 7.828351 0.449989 1.093594

 51 8 0 5.841749 -1.221082 2.384315

 52 8 0 5.107398 -1.829591 -0.396154

 53 6 0 -5.108171 -1.271110 -0.254755

 54 6 0 -4.034806 0.691823 0.090325

 55 7 0 -5.236493 0.053212 0.069342

 56 6 0 -6.351043 0.811353 0.295644

 57 6 0 -7.544926 0.120539 0.233453

 58 6 0 -7.506431 -1.268067 -0.066857

 59 6 0 -6.314110 -1.969810 -0.316753

 60 1 0 -8.489879 0.614340 0.398206

 61 1 0 -6.345826 -3.022214 -0.558109

 62 6 0 -4.374543 2.074665 0.361797

 63 6 0 -5.812009 2.144721 0.500818

 64 6 0 -3.620418 3.248193 0.480657

 65 6 0 -6.444918 3.359937 0.768407

 66 6 0 -5.669674 4.505480 0.890868

 67 6 0 -4.273375 4.446103 0.742678

 68 1 0 -3.692174 5.356189 0.833131

 69 1 0 -7.522289 3.406775 0.873736

 70 1 0 -2.545652 3.234851 0.360395

 71 7 0 -3.792865 -1.531069 -0.436535

 72 6 0 -3.117366 -0.355285 -0.229171

 73 1 0 -6.144572 5.456839 1.097333

 74 6 0 -8.768937 -2.052732 -0.143995

 75 8 0 -8.823649 -3.240447 -0.397520

 76 8 0 -9.856863 -1.304414 0.098234

 77 6 0 -11.129420 -1.982109 0.043131

 78 1 0 -11.871388 -1.218329 0.259622

 79 1 0 -11.289624 -2.402410 -0.949619

 80 1 0 -11.166356 -2.775405 0.789620

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**19·Ba(ClO4)2** (S0) wB97XD

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -0.288031 2.346384 -1.472328

 2 6 0 0.100259 3.142130 -0.392548

 3 6 0 0.663112 2.062300 -2.449803

 4 6 0 1.430624 3.465019 -0.196411

 5 1 0 -0.623369 3.393147 0.372678

 6 6 0 1.986651 2.431858 -2.287180

 7 1 0 0.385988 1.463886 -3.309250

 8 6 0 2.426716 3.015172 -1.086229

 9 1 0 1.691268 3.990791 0.710527

 10 1 0 2.684246 2.166182 -3.064986

 11 6 0 3.277397 -3.343218 1.197705

 12 1 0 3.616215 -3.197337 2.233099

 13 1 0 3.865467 -4.160782 0.759007

 14 6 0 1.816284 -3.726720 1.129554

 15 1 0 1.649251 -4.644323 1.706495

 16 1 0 1.541993 -3.903659 0.089455

 17 6 0 0.685436 -2.619665 2.968594

 18 1 0 0.771187 -3.610862 3.429620

 19 1 0 -0.343968 -2.276022 3.047858

 20 6 0 1.593241 -1.645526 3.697722

 21 1 0 2.618513 -2.028037 3.802106

 22 1 0 1.181628 -1.485009 4.702879

 23 6 0 2.198300 0.636984 3.710660

 24 1 0 3.208478 0.354515 4.043238

 25 1 0 1.582621 0.865514 4.590325

 26 6 0 2.257495 1.847374 2.805736

 27 1 0 2.708329 2.688579 3.343139

 28 1 0 1.244535 2.124535 2.507523

 29 6 0 4.264966 2.154359 1.487430

 30 1 0 4.929584 1.407703 1.056522

 31 1 0 4.654850 2.453374 2.469321

 32 6 0 4.216862 3.376635 0.569358

 33 1 0 5.228370 3.793239 0.521076

 34 1 0 3.596302 4.160280 1.006340

 35 6 0 4.768517 2.545192 -1.696479

 36 1 0 5.744094 2.805852 -1.280975

 37 1 0 4.702952 3.053682 -2.666692

 38 6 0 4.759896 1.037896 -1.984051

 39 1 0 5.716627 0.815351 -2.480250

 40 1 0 3.961615 0.730907 -2.662875

 41 6 0 5.057577 -1.053828 -0.988858

 42 1 0 4.497809 -1.514298 -1.809142

 43 1 0 6.130097 -1.075407 -1.234974

 44 6 0 4.845098 -1.850028 0.270686

 45 1 0 5.413943 -2.782611 0.170388

 46 1 0 5.226652 -1.305669 1.145629

 47 7 0 3.776780 3.095580 -0.786324

 48 8 0 2.998694 1.530949 1.634031

 49 8 0 1.622044 -0.427412 2.982600

 50 8 0 0.959161 -2.694462 1.578958

 51 8 0 3.473925 -2.156751 0.451590

 52 8 0 4.650005 0.286231 -0.793517

 53 56 0 1.164543 -0.278641 0.133186

 54 6 0 -2.838702 1.858089 -1.120492

 55 6 0 -2.542085 -0.366796 -1.228249

 56 6 0 -4.730929 0.613698 -0.650129

 57 6 0 -3.064451 -1.650172 -1.059533

 58 1 0 -2.447597 -2.530227 -1.178078

 59 6 0 -5.254750 -0.641789 -0.480530

 60 1 0 -6.276309 -0.793626 -0.165304

 61 6 0 -4.403369 -1.760538 -0.697242

 62 6 0 -5.061959 2.026441 -0.497150

 63 6 0 -3.891228 2.791925 -0.784742

 64 6 0 -6.243824 2.658822 -0.124514

 65 1 0 -7.132607 2.079951 0.099438

 66 6 0 -3.925643 4.181394 -0.694397

 67 6 0 -5.112043 4.792255 -0.322382

 68 1 0 -5.154329 5.873037 -0.246813

 69 6 0 -6.260276 4.041475 -0.039740

 70 1 0 -3.041204 4.769037 -0.911032

 71 7 0 -3.428697 0.640292 -1.036739

 72 1 0 -7.171584 4.550746 0.251351

 73 7 0 -1.335248 0.183543 -1.463692

 74 6 0 -1.509262 1.538773 -1.402043

 75 6 0 -4.922726 -3.145522 -0.500283

 76 8 0 -4.264956 -4.146589 -0.624899

 77 8 0 -6.220779 -3.160840 -0.160482

 78 6 0 -6.787760 -4.452345 0.056305

 79 1 0 -7.828105 -4.274950 0.320517

 80 1 0 -6.719873 -5.056771 -0.849695

 81 1 0 -6.268782 -4.965926 0.867257

 82 17 0 1.674032 -2.193731 -2.719855

 83 17 0 -1.629162 0.391609 2.286719

 84 8 0 2.799700 -3.129137 -2.758621

 85 8 0 2.194723 -0.812119 -2.429715

 86 8 0 0.781951 -2.522370 -1.567197

 87 8 0 0.929926 -2.195054 -3.965409

 88 8 0 -1.305892 -0.871002 1.562825

 89 8 0 -0.670501 1.410966 1.751721

 90 8 0 -1.410410 0.213213 3.723578

 91 8 0 -2.997626 0.802013 2.001516

 ---------------------------------------------------------------------

**19·Ba(ClO4)2** (S1) wB97XD

---------------------------------------------------------------------

 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 1 6 0 -0.368426 2.475186 -1.322086

 2 6 0 0.007083 3.208431 -0.187168

 3 6 0 0.587005 2.292291 -2.327565

 4 6 0 1.332887 3.551111 0.025808

 5 1 0 -0.718324 3.387760 0.595399

 6 6 0 1.905101 2.683499 -2.143247

 7 1 0 0.317807 1.756979 -3.229236

 8 6 0 2.338264 3.185391 -0.898411

 9 1 0 1.589477 4.017927 0.964546

 10 1 0 2.606258 2.494443 -2.939017

 11 6 0 3.516740 -3.323247 0.977044

 12 1 0 3.855573 -3.195775 2.013850

 13 1 0 4.148334 -4.087376 0.504955

 14 6 0 2.079447 -3.795503 0.902631

 15 1 0 1.977693 -4.748327 1.434557

 16 1 0 1.800208 -3.935651 -0.141146

 17 6 0 0.866924 -2.880523 2.819296

 18 1 0 0.993658 -3.898410 3.204028

 19 1 0 -0.176652 -2.588473 2.909043

 20 6 0 1.729843 -1.918875 3.620258

 21 1 0 2.771885 -2.257306 3.697130

 22 1 0 1.315194 -1.845492 4.633826

 23 6 0 2.262081 0.397521 3.764418

 24 1 0 3.304264 0.149590 4.012255

 25 1 0 1.694057 0.518451 4.695660

 26 6 0 2.187237 1.676462 2.955573

 27 1 0 2.611583 2.505268 3.530733

 28 1 0 1.145020 1.900331 2.729439

 29 6 0 4.163797 2.134724 1.610213

 30 1 0 4.819690 1.419633 1.119946

 31 1 0 4.553646 2.350954 2.612403

 32 6 0 4.122286 3.430723 0.793512

 33 1 0 5.134644 3.846883 0.784747

 34 1 0 3.496713 4.173981 1.288576

 35 6 0 4.699953 2.821544 -1.545685

 36 1 0 5.667803 3.084888 -1.115774

 37 1 0 4.604288 3.401388 -2.471972

 38 6 0 4.742387 1.342782 -1.956631

 39 1 0 5.674091 1.208594 -2.526214

 40 1 0 3.914408 1.054433 -2.605036

 41 6 0 5.136778 -0.838204 -1.172796

 42 1 0 4.525351 -1.217013 -1.994984

 43 1 0 6.190471 -0.831098 -1.489065

 44 6 0 5.008316 -1.756066 0.016156

 45 1 0 5.563035 -2.672984 -0.215357

 46 1 0 5.453091 -1.301133 0.911453

 47 7 0 3.690326 3.266287 -0.589369

 48 8 0 2.877575 1.512828 1.711205

 49 8 0 1.694542 -0.647551 2.984131

 50 8 0 1.153735 -2.842178 1.419565

 51 8 0 3.643379 -2.092889 0.268697

 52 8 0 4.745021 0.485576 -0.821853

 53 56 0 1.157387 -0.358529 0.155087

 54 6 0 -2.919030 1.922261 -1.028762

 55 6 0 -2.579515 -0.308866 -1.209843

 56 6 0 -4.803868 0.622642 -0.627794

 57 6 0 -3.082611 -1.603549 -1.089246

 58 1 0 -2.453006 -2.471005 -1.223522

 59 6 0 -5.306034 -0.654156 -0.506281

 60 1 0 -6.326929 -0.836403 -0.208671

 61 6 0 -4.433012 -1.752252 -0.747529

 62 6 0 -5.162811 2.020662 -0.426225

 63 6 0 -3.991216 2.823834 -0.671977

 64 6 0 -6.360100 2.623408 -0.044090

 65 1 0 -7.242428 2.023611 0.146205

 66 6 0 -4.054873 4.210533 -0.526707

 67 6 0 -5.260045 4.787955 -0.145947

 68 1 0 -5.321801 5.863753 -0.029545

 69 6 0 -6.400991 4.005629 0.093637

 70 1 0 -3.179479 4.822333 -0.708262

 71 7 0 -3.491748 0.684811 -1.000587

 72 1 0 -7.324281 4.487617 0.391897

 73 7 0 -1.372540 0.278298 -1.402050

 74 6 0 -1.569903 1.637069 -1.302241

 75 6 0 -4.926981 -3.149285 -0.601598

 76 8 0 -4.250614 -4.139999 -0.753656

 77 8 0 -6.238199 -3.199459 -0.272753

 78 6 0 -6.784196 -4.517769 -0.104180

 79 1 0 -7.829933 -4.367763 0.154709

 80 1 0 -6.693616 -5.088302 -1.029387

 81 1 0 -6.261397 -5.046311 0.693955

 82 17 0 1.732565 -1.977750 -2.852297

 83 17 0 -1.632866 0.117351 2.289092

 84 8 0 2.929309 -2.842321 -2.991287

 85 8 0 2.176615 -0.574609 -2.444474

 86 8 0 0.878311 -2.465667 -1.697289

 87 8 0 0.952136 -1.922026 -4.094278

 88 8 0 -1.240104 -1.134499 1.534580

 89 8 0 -0.686211 1.197084 1.787130

 90 8 0 -1.434920 -0.086913 3.743253

 91 8 0 -3.023865 0.488427 1.974072

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