

Optical and Electronic Properties of Clusters Type $[M_{25}(MPA)_{18}]^-$ ($M = Au, Ag$). A Quantum Chemistry Comparison Between TD-DFT and sTD-DFT

Carlos Orellana¹, Sebastián Miranda-Rojas², Dage Sundholm^{3*} and Fernando Mendizabal^{1*}

¹*Departamento de Química, Facultad de Ciencias, Universidad de Chile, P.O. Box 653, Las Palmeras 3425, Ñuñoa, Santiago, Chile.*

²*Departamento de Ciencias Químicas, Facultad de Ciencias Exactas, Universidad Andrés Bello, Avenida República 275, Santiago, Chile.*

³*Laboratory for Instruction in Swedish, Department of Chemistry, University of Helsinki, A.I. Virtasen aukio 1, P.O. Box 55, FI-00014 Helsinki, Finland.*

*Correspondence: hagua@uchile.cl (F.M.); sundholm@chem.helsinki.fi (D.S.)

Tables.

Table S1. Cartesian coordinates (in Angstroms) for the optimized geometries of the systems studied in this work.

$[Ag_{25}(MPA)_{18}]^-$ B3LYP S_0 (gas)

Au -0.046915 0.235528 0.212830
Au 0.918290 2.114730 2.155690
Au -2.116109 0.844305 -1.839264
Au 1.840989 -0.997280 2.205768
Au -1.064810 -1.789153 -1.606290
Au 0.635115 2.850240 -0.830145
Au 1.833507 -2.156503 -0.398290
Au -1.710328 2.438224 1.018178
Au -0.274068 -2.592712 1.431063
Au 2.691081 0.773623 -0.376970
Au -1.228617 0.129841 2.766943
Au 0.794551 0.492227 -2.515954
Au -2.794147 -0.764064 0.475650
Au 2.281256 -4.316360 2.656861
S 1.894457 -6.120148 1.176116
Au 0.501352 -5.109914 -0.466481
C 3.587728 -6.406172 0.484983
H 3.921994 -5.503386 -0.044762
H 4.238993 -6.512497 1.361215
Au 0.307177 5.383999 1.103914
S -1.372046 6.340953 -0.286588
Au -2.049673 4.513137 -1.661792
C -2.832597 6.537817 0.828604

H -3.008249 5.585977 1.342593
H -3.696639 6.742131 0.180920
Au -4.486029 1.118283 2.844327
S -5.221844 -0.974782 3.723828
Au -3.535733 -2.511757 3.031825
C -6.665833 -1.327902 2.607521
H -6.497998 -0.819513 1.654578
H -7.537536 -0.862394 3.088915
Au 3.150728 2.980244 -3.174983
S 4.881382 1.445818 -3.723193
Au 3.891327 -0.637276 -3.078253
C 6.074110 1.874678 -2.373092
H 5.505876 2.048618 -1.453819
H 6.544123 2.823982 -2.663698
Au -1.522187 -0.443922 -4.981645
S -3.292608 -2.076156 -5.058444
Au -4.065891 -1.915242 -2.806708
C -2.057993 -3.460083 -5.188081
H -1.272789 -3.251269 -4.457337
H -1.625679 -3.353756 -6.191017
Au 4.239027 0.818110 2.847749
S 3.644150 1.271080 5.115678
Au 1.346524 0.614505 5.147355
C 3.750847 3.121242 5.244573
H 3.956403 3.519635 4.244647
H 4.626494 3.330291 5.874661
S 1.425153 4.485850 -2.557520
S -3.791607 3.239624 2.027277
S 3.016214 -2.765961 -2.496271
S -2.050008 -4.087777 2.105505
S 1.979984 4.364769 2.465067
S -2.829214 2.799936 -3.101316
S 2.622666 -2.485119 4.130280
S -1.118990 -4.235231 -1.959692
S 0.517534 0.767604 -4.997535
S -4.913432 -1.606454 -0.582412
S 4.935939 0.435041 0.614212
S -0.925130 -0.089259 5.217991
C -5.702142 0.049559 -0.772534
H -4.980252 0.701430 -1.283065
H -5.845944 0.462857 0.235742
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H -0.289045 2.878228 -4.105907
H 0.954013 3.102225 -5.341074
C -0.826596 -1.928900 5.301696
H -0.252596 -2.285847 4.435654
H -1.865378 -2.269018 5.177500

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H 4.318226 -1.892883 1.008999
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H -0.636758 -4.670576 3.998989
H -0.640051 -5.876762 2.703953
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H -5.092343 3.111344 -2.206365
H -5.074909 2.259506 -3.773959
C 4.454484 -2.353351 4.253427
H 4.852589 -2.105945 3.267191
H 4.659229 -1.507612 4.925263
C 3.412233 4.018547 1.352336
H 3.031622 3.737944 0.360094
H 3.884347 3.118405 1.768861
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H -0.730587 2.594252 -7.145834
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O -0.865958 5.190057 -5.579129
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H -3.192966 -4.967622 -4.078157
C -1.372267 -5.823239 -4.779557
O -1.408434 -6.862439 -4.138480
O -0.286759 -5.386016 -5.395768
H 0.556548 -5.824595 -5.109824
C -7.034010 0.010852 -1.524526
H -6.950236 -0.586029 -2.443675
H -7.814230 -0.431916 -0.885999
C -7.380653 1.440749 -1.874826
O -7.425184 2.334821 -1.048408
O -7.529975 1.637136 -3.179098

H -7.536273 2.617285 -3.381653
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H -6.865719 3.774287 1.371821
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C -3.827142 7.817016 2.742724
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H -4.391121 5.247124 -3.363220
H -4.446979 4.425581 -4.923001
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C -2.025268 -7.168775 -0.727123
O -1.979941 -7.368803 0.467904
O -1.138082 -7.746678 -1.545344
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O 2.237309 -7.157416 -2.202713
H 2.192016 -6.817680 -3.141498
C 1.929010 -2.979680 -5.145461
H 1.007071 -3.273699 -5.670317
H 2.159311 -1.948687 -5.459785
C 3.098847 -3.878874 -5.583796
H 3.008396 -4.109637 -6.659286
H 4.060693 -3.365753 -5.447904
C 3.194296 -5.191838 -4.849931
O 2.212703 -5.897372 -4.561161
O 4.410716 -5.529839 -4.523265
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H 6.621353 -0.179031 -1.911702
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O 8.862277 0.099240 -0.733203
H 9.452971 0.356010 0.000234
C 6.487028 -1.849455 1.102537
H 7.345714 -1.532455 0.494336
H 6.636082 -1.421627 2.109815
C 6.523310 -3.348122 1.307599
O 5.554052 -4.039097 1.545578
O 7.766253 -3.838639 1.240200
H 7.732309 -4.795087 1.428812
C 5.109929 -3.626483 4.766218
H 4.876691 -4.470853 4.093816
H 4.747046 -3.910655 5.766116
C 6.615253 -3.513004 4.793271
O 7.261789 -2.652677 4.231603
O 7.181658 -4.507825 5.488112
H 8.150843 -4.404894 5.446131
C -6.900026 -2.806164 2.347673
H -5.993455 -3.275245 1.927504
H -7.142790 -3.364906 3.265797
C -7.998912 -3.023895 1.332032
O -8.581155 -2.146724 0.729995
O -8.246005 -4.325938 1.147476
H -8.938804 -4.420042 0.467343
C -0.248673 -2.493262 6.602529
H -0.763366 -2.055187 7.470171
H 0.830680 -2.295798 6.659367
C -0.532350 -3.980708 6.571962
O -1.640851 -4.445996 6.766257
O 0.512837 -4.716154 6.200202
H 0.198131 -5.636082 5.991362
C -2.325893 -6.059034 4.056589
H -2.956761 -5.411302 4.690388
H -2.992275 -6.571864 3.346106
C -1.715946 -7.088081 4.976344
O -0.579695 -7.059121 5.424464
O -2.566656 -8.063198 5.277073
H -2.139439 -8.677623 5.904187
C 3.401846 6.486970 -2.527129
H 4.167104 5.728265 -2.756019
H 3.044504 6.882977 -3.491802
C 4.108649 7.591536 -1.779893
O 3.849434 7.956866 -0.651864
O 5.086868 8.138099 -2.513329

H 5.521864 8.831185 -1.982926
C 4.452128 5.136832 1.251665
H 4.879886 5.342322 2.245041
H 4.026775 6.061995 0.842337
C 5.533570 4.635497 0.313632
O 5.659634 4.983098 -0.844808
O 6.281776 3.694251 0.886890
H 6.906119 3.270949 0.244056
C 2.501019 3.777774 5.808792
H 2.330024 3.491716 6.860647
H 1.604348 3.468522 5.251437
C 2.589406 5.285525 5.738243
O 3.603977 5.918125 5.541175
O 1.393205 5.858464 5.929904
H 1.501778 6.826715 5.889711

[Ag₂₅(MPA)₁₈]⁻ B3LYP T₁ (gas)

Ag 0.031985 0.212406 0.265875
Ag 1.546752 2.167178 1.729380
Ag -2.076116 0.875668 -1.511006
Ag 1.627565 -0.715863 2.376745
Ag -1.167145 -1.763701 -1.422040
Ag 0.637991 2.903739 -0.863215
Ag 1.664038 -2.091288 -0.295054
Ag -1.209155 2.499866 1.319253
Ag -0.436019 -2.461846 1.491111
Ag 2.786875 0.838384 -0.687709
Ag -1.126182 0.054766 2.959176
Ag 0.622985 0.520755 -2.521197
Ag -2.796074 -0.850763 0.890800
Ag 2.273153 -3.977161 2.750594
S 2.024790 -5.872388 1.271223
Ag 0.460054 -5.022812 -0.403160
C 3.671772 -6.001521 0.447723
H 3.867339 -5.092166 -0.140987
H 4.417072 -6.025713 1.252112
Ag 0.928656 5.377890 0.822899
S -1.015616 6.342546 -0.310002
Ag -1.807590 4.499207 -1.735213
C -2.293315 6.343348 1.019282
H -2.354368 5.339168 1.454191
H -3.258567 6.572813 0.546397
Ag -3.992591 0.887670 3.203664
S -5.136552 -1.129194 4.061312
Ag -3.500145 -2.742260 3.222601

C -6.567201 -1.287450 2.891913
H -6.387872 -0.667170 2.008482
H -7.446835 -0.870144 3.404730
Ag 3.259796 2.728265 -3.184403
S 5.085552 1.190004 -3.760734
Ag 3.875956 -0.758507 -2.927008
C 6.308457 1.553060 -2.424408
H 5.781826 1.862794 -1.513302
H 6.908242 2.407747 -2.763926
Ag -1.690029 -0.211992 -4.799859
S -3.390729 -1.996322 -5.002663
Ag -3.979417 -1.874977 -2.640258
C -2.066183 -3.280322 -5.193176
H -1.297836 -3.092504 -4.436948
H -1.613275 -3.114471 -6.179891
Ag 3.959261 1.196645 2.958854
S 3.120176 1.871086 5.167740
Ag 1.272268 0.214755 5.334627
C 2.202726 3.486820 5.043234
H 2.631150 4.051055 4.205841
H 2.433027 4.030488 5.972236
S 1.569772 4.406795 -2.719718
S -3.339558 3.131577 2.470822
S 2.872414 -2.891538 -2.370963
S -2.040079 -4.280053 2.063500
S 2.946276 4.337703 1.748386
S -2.958434 2.696569 -2.959421
S 2.449642 -2.169392 4.372079
S -1.273159 -4.216150 -1.925806
S 0.432860 0.966444 -5.056545
S -4.865634 -1.585200 -0.395085
S 4.827514 0.401489 0.801119
S -1.123992 -0.337111 5.477217
C -5.567923 0.118825 -0.500714
H -4.813708 0.784459 -0.944031
H -5.738503 0.474068 0.524754
C -0.094070 2.739134 -5.058937
H -0.379693 3.026360 -4.043244
H 0.790435 3.337947 -5.312803
C -1.102423 -2.178994 5.410940
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H 4.160607 -1.849711 1.506015
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C -1.163229 -5.487796 3.132806
H -0.589882 -4.959516 3.900499

H -0.453156 -6.005164 2.473630
C 1.470074 -2.955182 -3.585535
H 0.733678 -2.181845 -3.324676
H 0.987777 -3.925187 -3.420639
C -4.367278 3.536052 0.982178
H -4.801271 2.624458 0.560164
H -3.698280 3.962135 0.223283
C 2.428566 5.919118 -2.116041
H 2.769020 5.787179 -1.081965
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C -2.849409 -4.911147 -1.258419
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H -5.070106 3.276515 -1.879541
H -5.316621 2.366878 -3.388321
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H 4.732220 -1.727137 3.651043
H 4.367093 -0.993339 5.221811
C 4.179796 4.007125 0.424971
H 3.673072 3.847411 -0.536505
H 4.683688 3.068674 0.688598
C -1.249099 3.061367 -5.996213
H -0.968127 2.978651 -7.059576
H -2.085264 2.358323 -5.843936
C -1.820947 4.438547 -5.742153
O -1.461741 5.226998 -4.902281
O -2.859029 4.707530 -6.574967
H -3.172590 5.598142 -6.340072
C -2.518596 -4.735293 -5.060463
H -3.102413 -5.054226 -5.942117
H -3.159809 -4.878762 -4.180430
C -1.322494 -5.662674 -4.901743
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H -6.764229 -0.199782 -2.302362
H -7.670848 -0.337727 -0.773187
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O -7.744919 2.037550 -2.567343
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H -5.082547 5.358094 1.924111
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C -5.975680 5.190239 0.021078

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H -4.226608 5.246947 -3.271688
H -4.681306 4.384417 -4.732368
C -6.284349 5.129704 -3.557632
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H -3.915861 -6.750687 -0.964837
H -3.082911 -6.654317 -2.547023
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H 0.949255 -3.046088 -5.637488
H 2.059805 -1.723267 -5.265163
C 3.053242 -3.610223 -5.550648
H 2.972011 -3.767459 -6.640656
H 3.996244 -3.074865 -5.374468
C 3.194805 -4.966095 -4.903953
O 2.233292 -5.714088 -4.658787
O 4.420890 -5.292437 -4.607535
H 4.438256 -6.104257 -4.002458
C 7.183641 0.350085 -2.107021
H 7.651008 -0.059696 -3.020994
H 6.589528 -0.471329 -1.675330
C 8.299745 0.679713 -1.149183
O 8.709663 1.790141 -0.880892
O 8.853861 -0.420969 -0.613752

H 9.555256 -0.127600 -0.005580
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H 7.144918 -1.661048 0.729879
H 6.565407 -1.337317 2.367164
C 6.346131 -3.332289 1.819625
O 5.393909 -3.960064 2.236284
O 7.561414 -3.888180 1.691023
H 7.489981 -4.801759 2.018341
C 4.913907 -3.096558 5.301099
H 4.720716 -4.011557 4.713357
H 4.508514 -3.274872 6.307868
C 6.414211 -2.950047 5.366172
O 7.095227 -2.317719 4.589314
O 6.957135 -3.646208 6.384293
H 7.920281 -3.518527 6.326696
C -6.837849 -2.714527 2.439049
H -5.933256 -3.153286 1.983257
H -7.111707 -3.377672 3.276393
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H -8.836481 -4.011467 0.306774
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H -1.120114 -2.558285 7.546684
H 0.518468 -2.604547 6.797275
C -0.707447 -4.354705 6.449767
O -1.788781 -4.909281 6.448915
O 0.436379 -4.977733 6.153874
H 0.224841 -5.898652 5.847433
C -2.123650 -6.499041 3.741929
H -2.856014 -5.991051 4.393965
H -2.675549 -7.027604 2.950073
C -1.426230 -7.510617 4.611751
O -0.347219 -7.373977 5.161724
O -2.134137 -8.637625 4.761906
H -1.627731 -9.208542 5.366029
C 3.606110 6.303399 -3.004476
H 4.375665 5.509548 -2.990194
H 3.304515 6.436545 -4.054545
C 4.314285 7.542463 -2.518157
O 4.281115 7.980614 -1.390569
O 5.052662 8.119995 -3.488372
H 5.522741 8.861760 -3.069863
C 5.238435 5.114192 0.301905
H 5.664654 5.321891 1.293912
H 4.813380 6.038151 -0.111080
C 6.315903 4.580193 -0.612815

O 6.328789 4.707897 -1.821676
O 7.203484 3.847946 0.064721
H 7.783890 3.324886 -0.533134
C 0.690485 3.338566 4.879262
H 0.224623 2.899623 5.772369
H 0.472872 2.644101 4.044935
C -0.049775 4.604997 4.498546
O 0.342880 5.400299 3.662581
O -1.209610 4.714750 5.130376
H -1.720707 5.495922 4.794029

[Ag₂₅(MPA)₁₈]⁻ B3LYP S₀ (acetonitrile)

Ag 0.066025 0.167229 0.251220
Ag 1.476879 2.108695 1.791619
Ag -2.065921 0.958900 -1.402781
Ag 1.764368 -0.855314 2.245326
Ag -1.102917 -1.750918 -1.486473
Ag 0.695905 2.857319 -0.875768
Ag 1.788452 -2.082705 -0.417797
Ag -1.324232 2.418799 1.220848
Ag -0.342974 -2.521926 1.378343
Ag 2.773183 0.674707 -0.486376
Ag -0.973671 0.100877 2.879983
Ag 0.697207 0.473379 -2.493890
Ag -2.665808 -0.819932 0.753099
Ag 2.310814 -3.941147 2.730972
S 2.070858 -5.809098 1.212731
Ag 0.501253 -4.995197 -0.467759
C 3.724471 -5.906366 0.387116
H 3.885877 -4.998041 -0.212457
H 4.467199 -5.895889 1.193259
Ag 0.838145 5.318238 0.835137
S -1.045876 6.304640 -0.355520
Ag -1.830572 4.476025 -1.798629
C -2.362480 6.401029 0.932086
H -2.528215 5.392840 1.325748
H -3.285391 6.733089 0.436704
Ag -4.041862 1.079744 3.204031
S -4.992507 -1.018955 4.019070
Ag -3.438782 -2.648503 3.099386
C -6.523057 -1.207170 2.986274
H -6.404944 -0.630111 2.064188
H -7.348224 -0.755039 3.555667
Ag 3.299501 2.813855 -3.154983
S 5.055791 1.217214 -3.675402

Ag 3.935753 -0.821331 -2.988615
C 6.313148 1.540345 -2.358902
H 5.799269 1.838029 -1.437877
H 6.916359 2.391795 -2.698959
Ag -1.658130 -0.181829 -4.749818
S -3.394601 -1.926619 -4.940928
Ag -3.991329 -1.877603 -2.573530
C -2.106761 -3.236205 -5.221019
H -1.303492 -3.070082 -4.497554
H -1.700210 -3.055056 -6.224921
Ag 3.991116 1.198333 2.996054
S 3.076333 1.861188 5.189089
Ag 1.255428 0.155163 5.236770
C 2.161293 3.479197 5.093664
H 2.605240 4.064174 4.279931
H 2.366723 3.998515 6.041538
S 1.583093 4.450360 -2.683138
S -3.383378 3.280546 2.394733
S 2.946421 -2.972494 -2.502937
S -2.015253 -4.256777 2.003038
S 2.848326 4.327056 1.805418
S -2.925899 2.645102 -3.016741
S 2.459783 -2.159750 4.393161
S -1.222874 -4.199460 -2.001084
S 0.501523 0.947627 -5.004305
S -4.855324 -1.620294 -0.295813
S 4.952408 0.454134 0.846834
S -1.178744 -0.336787 5.368126
C -5.556620 0.084498 -0.423776
H -4.815759 0.735891 -0.910745
H -5.691004 0.472673 0.595527
C -0.016684 2.724800 -5.039689
H -0.321789 3.018978 -4.031482
H 0.874095 3.317845 -5.285099
C -1.143799 -2.180393 5.361889
H -0.574200 -2.523310 4.485865
H -2.183397 -2.522322 5.238162
C 5.105615 -1.387203 0.917406
H 4.258915 -1.808731 1.475296
H 5.017836 -1.759887 -0.114298
C -1.155140 -5.427966 3.127002
H -0.603963 -4.876654 3.894807
H -0.419615 -5.944149 2.494684
C 1.514301 -2.992192 -3.681963
H 0.810541 -2.193218 -3.404582
H 1.004562 -3.944247 -3.499310
C -4.436895 3.617051 0.904229

H -4.867974 2.685094 0.525910
H -3.772785 4.009676 0.122890
C 2.416535 5.953811 -2.020379
H 2.710323 5.804187 -0.974371
H 1.655336 6.748296 -2.028708
C -2.802146 -4.873553 -1.319556
H -2.847337 -4.634425 -0.251290
H -3.629187 -4.351650 -1.825141
C -4.715877 3.094499 -2.969880
H -5.034800 3.229563 -1.931250
H -5.278744 2.256014 -3.401315
C 4.263414 -1.901395 4.663346
H 4.745840 -1.706941 3.701814
H 4.370658 -0.999654 5.283991
C 4.090871 3.982536 0.491820
H 3.593835 3.840576 -0.477316
H 4.566240 3.030159 0.752501
C -1.150730 3.030085 -6.007749
H -0.833586 2.963138 -7.061960
H -1.977098 2.309762 -5.888046
C -1.759351 4.394613 -5.770721
O -1.405287 5.200711 -4.939064
O -2.798170 4.616680 -6.598448
H -3.149878 5.508117 -6.419761
C -2.579317 -4.684746 -5.092662
H -3.178320 -4.993111 -5.967160
H -3.210911 -4.829978 -4.205577
C -1.397321 -5.630440 -4.961544
O -1.436695 -6.706206 -4.381057
O -0.308839 -5.166876 -5.550761
H 0.525702 -5.636847 -5.282749
C -6.886131 0.156530 -1.175002
H -6.817219 -0.328703 -2.159845
H -7.673728 -0.353643 -0.596010
C -7.242056 1.617025 -1.349709
O -7.083391 2.445477 -0.471775
O -7.667732 1.923217 -2.571366
H -7.656726 2.913455 -2.684943
C -5.547058 4.633977 1.173507
H -5.160776 5.473201 1.777946
H -6.388101 4.186620 1.719145
C -6.031125 5.243536 -0.125039
O -5.282345 5.578561 -1.025272
O -7.350081 5.413242 -0.182986
H -7.583707 5.712851 -1.082432
C -1.991107 7.325719 2.098884
H -1.915719 8.369863 1.758083

H -1.039245 7.016118 2.552187
C -3.050427 7.223590 3.165871
O -2.916197 6.650341 4.235143
O -4.204207 7.786780 2.811326
H -4.857311 7.663589 3.526552
C -4.941145 4.375243 -3.767488
H -4.230274 5.153169 -3.447079
H -4.744045 4.214712 -4.840981
C -6.306527 5.000132 -3.643182
O -7.297083 4.516464 -3.110350
O -6.340512 6.203525 -4.204449
H -7.242085 6.569139 -4.128451
C -2.973717 -6.384607 -1.531092
H -3.875834 -6.702316 -0.985106
H -3.109988 -6.612728 -2.596701
C -1.804480 -7.179366 -0.974986
O -1.645535 -7.397926 0.208402
O -0.906104 -7.613863 -1.865654
H -1.110624 -7.305096 -2.780568
C 3.911090 -7.183862 -0.456866
H 4.962923 -7.498457 -0.418400
H 3.295411 -8.003075 -0.050582
C 3.577134 -6.993852 -1.912529
O 4.421133 -7.109735 -2.797526
O 2.320708 -6.670737 -2.157176
H 2.191584 -6.484212 -3.127693
C 1.856217 -2.842719 -5.163332
H 0.924665 -3.037487 -5.715570
H 2.134100 -1.796691 -5.374561
C 2.988291 -3.742950 -5.702864
H 2.824525 -3.939066 -6.776464
H 3.963551 -3.244976 -5.618022
C 3.115927 -5.078337 -5.018388
O 2.148138 -5.789531 -4.699658
O 4.346520 -5.435459 -4.765922
H 4.366920 -6.240056 -4.158790
C 7.182725 0.325700 -2.078958
H 7.655967 -0.058225 -2.999759
H 6.589453 -0.508880 -1.671083
C 8.295171 0.625892 -1.105912
O 8.641307 1.738864 -0.748556
O 8.902639 -0.478807 -0.676962
H 9.626766 -0.233945 -0.069710
C 6.423014 -1.838579 1.538504
H 7.278514 -1.651815 0.873876
H 6.625382 -1.290061 2.475122
C 6.393091 -3.293313 1.945180

O 5.391063 -3.900032 2.273368
O 7.607228 -3.847487 1.953222
H 7.532502 -4.765480 2.275159
C 4.918703 -3.099449 5.334545
H 4.732907 -4.014364 4.745763
H 4.511207 -3.284258 6.340205
C 6.419342 -2.951255 5.419616
O 7.080350 -2.167403 4.768856
O 6.963580 -3.820372 6.278831
H 7.932329 -3.704829 6.269210
C -6.837355 -2.652049 2.630837
H -5.971191 -3.126641 2.136859
H -7.063912 -3.263674 3.519284
C -7.981375 -2.764666 1.649559
O -8.544981 -1.831496 1.117467
O -8.294107 -4.042940 1.401911
H -9.013318 -4.066033 0.743456
C -0.566499 -2.819379 6.631080
H -1.134172 -2.488650 7.513594
H 0.494375 -2.557291 6.744624
C -0.734181 -4.314263 6.467558
O -1.815656 -4.872205 6.527520
O 0.391622 -4.944002 6.137057
H 0.169696 -5.871812 5.848055
C -2.119605 -6.439230 3.732673
H -2.844516 -5.933457 4.394522
H -2.688866 -6.949577 2.941607
C -1.427813 -7.477268 4.580836
O -0.361297 -7.327728 5.160442
O -2.113593 -8.611993 4.660068
H -1.643479 -9.228635 5.253656
C 3.628949 6.364292 -2.845522
H 4.406117 5.578859 -2.811732
H 3.374391 6.515602 -3.905603
C 4.296662 7.605622 -2.306006
O 4.154499 8.041170 -1.180865
O 5.115918 8.166831 -3.202728
H 5.557757 8.930442 -2.786210
C 5.179689 5.061940 0.393523
H 5.586618 5.265696 1.394776
H 4.790136 5.994809 -0.033066
C 6.275383 4.505729 -0.486864
O 6.360656 4.686953 -1.687673
O 7.084565 3.703026 0.201523
H 7.682157 3.166594 -0.377242
C 0.655663 3.336326 4.888507
H 0.164232 2.885000 5.761757

H 0.450730 2.652885 4.040818
C -0.070439 4.608077 4.503307
O 0.409680 5.488148 3.807889
O -1.319311 4.622395 4.945392
H -1.812999 5.424469 4.615292

[Ag₂₅(MPA)₁₈]⁻ B3LYP T₁ (acetonitrile)

Ag 0.058088 0.207819 0.245166
Ag 1.544486 2.175252 1.714408
Ag -2.059690 0.862954 -1.538927
Ag 1.648689 -0.718136 2.366018
Ag -1.130706 -1.777020 -1.449047
Ag 0.659951 2.891441 -0.908463
Ag 1.690728 -2.114165 -0.332171
Ag -1.201436 2.514641 1.267032
Ag -0.402839 -2.462352 1.478741
Ag 2.796797 0.829514 -0.701995
Ag -1.090356 0.090253 2.929622
Ag 0.651588 0.501465 -2.537112
Ag -2.738483 -0.849620 0.867901
Ag 2.284295 -3.932019 2.727107
S 2.046317 -5.830515 1.247946
Ag 0.479897 -5.020716 -0.440039
C 3.706789 -5.963011 0.444673
H 3.901945 -5.052948 -0.141891
H 4.438020 -5.978966 1.261101
Ag 0.898011 5.370859 0.799974
S -1.027621 6.346557 -0.353169
Ag -1.815442 4.491993 -1.770409
C -2.322512 6.369365 0.961103
H -2.415938 5.356944 1.369126
H -3.274448 6.634404 0.480532
Ag -3.960768 0.897583 3.143555
S -5.075186 -1.109344 4.055179
Ag -3.470705 -2.739668 3.186672
C -6.554315 -1.278587 2.946404
H -6.398441 -0.675233 2.046511
H -7.408133 -0.846117 3.488305
Ag 3.271808 2.771950 -3.164760
S 5.089692 1.232107 -3.753453
Ag 3.878192 -0.742437 -2.981253
C 6.327449 1.537200 -2.413050
H 5.802985 1.847893 -1.501607
H 6.951914 2.377630 -2.742373
Ag -1.662613 -0.204195 -4.794893
S -3.381507 -1.968892 -4.989568

Ag -3.960687 -1.874995 -2.622767
C -2.078822 -3.271034 -5.223235
H -1.293539 -3.089586 -4.483427
H -1.650992 -3.101355 -6.220165
Ag 3.959219 1.201525 2.960505
S 3.142737 1.901589 5.170971
Ag 1.316384 0.208521 5.318788
C 2.211987 3.509189 5.047837
H 2.649968 4.081944 4.222008
H 2.416236 4.046869 5.985590
S 1.585300 4.465255 -2.726217
S -3.336212 3.143996 2.408527
S 2.885789 -2.874854 -2.424419
S -2.006876 -4.287601 2.046858
S 2.929491 4.369959 1.744541
S -2.957673 2.679775 -2.969581
S 2.440692 -2.153040 4.387918
S -1.255491 -4.223754 -1.962396
S 0.462479 0.974084 -5.064391
S -4.826649 -1.593876 -0.364312
S 4.815144 0.421691 0.801794
S -1.108603 -0.248847 5.463348
C -5.547043 0.103948 -0.469132
H -4.813819 0.767206 -0.949318
H -5.683154 0.472876 0.556801
C -0.074786 2.745465 -5.062462
H -0.355814 3.026263 -4.043305
H 0.805343 3.347513 -5.323728
C -1.142642 -2.091343 5.420520
H -0.587363 -2.440521 4.537463
H -2.195054 -2.387686 5.288438
C 4.982700 -1.417029 0.884469
H 4.163469 -1.838513 1.480841
H 4.863074 -1.800335 -0.139467
C -1.137771 -5.479875 3.139710
H -0.581744 -4.941803 3.913891
H -0.409087 -5.989035 2.493835
C 1.474474 -2.953140 -3.628354
H 0.741571 -2.175515 -3.369179
H 0.994019 -3.920854 -3.446957
C -4.382459 3.545212 0.931763
H -4.817633 2.630812 0.517738
H -3.718038 3.968261 0.167225
C 2.440018 5.960257 -2.071056
H 2.730089 5.811168 -1.023606
H 1.693242 6.768517 -2.083761
C -2.830989 -4.912802 -1.285253

H -2.874934 -4.685563 -0.213914
H -3.661645 -4.391306 -1.785459
C -4.744814 3.137237 -2.913578
H -5.062310 3.249972 -1.872415
H -5.311930 2.311776 -3.363860
C 4.247513 -1.890960 4.632238
H 4.716002 -1.695762 3.664102
H 4.362393 -0.988576 5.250597
C 4.167129 4.017611 0.428168
H 3.663834 3.880755 -0.538267
H 4.635262 3.060845 0.688408
C -1.235084 3.054349 -5.996896
H -0.948731 2.983353 -7.059516
H -2.060927 2.338320 -5.850088
C -1.827392 4.423324 -5.745285
O -1.448271 5.225059 -4.919970
O -2.881332 4.656391 -6.549863
H -3.220550 5.551071 -6.362845
C -2.544605 -4.720849 -5.086412
H -3.132592 -5.040495 -5.964346
H -3.183213 -4.862473 -4.203634
C -1.356680 -5.656156 -4.937251
O -1.390999 -6.727570 -4.349283
O -0.267691 -5.185863 -5.521201
H 0.570631 -5.641983 -5.244938
C -6.879929 0.177302 -1.212761
H -6.809048 -0.273138 -2.213827
H -7.657931 -0.361622 -0.647146
C -7.255186 1.639004 -1.334667
O -7.090427 2.440111 -0.432808
O -7.703047 1.979949 -2.538668
H -7.694140 2.973233 -2.621139
C -5.489872 4.549740 1.252734
H -5.100913 5.361811 1.891790
H -6.327238 4.078588 1.783586
C -5.985461 5.217450 -0.012794
O -5.247145 5.578253 -0.911489
O -7.301814 5.408838 -0.038221
H -7.547836 5.756242 -0.916897
C -1.990625 7.334298 2.106907
H -1.959937 8.371714 1.740959
H -1.027026 7.070564 2.564259
C -3.049423 7.207011 3.170496
O -2.917557 6.599956 4.221726
O -4.202685 7.779674 2.831289
H -4.855466 7.639760 3.543848
C -4.964309 4.436601 -3.681628

H -4.243017 5.200924 -3.351571
H -4.779816 4.296457 -4.760116
C -6.322867 5.070680 -3.528992
O -7.311097 4.585322 -2.993975
O -6.351979 6.285610 -4.065296
H -7.249414 6.657471 -3.972050
C -2.989541 -6.422697 -1.512886
H -3.897937 -6.752723 -0.984629
H -3.107400 -6.641766 -2.582573
C -1.822734 -7.212797 -0.944641
O -1.677580 -7.433028 0.240100
O -0.910682 -7.640065 -1.824948
H -1.102487 -7.328144 -2.741369
C 3.870115 -7.236899 -0.411365
H 4.910382 -7.585094 -0.354472
H 3.216612 -8.039283 -0.032691
C 3.576600 -7.000224 -1.867875
O 4.451241 -7.056547 -2.728987
O 2.321435 -6.694260 -2.138458
H 2.218161 -6.474140 -3.105728
C 1.840943 -2.802678 -5.103760
H 0.929282 -3.038491 -5.672643
H 2.082593 -1.748534 -5.319300
C 3.016498 -3.662998 -5.610800
H 2.897188 -3.852447 -6.691493
H 3.973103 -3.137574 -5.486191
C 3.157934 -5.000764 -4.933515
O 2.199205 -5.737128 -4.646703
O 4.389016 -5.328773 -4.648120
H 4.413241 -6.144612 -4.054527
C 7.171208 0.308134 -2.115232
H 7.639079 -0.095380 -3.030421
H 6.558071 -0.509667 -1.702379
C 8.288314 0.591663 -1.142612
O 8.661970 1.699336 -0.796886
O 8.865239 -0.523253 -0.697977
H 9.592632 -0.289897 -0.090065
C 6.329869 -1.841483 1.459655
H 7.156690 -1.651382 0.760517
H 6.561123 -1.278324 2.380877
C 6.338019 -3.290774 1.886001
O 5.356343 -3.912279 2.245533
O 7.563223 -3.819199 1.873339
H 7.515452 -4.733956 2.209222
C 4.916081 -3.086687 5.294275
H 4.715342 -4.005029 4.715843
H 4.533596 -3.264318 6.311034

C 6.418612 -2.939545 5.340945
O 7.062853 -2.153490 4.676184
O 6.984015 -3.812365 6.182175
H 7.952304 -3.697471 6.148805
C -6.845662 -2.714092 2.537792
H -5.964784 -3.163195 2.045809
H -7.080420 -3.355934 3.402353
C -7.972156 -2.807692 1.534632
O -8.527318 -1.863683 1.012679
O -8.279871 -4.080360 1.254636
H -8.987775 -4.089545 0.583614
C -0.590928 -2.781226 6.672772
H -1.149570 -2.454730 7.563049
H 0.477226 -2.556337 6.797983
C -0.804691 -4.266715 6.474529
O -1.908581 -4.782566 6.464407
O 0.313125 -4.937766 6.206947
H 0.076148 -5.862401 5.914172
C -2.101804 -6.497835 3.737899
H -2.822584 -5.992090 4.404541
H -2.667954 -7.004558 2.943232
C -1.401618 -7.532302 4.582687
O -0.394970 -7.337881 5.250676
O -2.001677 -8.716358 4.553957
H -1.529271 -9.329181 5.149880
C 3.661161 6.346946 -2.895399
H 4.430301 5.553816 -2.849941
H 3.413943 6.488417 -3.958658
C 4.337336 7.589749 -2.369321
O 4.195350 8.040299 -1.250183
O 5.162035 8.134501 -3.271057
H 5.607534 8.900616 -2.863034
C 5.264488 5.087509 0.325063
H 5.674193 5.290734 1.325246
H 4.880666 6.021495 -0.103722
C 6.354141 4.518699 -0.554215
O 6.446612 4.702743 -1.753873
O 7.148352 3.700744 0.134746
H 7.738987 3.156700 -0.443613
C 0.707923 3.346985 4.850033
H 0.225955 2.901905 5.731576
H 0.507963 2.652252 4.010498
C -0.034877 4.606468 4.458294
O 0.427618 5.484182 3.748088
O -1.277274 4.612077 4.917406
H -1.786657 5.405041 4.588337

[Ag₂₅(MPA)₁₈]⁻ TPSSh S_o (gas)

Ag 0.050290 0.174664 0.441672
Ag 1.323319 2.042058 2.020298
Ag -1.928606 1.121480 -1.183421
Ag 1.846338 -0.780371 2.253461
Ag -1.144453 -1.655984 -1.258279
Ag 0.590931 2.694683 -0.624050
Ag 1.648806 -1.937813 -0.443326
Ag -1.421482 2.310372 1.381804
Ag -0.312758 -2.406442 1.471432
Ag 2.692976 0.739030 -0.194857
Ag -0.788569 0.074752 3.047794
Ag 0.724842 0.359830 -2.218388
Ag -2.569414 -0.601649 0.955310
Ag 2.285879 -3.635783 2.497387
S 1.946856 -5.522790 1.071612
Ag 0.342850 -4.651109 -0.514191
C 3.547482 -5.784273 0.202780
H 3.726429 -4.951921 -0.495529
H 4.325032 -5.751762 0.975729
Ag 0.568503 4.962885 1.143311
S -1.128518 6.087442 -0.144240
Ag -1.724902 4.182298 -1.542970
C -2.474879 6.514285 1.020512
H -2.805754 5.601660 1.532476
H -3.312888 6.901922 0.423982
Ag -3.608831 1.108385 3.132929
S -4.484812 -0.945908 4.079735
Ag -2.993210 -2.527915 3.036118
C -6.061673 -1.158308 3.134571
H -6.008325 -0.565470 2.215407
H -6.864410 -0.735273 3.755975
Ag 2.677340 2.538131 -2.667965
S 4.651886 1.340199 -3.411974
Ag 3.515538 -0.658310 -2.659203
C 5.950099 1.724168 -2.166258
H 5.478860 1.978925 -1.208901
H 6.486976 2.610678 -2.530239
Ag -1.752049 -0.008552 -3.793197
S -3.454195 -1.596683 -4.773107
Ag -3.787377 -1.640013 -2.380148
C -2.191644 -2.881535 -5.191577
H -1.357255 -2.779933 -4.488939
H -1.816358 -2.637810 -6.195095
Ag 3.804897 1.250750 3.139409

S 3.004355 1.957739 5.351908
Ag 1.398224 0.087092 5.031313
C 1.924763 3.465005 5.244599
H 2.233781 4.042783 4.363410
H 2.163617 4.059871 6.138681
S 1.059661 4.348107 -2.495282
S -3.396930 3.415483 2.396007
S 2.818759 -2.962806 -2.421660
S -1.834715 -4.299740 1.925894
S 2.686971 4.189346 2.026915
S -2.678349 2.552040 -3.092582
S 2.591823 -2.129644 4.365741
S -1.404312 -3.995366 -2.061044
S 0.568911 0.467556 -4.709021
S -4.676591 -1.467640 -0.121621
S 4.883594 0.493427 1.055705
S -0.995352 -0.435471 5.479963
C -5.444689 0.197018 -0.319123
H -4.691125 0.873403 -0.753649
H -5.691995 0.589213 0.677742
C 0.238031 2.232515 -5.137938
H -0.063664 2.775831 -4.233341
H 1.173991 2.685429 -5.494102
C -0.933785 -2.275399 5.398681
H -0.394922 -2.576397 4.484475
H -1.974327 -2.633546 5.321585
C 5.007603 -1.349452 1.019676
H 4.229149 -1.788036 1.663524
H 4.782618 -1.675073 -0.008023
C -0.981809 -5.457451 3.067175
H -0.421108 -4.894741 3.820916
H -0.262622 -6.004264 2.441693
C 1.424031 -2.985220 -3.643925
H 0.705258 -2.191539 -3.383567
H 0.913389 -3.943445 -3.488718
C -4.378518 3.693670 0.857055
H -4.746124 2.734042 0.480258
H -3.686261 4.106976 0.106839
C 1.999353 5.828383 -1.926893
H 2.302866 5.708370 -0.878261
H 1.289413 6.667231 -1.963802
C -2.930217 -4.711433 -1.307021
H -2.904399 -4.523633 -0.226103
H -3.793387 -4.175558 -1.735037
C -4.478108 2.951125 -3.155627
H -4.860194 3.064213 -2.134668
H -4.991734 2.113121 -3.645938

C 4.396619 -1.920426 4.636970
H 4.887752 -1.674951 3.690023
H 4.518296 -1.061590 5.313710
C 3.879758 3.956150 0.647837
H 3.343192 3.819925 -0.305411
H 4.427784 3.027119 0.854856
C -0.861336 2.360335 -6.189940
H -0.552073 1.892579 -7.141224
H -1.778957 1.845573 -5.866801
C -1.188820 3.809563 -6.464079
O -0.428250 4.743974 -6.360863
O -2.476530 3.976908 -6.871005
H -2.576765 4.934188 -7.033409
C -2.712699 -4.320092 -5.128763
H -3.329701 -4.562824 -6.011463
H -3.349298 -4.468096 -4.244859
C -1.583101 -5.329374 -5.026447
O -1.683311 -6.421611 -4.482799
O -0.466682 -4.904244 -5.603269
H 0.337678 -5.431378 -5.334406
C -6.699958 0.179889 -1.192493
H -6.528319 -0.369647 -2.130162
H -7.523156 -0.313562 -0.650944
C -7.057916 1.613131 -1.509960
O -6.918649 2.523981 -0.711765
O -7.456917 1.799888 -2.768890
H -7.447621 2.778762 -2.953901
C -5.540229 4.663921 1.063328
H -5.214861 5.532460 1.664239
H -6.383242 4.188782 1.581214
C -5.999988 5.188676 -0.276888
O -5.259835 5.403400 -1.221750
O -7.315480 5.439592 -0.334246
H -7.510137 5.644153 -1.268757
C -2.015043 7.519929 2.066990
H -1.611746 8.441946 1.618228
H -1.202736 7.088374 2.679015
C -3.138504 7.883390 3.006516
O -4.230144 7.355656 3.050542
O -2.796182 8.887797 3.844337
H -3.568264 9.030805 4.423503
C -4.641818 4.254909 -3.928261
H -4.003083 5.033481 -3.479074
H -4.297721 4.143990 -4.970662
C -6.027958 4.839420 -3.946787
O -7.060960 4.368421 -3.490870
O -6.042785 6.029052 -4.568364

H -6.964530 6.347056 -4.541637
C -3.069317 -6.213532 -1.582152
H -3.940746 -6.581732 -1.017790
H -3.233285 -6.394091 -2.654251
C -1.852266 -6.992383 -1.094098
O -1.630870 -7.207751 0.079631
O -1.008229 -7.418776 -2.042388
H -1.272951 -7.088469 -2.936507
C 3.589697 -7.150085 -0.518783
H 4.604801 -7.568479 -0.482625
H 2.901696 -7.853376 -0.021852
C 3.227780 -7.041739 -1.975792
O 4.014363 -7.351405 -2.871960
O 2.024346 -6.553348 -2.201322
H 1.880158 -6.426492 -3.181348
C 1.849434 -2.816286 -5.101192
H 0.949074 -2.980738 -5.710963
H 2.159886 -1.774066 -5.274569
C 2.992736 -3.730453 -5.576511
H 2.960895 -3.819376 -6.676503
H 3.972324 -3.305125 -5.317976
C 2.968469 -5.123649 -5.002363
O 1.926880 -5.767316 -4.771622
O 4.152952 -5.609329 -4.740698
H 4.072849 -6.447572 -4.170091
C 6.885741 0.542609 -1.966425
H 7.291444 0.187141 -2.930511
H 6.348629 -0.313448 -1.526982
C 8.060994 0.876996 -1.085283
O 8.437668 1.991810 -0.773341
O 8.723391 -0.221660 -0.678161
H 9.457905 0.085249 -0.112895
C 6.386634 -1.836727 1.452898
H 7.165099 -1.596630 0.715371
H 6.686867 -1.362682 2.404020
C 6.381058 -3.316690 1.737135
O 5.428236 -3.948841 2.155544
O 7.572052 -3.897002 1.507235
H 7.478228 -4.832309 1.769807
C 5.001303 -3.187236 5.232562
H 4.771147 -4.043882 4.574991
H 4.581070 -3.419036 6.221548
C 6.505044 -3.103891 5.314555
O 7.219640 -2.452987 4.579629
O 7.012026 -3.877211 6.298367
H 7.981847 -3.778672 6.247210
C -6.355279 -2.604138 2.763478

H -5.472721 -3.061863 2.280371
H -6.587248 -3.229145 3.641233
C -7.479857 -2.703342 1.760166
O -8.085408 -1.772437 1.274038
O -7.740873 -3.986596 1.428777
H -8.437391 -3.953014 0.746774
C -0.279464 -2.940310 6.617446
H -0.815194 -2.647327 7.531930
H 0.778799 -2.653817 6.686282
C -0.427623 -4.432167 6.407084
O -1.496622 -5.012650 6.480797
O 0.706193 -5.027339 6.017773
H 0.477033 -5.947331 5.706824
C -1.970859 -6.427307 3.698719
H -2.680349 -5.891764 4.352733
H -2.552509 -6.944337 2.920493
C -1.293860 -7.458250 4.562125
O -0.172847 -7.387294 5.042769
O -2.068307 -8.530713 4.784271
H -1.562114 -9.114230 5.380932
C 3.207911 6.079702 -2.820766
H 3.914764 5.231271 -2.770529
H 2.917138 6.184568 -3.876901
C 4.001377 7.286510 -2.387974
O 3.962704 7.807938 -1.292865
O 4.812505 7.736529 -3.368399
H 5.332903 8.460134 -2.972069
C 4.878195 5.120848 0.564462
H 5.283343 5.315957 1.567777
H 4.407151 6.031385 0.172779
C 5.995454 4.672552 -0.348951
O 6.050893 4.885140 -1.546835
O 6.874820 3.914159 0.315246
H 7.479843 3.432972 -0.301635
C 0.436386 3.142184 5.187628
H 0.031253 2.805493 6.152573
H 0.276437 2.279364 4.504081
C -0.463212 4.190626 4.583593
O -0.119288 5.068670 3.811249
O -1.743435 3.970968 4.914782
H -2.325126 4.464669 4.293975

[Ag₂₅(MPA)₁₈]⁻ TPSSh T₁ (gas)

Ag 0.009177 0.452905 0.294354
Ag 1.385066 2.334163 1.836304

Ag -1.983157 1.333943 -1.337736
Ag 1.926289 -0.455914 2.042207
Ag -1.175372 -1.448781 -1.259182
Ag 0.585723 2.903842 -0.806872
Ag 1.577157 -1.849670 -0.473882
Ag -1.300998 2.751540 1.217612
Ag -0.416308 -1.991396 1.505464
Ag 2.632834 0.834642 -0.600276
Ag -0.622215 0.490454 2.928059
Ag 0.544845 0.553935 -2.447950
Ag -2.667617 -0.212044 1.031634
Ag 2.067517 -3.276912 2.096656
S 2.181348 -5.459734 1.050191
Ag 0.260119 -4.414470 -0.192190
C 3.520779 -5.416204 -0.222059
H 3.321427 -4.602171 -0.933468
H 4.461490 -5.187616 0.299460
Ag 0.624603 5.154011 1.054190
S -1.278552 6.263711 -0.026704
Ag -1.859382 4.295502 -1.369131
C -2.525704 6.471711 1.306855
H -2.662849 5.513928 1.830821
H -3.477233 6.755184 0.831976
Ag -3.282115 0.991466 3.697474
S -4.575145 -1.071948 4.173518
Ag -2.914139 -2.372587 2.967016
C -6.008275 -1.088150 3.017603
H -5.768225 -0.472385 2.142962
H -6.859541 -0.624589 3.536403
Ag 2.614954 2.690912 -2.778590
S 4.594912 1.668963 -3.829642
Ag 3.183706 -0.258164 -3.222992
C 5.867662 1.516058 -2.503689
H 5.383320 1.610271 -1.521390
H 6.553249 2.366075 -2.618995
Ag -1.786109 0.651087 -4.149087
S -3.436073 -1.095482 -4.912040
Ag -3.694377 -1.137242 -2.516796
C -2.220264 -2.444820 -5.243189
H -1.416075 -2.385934 -4.499278
H -1.776865 -2.252930 -6.229540
Ag 3.723880 1.501459 3.247235
S 2.992764 2.304095 5.422991
Ag 1.424725 0.420444 4.898434
C 1.982242 3.831811 5.147533
H 2.384572 4.356530 4.270178
H 2.162356 4.459589 6.033405

S 1.005690 4.581480 -2.627971
S -3.273904 3.202220 2.631506
S 2.927037 -2.552279 -2.449830
S -1.595694 -4.169239 2.016751
S 2.827252 4.396406 1.836025
S -2.712566 2.909959 -3.232508
S 2.226250 -1.939832 4.199512
S -1.380111 -3.794909 -1.992588
S 0.622036 0.138061 -4.926932
S -4.633456 -1.122833 -0.276803
S 4.414099 0.476165 1.128465
S -1.101077 0.362665 5.422866
C -5.949951 0.135393 -0.586727
H -5.467568 1.043102 -0.970557
H -6.421587 0.371165 0.375717
C 1.228836 1.684569 -5.734116
H 2.207235 1.952172 -5.308824
H 1.396141 1.430020 -6.791369
C -1.296806 -1.461100 5.583983
H -0.962862 -1.923043 4.638492
H -2.364042 -1.685679 5.717681
C 5.117812 -1.225235 1.132228
H 4.464033 -1.910845 1.691341
H 5.111523 -1.552248 0.082294
C -0.699856 -5.089674 3.337414
H -0.243825 -4.390305 4.048619
H 0.108440 -5.633512 2.826486
C 1.598284 -3.108118 -3.613877
H 0.785766 -2.367628 -3.584052
H 1.201636 -4.053646 -3.217591
C -4.468279 3.151877 1.228844
H -4.260202 2.265214 0.612458
H -4.272150 4.031115 0.598350
C 2.090995 5.970158 -2.085796
H 2.294645 5.892746 -1.008182
H 1.507035 6.890155 -2.235370
C -2.905330 -4.545168 -1.262503
H -2.846179 -4.463620 -0.168862
H -3.778922 -3.970449 -1.605744
C -4.554198 2.954283 -3.294442
H -4.968543 2.327192 -2.498271
H -4.845678 2.516945 -4.258714
C 4.010773 -1.974818 4.656264
H 4.561018 -1.262017 4.026352
H 4.076390 -1.613814 5.692842
C 3.985055 4.037059 0.447416
H 3.519599 4.305725 -0.509528

H 4.170880 2.954543 0.432625
C 0.271682 2.859065 -5.606420
H -0.643899 2.719133 -6.201016
H -0.063851 2.966774 -4.558839
C 0.909178 4.184280 -5.948381
O 2.098783 4.405697 -6.017956
O -0.019016 5.147192 -6.136897
H 0.475717 5.979623 -6.252257
C -2.868643 -3.825484 -5.178990
H -3.548383 -3.989908 -6.033043
H -3.480185 -3.923452 -4.269206
C -1.861172 -4.953070 -5.137471
O -2.121553 -6.061909 -4.673676
O -0.689935 -4.635331 -5.646425
H 0.027524 -5.313349 -5.445333
C -7.032050 -0.367988 -1.568575
H -6.574602 -0.994875 -2.348045
H -7.785475 -0.940743 -1.014031
C -7.673348 0.830351 -2.229445
O -8.548138 1.525870 -1.726192
O -7.125909 1.104177 -3.405446
H -7.345883 2.042388 -3.671788
C -5.924353 3.142369 1.677888
H -6.164527 4.064738 2.233585
H -6.131767 2.298672 2.353563
C -6.818824 3.043163 0.457193
O -6.480870 3.453570 -0.642644
O -7.964798 2.414204 0.692502
H -8.377084 2.168714 -0.187551
C -2.075582 7.551657 2.307002
H -2.000047 8.527763 1.808337
H -1.105341 7.259327 2.731912
C -3.059780 7.625489 3.439300
O -3.050905 6.923572 4.438963
O -4.033794 8.530525 3.247374
H -4.635657 8.457128 4.012874
C -5.058036 4.382809 -3.150266
H -4.818616 4.782240 -2.153291
H -4.567083 5.046797 -3.883803
C -6.544785 4.526613 -3.354455
O -7.299381 3.708528 -3.857698
O -6.991242 5.729181 -2.972673
H -7.954505 5.727765 -3.129864
C -3.047142 -6.018372 -1.683034
H -3.831397 -6.483101 -1.064491
H -3.334558 -6.088098 -2.740648
C -1.757835 -6.789310 -1.433370

O -1.361871 -7.093978 -0.331202
O -1.023644 -7.101691 -2.527680
H -1.428880 -6.758682 -3.376720
C 3.661815 -6.752054 -0.946811
H 4.552662 -6.724935 -1.598628
H 3.831970 -7.576390 -0.234149
C 2.526426 -7.203927 -1.843981
O 2.584821 -8.230970 -2.506376
O 1.499452 -6.366850 -1.898537
H 0.707279 -6.776799 -2.342497
C 2.107787 -3.260035 -5.046701
H 1.238832 -3.405531 -5.703345
H 2.577705 -2.315060 -5.363405
C 3.111198 -4.400074 -5.233868
H 3.458922 -4.434449 -6.281850
H 4.005109 -4.248334 -4.610099
C 2.555203 -5.770799 -4.918256
O 1.380463 -6.109958 -5.019727
O 3.490449 -6.621524 -4.511215
H 3.061551 -7.443969 -4.160720
C 6.596419 0.181697 -2.593365
H 7.139020 0.087661 -3.550273
H 5.883795 -0.660418 -2.571212
C 7.584822 -0.020760 -1.475004
O 8.035543 0.850638 -0.749304
O 7.921998 -1.309793 -1.330599
H 8.493649 -1.409625 -0.538895
C 6.534357 -1.222645 1.705162
H 7.157196 -0.447649 1.238017
H 6.512977 -1.015271 2.788767
C 7.164939 -2.581537 1.555022
O 6.613022 -3.646123 1.715549
O 8.480723 -2.509995 1.199696
H 8.800401 -3.431939 1.149504
C 4.593131 -3.376917 4.530485
H 4.468085 -3.757046 3.498312
H 4.073321 -4.091936 5.184883
C 6.075162 -3.407220 4.805813
O 6.835563 -2.465980 4.698572
O 6.500417 -4.633364 5.169914
H 7.468404 -4.565908 5.270802
C -6.342285 -2.504687 2.571548
H -5.467936 -2.969043 2.082176
H -6.593287 -3.153624 3.427261
C -7.475137 -2.547098 1.578537
O -8.120345 -1.594238 1.193972
O -7.705737 -3.800847 1.132926

H -8.433978 -3.732627 0.487554
C -0.502170 -2.070380 6.742499
H -0.922367 -1.737185 7.704575
H 0.556286 -1.779534 6.693452
C -0.625368 -3.576457 6.623734
O -1.694807 -4.150500 6.501946
O 0.552477 -4.200545 6.581011
H 0.391250 -5.151392 6.322690
C -1.650283 -6.064637 4.028656
H -2.403785 -5.502387 4.606599
H -2.176731 -6.687092 3.291020
C -0.951379 -6.961758 5.014675
O 0.021990 -6.678680 5.697233
O -1.519930 -8.172898 5.106332
H -1.021701 -8.660005 5.790517
C 3.392521 6.002675 -2.880125
H 3.898787 5.018550 -2.835000
H 3.223500 6.186213 -3.951351
C 4.390563 6.986891 -2.322944
O 4.377984 7.444992 -1.199068
O 5.355028 7.285206 -3.215633
H 6.010246 7.825686 -2.735961
C 5.313239 4.784844 0.647636
H 5.630217 4.684385 1.695382
H 5.200031 5.844171 0.385063
C 6.333592 4.123655 -0.250952
O 6.543334 4.433131 -1.409393
O 6.908438 3.084919 0.368352
H 7.409790 2.502303 -0.253462
C 0.489362 3.564507 4.979010
H 0.045297 3.110386 5.874614
H 0.344885 2.835805 4.153125
C -0.309486 4.773791 4.552722
O 0.048827 5.535967 3.661277
O -1.453200 4.896809 5.205779
H -1.989978 5.658123 4.841037

[Ag₂₅(MPA)₁₈]⁻ TPSSh S_o (acetonitrile)

Ag 0.094329 0.201272 0.374432
Ag 1.383092 2.076960 1.943560
Ag -1.880812 1.144522 -1.251131
Ag 1.873235 -0.740398 2.201858
Ag -1.086853 -1.640096 -1.318040
Ag 0.637077 2.712907 -0.699745
Ag 1.689331 -1.935777 -0.496158

Ag -1.367617 2.366609 1.298317
Ag -0.273316 -2.368719 1.445572
Ag 2.749072 0.728372 -0.247156
Ag -0.780889 0.132434 2.960903
Ag 0.791583 0.367236 -2.273747
Ag -2.522335 -0.596020 0.873583
Ag 2.296335 -3.602850 2.432231
S 1.996284 -5.481040 0.980133
Ag 0.362237 -4.625919 -0.586711
C 3.607762 -5.721555 0.118252
H 3.770452 -4.887563 -0.580846
H 4.377856 -5.669547 0.896864
Ag 0.622107 4.939131 1.115227
S -1.105571 6.094920 -0.124270
Ag -1.692319 4.217925 -1.580654
C -2.454342 6.422504 1.072690
H -2.759918 5.457581 1.497801
H -3.299027 6.854846 0.518655
Ag -3.618676 1.048482 3.051866
S -4.483020 -1.022649 3.968035
Ag -2.953828 -2.572703 2.918290
C -6.072929 -1.275808 3.055054
H -6.049087 -0.676067 2.138915
H -6.872899 -0.880755 3.697321
Ag 2.746915 2.596813 -2.683750
S 4.677103 1.328002 -3.422360
Ag 3.546730 -0.689570 -2.723040
C 6.016447 1.641384 -2.198018
H 5.563161 1.915874 -1.237679
H 6.589549 2.500360 -2.571031
Ag -1.651120 0.010324 -3.849469
S -3.415239 -1.503584 -4.834036
Ag -3.736399 -1.584605 -2.438837
C -2.205103 -2.833662 -5.273640
H -1.356104 -2.746603 -4.586662
H -1.846564 -2.607956 -6.287183
Ag 3.843138 1.242557 3.097872
S 3.009280 1.950116 5.293281
Ag 1.326206 0.157434 4.950333
C 2.027909 3.519890 5.192753
H 2.448974 4.123891 4.378461
H 2.211058 4.042483 6.143079
S 1.159972 4.435737 -2.494968
S -3.371185 3.359407 2.366154
S 2.805126 -2.972295 -2.504574
S -1.690732 -4.344125 1.918874
S 2.783113 4.215663 1.968345

S -2.666571 2.593749 -3.118453
S 2.460149 -2.105946 4.330948
S -1.406958 -3.970055 -2.114078
S 0.653754 0.579399 -4.760209
S -4.629520 -1.475791 -0.175367
S 4.920986 0.478607 1.029030
S -1.097594 -0.217989 5.416925
C -5.432529 0.175552 -0.345668
H -4.705499 0.861783 -0.808061
H -5.649904 0.565075 0.659707
C 0.239117 2.350372 -5.097421
H -0.088738 2.825665 -4.163978
H 1.155382 2.863635 -5.421628
C -1.113492 -2.061473 5.441909
H -0.602419 -2.425208 4.534752
H -2.166838 -2.380641 5.400250
C 5.042081 -1.366099 1.035818
H 4.217754 -1.786540 1.633440
H 4.887628 -1.706454 0.000509
C -0.861615 -5.406644 3.169083
H -0.385114 -4.786138 3.935705
H -0.069575 -5.935003 2.619716
C 1.400113 -2.970437 -3.714761
H 0.699421 -2.162800 -3.446643
H 0.875191 -3.919327 -3.551076
C -4.369750 3.615210 0.825489
H -4.706916 2.652785 0.428679
H -3.698866 4.065787 0.077104
C 2.113867 5.883000 -1.864752
H 2.382448 5.736033 -0.809542
H 1.424578 6.738443 -1.910875
C -2.917993 -4.667524 -1.311104
H -2.849062 -4.497636 -0.229170
H -3.789109 -4.115762 -1.698180
C -4.474139 2.965087 -3.150254
H -4.838955 3.074464 -2.122212
H -4.976913 2.113289 -3.626757
C 4.254856 -1.906560 4.691743
H 4.783872 -1.661152 3.765228
H 4.348099 -1.050552 5.375532
C 3.962075 3.935787 0.585802
H 3.417968 3.848426 -0.368815
H 4.453771 2.972070 0.773060
C -0.862623 2.476640 -6.143888
H -0.510255 2.173189 -7.144686
H -1.712538 1.817221 -5.902260
C -1.394923 3.886337 -6.238431

O -0.864505 4.878042 -5.782810
O -2.563564 3.931836 -6.913212
H -2.833235 4.869062 -6.980860
C -2.765857 -4.254777 -5.188063
H -3.397021 -4.495589 -6.060497
H -3.393734 -4.380820 -4.293894
C -1.659720 -5.286637 -5.090859
O -1.797021 -6.390688 -4.570888
O -0.525774 -4.876298 -5.632034
H 0.268703 -5.428321 -5.376408
C -6.717039 0.128034 -1.176189
H -6.571922 -0.451466 -2.099493
H -7.521420 -0.348192 -0.593680
C -7.084879 1.551409 -1.526207
O -7.022944 2.469142 -0.722041
O -7.391785 1.718600 -2.808984
H -7.385423 2.700042 -3.027770
C -5.559729 4.539695 1.061388
H -5.270637 5.386050 1.710299
H -6.393268 4.022813 1.554644
C -6.034673 5.153008 -0.237786
O -5.312497 5.387389 -1.191280
O -7.330286 5.478126 -0.214054
H -7.557762 5.871879 -1.079635
C -2.005938 7.339090 2.221745
H -1.863878 8.370521 1.868487
H -1.074711 6.962731 2.665545
C -3.059286 7.304089 3.296806
O -2.985391 6.655444 4.333999
O -4.146378 8.010347 2.989918
H -4.804397 7.909679 3.707907
C -4.682407 4.257911 -3.931054
H -4.036346 5.052472 -3.526651
H -4.387676 4.125975 -4.985858
C -6.088084 4.802614 -3.921839
O -7.107121 4.226830 -3.558574
O -6.129984 6.043180 -4.402779
H -7.060861 6.344200 -4.413048
C -3.092715 -6.160723 -1.612282
H -3.950496 -6.529296 -1.028649
H -3.300257 -6.312128 -2.680818
C -1.875451 -6.971683 -1.196330
O -1.617943 -7.247576 -0.039598
O -1.061445 -7.370608 -2.180733
H -1.350664 -7.019790 -3.063428
C 3.696340 -7.084968 -0.593957
H 4.738669 -7.430494 -0.604588

H 3.095744 -7.835513 -0.053892
C 3.248487 -7.037792 -2.029714
O 3.969633 -7.405231 -2.959119
O 2.038370 -6.542166 -2.214790
H 1.850624 -6.448842 -3.190736
C 1.810371 -2.815164 -5.176964
H 0.894516 -2.942572 -5.772282
H 2.161016 -1.786241 -5.352987
C 2.908459 -3.771002 -5.678478
H 2.825917 -3.886527 -6.772685
H 3.908702 -3.362962 -5.479056
C 2.877917 -5.150151 -5.077500
O 1.838674 -5.779008 -4.800765
O 4.065222 -5.648674 -4.841035
H 3.989466 -6.497238 -4.294339
C 6.901549 0.420195 -2.013375
H 7.293246 0.056512 -2.979046
H 6.335120 -0.418338 -1.576139
C 8.093423 0.701407 -1.133654
O 8.472525 1.809290 -0.780409
O 8.740405 -0.411557 -0.787521
H 9.514612 -0.170203 -0.239218
C 6.382489 -1.850586 1.574234
H 7.205920 -1.652543 0.873642
H 6.634869 -1.338114 2.519351
C 6.339026 -3.320195 1.918686
O 5.331045 -3.927922 2.240623
O 7.544589 -3.892586 1.872460
H 7.457456 -4.825621 2.153805
C 4.827973 -3.173312 5.311244
H 4.616943 -4.039103 4.660090
H 4.377673 -3.391904 6.290552
C 6.330135 -3.096246 5.446835
O 7.049394 -2.340164 4.819697
O 6.804273 -3.991797 6.323217
H 7.779772 -3.918693 6.340090
C -6.322944 -2.730814 2.691325
H -5.438354 -3.156156 2.182795
H -6.510247 -3.359881 3.576226
C -7.474570 -2.877832 1.724103
O -8.122407 -1.961894 1.254833
O -7.695549 -4.164003 1.413046
H -8.430851 -4.200363 0.769397
C -0.454259 -2.684660 6.678395
H -0.973488 -2.353884 7.589990
H 0.608580 -2.412203 6.729132
C -0.616694 -4.180825 6.523799

O -1.703920 -4.738484 6.549244
O 0.521082 -4.816549 6.247217
H 0.298536 -5.753866 5.966672
C -1.853644 -6.399904 3.765481
H -2.607181 -5.870446 4.373686
H -2.386939 -6.937748 2.968237
C -1.197985 -7.406000 4.677691
O -0.181086 -7.219921 5.337626
O -1.851472 -8.563487 4.715654
H -1.403322 -9.156573 5.353063
C 3.351512 6.129737 -2.718372
H 4.054525 5.279595 -2.645718
H 3.092908 6.232862 -3.782946
C 4.129804 7.343602 -2.273674
O 4.028163 7.882327 -1.186222
O 4.986994 7.761122 -3.214902
H 5.492499 8.516754 -2.854099
C 5.026784 5.041528 0.526038
H 5.427824 5.211402 1.535753
H 4.612091 5.979237 0.135574
C 6.138065 4.545929 -0.369552
O 6.246378 4.803401 -1.556951
O 6.939155 3.706580 0.288937
H 7.540048 3.194477 -0.317219
C 0.531105 3.311324 4.980879
H 0.047560 2.843709 5.849227
H 0.371421 2.615103 4.127803
C -0.215167 4.561984 4.573785
O 0.248830 5.404641 3.812993
O -1.441219 4.620079 5.067368
H -1.933278 5.423963 4.713391

[Ag₂₅(MPA)₁₈]- TPSSh T₁ (acetonitrile)

Ag -0.007013 0.487957 0.273448
Ag 1.361143 2.358071 1.825958
Ag -2.006666 1.355392 -1.359680
Ag 1.906021 -0.436079 2.004214
Ag -1.184922 -1.411123 -1.284733
Ag 0.558099 2.929571 -0.828644
Ag 1.542695 -1.806090 -0.512355
Ag -1.325732 2.761049 1.211156
Ag -0.435616 -1.964767 1.470156
Ag 2.611073 0.866851 -0.630689
Ag -0.634984 0.508232 2.909033
Ag 0.525203 0.575574 -2.463291

Ag -2.672291 -0.163800 1.014454
Ag 2.042123 -3.245211 2.008060
S 2.249668 -5.446995 0.998734
Ag 0.293683 -4.409115 -0.197273
C 3.558315 -5.357265 -0.309059
H 3.302804 -4.545106 -1.002489
H 4.511488 -5.106714 0.177629
Ag 0.594028 5.147364 1.041481
S -1.320237 6.257691 -0.009462
Ag -1.934837 4.274098 -1.312197
C -2.550050 6.501358 1.336768
H -2.686537 5.548826 1.869742
H -3.502844 6.784235 0.865582
Ag -3.299692 0.996140 3.652244
S -4.547985 -1.079044 4.165612
Ag -2.891599 -2.352587 2.923051
C -5.998848 -1.087916 3.028390
H -5.757134 -0.466956 2.157831
H -6.840085 -0.622658 3.561039
Ag 2.593753 2.737279 -2.789593
S 4.569395 1.711782 -3.846102
Ag 3.127999 -0.207666 -3.266867
C 5.844794 1.517446 -2.525324
H 5.367062 1.666406 -1.546962
H 6.575209 2.323920 -2.669923
Ag -1.789541 0.721713 -4.159411
S -3.426538 -1.041651 -4.919670
Ag -3.689275 -1.081174 -2.525211
C -2.200437 -2.385646 -5.245722
H -1.385311 -2.293799 -4.516750
H -1.781948 -2.208112 -6.245439
Ag 3.698156 1.486855 3.224561
S 2.998835 2.300946 5.412313
Ag 1.434679 0.412863 4.846225
C 1.997738 3.839792 5.160322
H 2.405068 4.368926 4.288276
H 2.174946 4.456021 6.054107
S 1.028252 4.653723 -2.588172
S -3.300428 3.212885 2.620806
S 2.935122 -2.487555 -2.437226
S -1.565325 -4.163673 2.007845
S 2.809628 4.425719 1.836080
S -2.729857 2.953861 -3.245622
S 2.183205 -1.943446 4.141203
S -1.338828 -3.756879 -1.986440
S 0.607217 0.158781 -4.944639
S -4.592493 -1.150888 -0.274455

S 4.373102 0.480909 1.098468
S -1.094037 0.410650 5.409957
C -5.954992 0.063527 -0.560859
H -5.502259 0.990939 -0.933344
H -6.428805 0.271206 0.406918
C 1.220492 1.704441 -5.753941
H 2.221878 1.931835 -5.360452
H 1.334135 1.467269 -6.822010
C -1.298400 -1.410167 5.594315
H -0.977970 -1.880982 4.648636
H -2.365701 -1.625700 5.740249
C 5.077181 -1.221745 1.105202
H 4.420722 -1.902441 1.666343
H 5.067353 -1.550621 0.056157
C -0.669763 -5.046606 3.355787
H -0.227244 -4.326719 4.055022
H 0.151672 -5.585292 2.860072
C 1.681482 -3.145725 -3.633902
H 0.882640 -2.398242 -3.739655
H 1.248337 -4.047041 -3.180072
C -4.507966 3.199029 1.227143
H -4.236575 2.393877 0.528048
H -4.381004 4.148021 0.686127
C 2.131298 6.017458 -2.018344
H 2.318680 5.923149 -0.938737
H 1.567641 6.949322 -2.171667
C -2.883885 -4.483367 -1.271538
H -2.837589 -4.393957 -0.178171
H -3.746673 -3.903062 -1.629988
C -4.573709 2.950253 -3.322931
H -4.970952 2.285133 -2.549205
H -4.838461 2.535319 -4.304927
C 3.969066 -1.998588 4.602679
H 4.516836 -1.253904 4.008228
H 4.029177 -1.691835 5.656388
C 3.967316 4.035819 0.455279
H 3.506152 4.300059 -0.505175
H 4.135619 2.950367 0.452346
C 0.305813 2.904057 -5.564965
H -0.621767 2.814913 -6.150498
H -0.006248 2.987744 -4.507380
C 0.982074 4.217815 -5.879638
O 2.183306 4.386811 -5.967898
O 0.092058 5.211608 -6.015601
H 0.585729 6.044529 -6.151190
C -2.826845 -3.772428 -5.142882
H -3.519855 -3.966600 -5.979361

H -3.416325 -3.869367 -4.218023
C -1.801459 -4.880605 -5.114003
O -2.056121 -6.011215 -4.691779
O -0.625120 -4.534599 -5.584270
H 0.077312 -5.247577 -5.452401
C -7.026122 -0.462678 -1.543789
H -6.564823 -1.101192 -2.311134
H -7.785152 -1.032045 -0.994087
C -7.660909 0.727469 -2.222704
O -8.578557 1.393597 -1.752992
O -7.058306 1.034348 -3.361380
H -7.286284 1.974822 -3.634852
C -5.953851 3.032845 1.674419
H -6.282937 3.886542 2.290310
H -6.082450 2.129980 2.292415
C -6.842891 2.928718 0.453210
O -6.502081 3.318815 -0.652284
O -7.999545 2.314310 0.690961
H -8.418605 2.085166 -0.186625
C -2.080202 7.589844 2.314114
H -2.016352 8.564383 1.812776
H -1.097848 7.306839 2.719043
C -3.034308 7.663400 3.475031
O -3.063280 6.854773 4.397870
O -3.895581 8.672137 3.401918
H -4.497729 8.632043 4.173387
C -5.119433 4.358889 -3.149549
H -4.899911 4.743915 -2.141831
H -4.648497 5.053854 -3.866103
C -6.609433 4.465809 -3.363068
O -7.339442 3.604995 -3.839644
O -7.073082 5.663362 -3.019601
H -8.034895 5.689575 -3.198073
C -3.040040 -5.956335 -1.686884
H -3.832599 -6.412265 -1.073958
H -3.323836 -6.026069 -2.744987
C -1.758512 -6.730778 -1.436580
O -1.365808 -7.051228 -0.333376
O -1.012323 -7.029729 -2.521725
H -1.411827 -6.684454 -3.376321
C 3.680014 -6.691016 -1.044541
H 4.369620 -6.566974 -1.899176
H 4.097432 -7.475694 -0.398581
C 2.378417 -7.228652 -1.600643
O 2.072890 -8.406440 -1.603339
O 1.594266 -6.278087 -2.125987
H 0.712077 -6.671974 -2.362528

C 2.324380 -3.445933 -4.988932
H 1.529028 -3.581245 -5.735871
H 2.908195 -2.570387 -5.314865
C 3.237582 -4.670450 -4.971037
H 3.843352 -4.719655 -5.892730
H 3.957751 -4.621720 -4.138494
C 2.520137 -5.993643 -4.893945
O 1.339203 -6.202711 -5.151672
O 3.332826 -6.990601 -4.547191
H 2.825967 -7.827790 -4.554445
C 6.506838 0.148685 -2.578906
H 7.012825 -0.015441 -3.545417
H 5.760635 -0.659808 -2.490175
C 7.530110 -0.042898 -1.490522
O 8.000367 0.845388 -0.792092
O 7.869847 -1.323141 -1.343498
H 8.511254 -1.424553 -0.606017
C 6.491296 -1.217752 1.679177
H 7.116898 -0.446773 1.209763
H 6.469369 -1.000410 2.760559
C 7.123937 -2.579892 1.528942
O 6.536736 -3.634742 1.656961
O 8.435561 -2.501303 1.230701
H 8.801010 -3.407954 1.170170
C 4.552573 -3.390542 4.407344
H 4.440847 -3.718584 3.356583
H 4.029163 -4.137432 5.022352
C 6.032764 -3.437936 4.700791
O 6.767552 -2.468186 4.743860
O 6.466327 -4.691397 4.882127
H 7.433680 -4.664327 5.024237
C -6.344354 -2.499648 2.578091
H -5.481089 -2.970133 2.075892
H -6.598477 -3.148144 3.433143
C -7.495489 -2.522388 1.602937
O -8.160928 -1.555424 1.281588
O -7.705272 -3.750738 1.108612
H -8.463451 -3.708577 0.492505
C -0.494141 -2.010359 6.751249
H -0.895463 -1.662475 7.715854
H 0.567192 -1.735188 6.680111
C -0.639747 -3.513766 6.650952
O -1.724472 -4.076080 6.598044
O 0.520389 -4.152659 6.537924
H 0.340712 -5.111742 6.298514
C -1.614982 -6.026002 4.053531
H -2.354960 -5.467673 4.651465

H -2.160462 -6.632150 3.317136
C -0.900164 -6.947287 5.009354
O 0.028798 -6.631039 5.745449
O -1.386399 -8.184111 4.994975
H -0.906596 -8.718324 5.661055
C 3.442548 6.040578 -2.795211
H 3.951304 5.059043 -2.732285
H 3.278901 6.221967 -3.867418
C 4.427182 7.042185 -2.242380
O 4.379077 7.525190 -1.126016
O 5.401715 7.320515 -3.117690
H 6.039276 7.922053 -2.683872
C 5.308606 4.760669 0.650605
H 5.636188 4.647928 1.694009
H 5.214935 5.824302 0.398752
C 6.310045 4.093387 -0.263549
O 6.522154 4.426547 -1.416824
O 6.861054 3.029292 0.326600
H 7.359042 2.444954 -0.302968
C 0.507657 3.578486 4.978814
H 0.051162 3.138290 5.875109
H 0.363168 2.840342 4.160627
C -0.281341 4.785405 4.528869
O 0.139419 5.598106 3.711136
O -1.489334 4.840207 5.061643
H -2.019688 5.616795 4.696924

[Ag₂₅(MPA)₁₈]⁻ PBEh-3c S₀ (gas)

Ag 0.138842 0.271995 0.291849
Ag 1.512993 2.134583 1.909996
Ag -1.736507 1.334260 -1.448553
Ag 1.930365 -0.770854 2.135499
Ag -1.141601 -1.535079 -1.425020
Ag 0.762234 2.811228 -0.723212
Ag 1.673072 -1.917810 -0.629124
Ag -1.293915 2.453438 1.314710
Ag -0.411862 -2.280745 1.353004
Ag 2.862864 0.719687 -0.275769
Ag -0.694795 0.156675 2.921736
Ag 0.920512 0.448353 -2.412921
Ag -2.623878 -0.293141 0.742384
Ag 2.275727 -3.745583 2.347003
S 1.821395 -5.548906 0.857301
Ag 0.051302 -4.611977 -0.550043
C 3.270359 -5.831801 -0.222472

H 3.317957 -5.060754 -1.000829
H 4.168887 -5.712655 0.393634
Ag 0.886563 5.105678 1.404276
S -0.973548 6.174522 0.276752
Ag -1.607850 4.491128 -1.365105
C -2.266796 6.436759 1.530642
H -2.504440 5.485446 2.022917
H -3.170432 6.783930 1.014112
Ag -3.494186 0.882263 3.565573
S -4.664679 -1.206828 4.030141
Ag -3.263228 -2.633804 2.702569
C -6.253811 -1.183873 3.134002
H -6.074888 -1.031643 2.065262
H -6.837484 -0.329127 3.497408
Ag 2.870312 2.815349 -2.879370
S 4.790799 1.499830 -3.483056
Ag 3.823922 -0.607864 -2.854311
C 6.098328 2.011013 -2.318109
H 5.673525 2.235600 -1.333634
H 6.515478 2.939067 -2.724424
Ag -1.695089 0.929826 -4.337636
S -3.353861 -0.857678 -4.958043
Ag -3.816610 -1.059413 -2.607048
C -2.137932 -2.158898 -5.383525
H -1.353690 -2.194119 -4.621827
H -1.653890 -1.853385 -6.318511
Ag 4.019448 1.366196 3.156825
S 3.114434 1.780416 5.384175
Ag 1.382820 0.044018 5.062423
C 2.270370 3.411035 5.415626
H 2.652762 4.010664 4.583527
H 2.608771 3.903776 6.336274
S 1.085513 4.442788 -2.615101
S -3.233445 3.162779 2.721175
S 3.077077 -2.863417 -2.471782
S -1.815701 -4.311616 1.779384
S 3.027139 4.187672 2.111200
S -2.582936 3.067084 -3.121638
S 2.560070 -2.185629 4.185684
S -1.520564 -3.834474 -2.273034
S 0.706784 0.375804 -4.885011
S -4.722849 -1.198681 -0.343949
S 5.024665 0.660203 1.025406
S -1.102113 -0.126503 5.373549
C -5.966441 0.139400 -0.425348
H -5.505623 1.021136 -0.886034
H -6.231757 0.424327 0.599289

C 1.350747 1.864092 -5.728302
H 1.046311 2.775825 -5.201618
H 2.447520 1.825282 -5.716463
C -1.339956 -1.929223 5.543947
H -0.926792 -2.438982 4.663433
H -2.418865 -2.124309 5.568978
C 5.440193 -1.120025 1.048123
H 4.666896 -1.692751 1.570972
H 5.426302 -1.477098 0.009989
C -1.140586 -5.314899 3.147791
H -0.626750 -4.676572 3.873040
H -0.382641 -5.970696 2.700792
C 1.874039 -3.144803 -3.828224
H 1.206379 -2.282648 -3.929958
H 1.247375 -3.993846 -3.528592
C -4.448461 3.312948 1.363902
H -4.308562 2.495593 0.644707
H -4.223682 4.238934 0.819678
C 1.955848 5.949118 -2.049339
H 2.534369 5.734541 -1.146220
H 1.189495 6.680652 -1.765074
C -3.079015 -4.561428 -1.637363
H -3.070042 -4.562920 -0.542142
H -3.925186 -3.937373 -1.948347
C -4.410575 3.065385 -3.083640
H -4.772695 2.533275 -2.198849
H -4.742682 2.503986 -3.964278
C 4.338337 -2.093457 4.583912
H 4.904980 -1.790274 3.700912
H 4.461400 -1.300838 5.332799
C 4.163292 4.164507 0.688932
H 3.624303 3.941519 -0.240084
H 4.877932 3.348108 0.848161
C 0.855234 1.908254 -7.160901
H 1.117879 0.983230 -7.695476
H -0.244464 1.949500 -7.192713
C 1.393686 3.081797 -7.935861
O 2.124273 3.925964 -7.508139
O 0.957554 3.087745 -9.198057
H 1.326163 3.858166 -9.639210
C -2.781195 -3.530220 -5.519662
H -3.387306 -3.587673 -6.437569
H -3.481698 -3.711551 -4.694837
C -1.808924 -4.684282 -5.523723
O -2.123473 -5.805913 -5.185670
O -0.614115 -4.376174 -5.945878
H 0.048021 -5.091025 -5.813130

C -7.238397 -0.283437 -1.181410
H -6.995190 -1.057645 -1.919606
H -7.970259 -0.697222 -0.480153
C -7.814036 0.911727 -1.896952
O -8.666401 1.640297 -1.445922
O -7.233384 1.116239 -3.054910
H -7.383279 2.026619 -3.387483
C -5.888668 3.329005 1.844714
H -6.082947 4.228317 2.448776
H -6.093582 2.475628 2.504704
C -6.844049 3.300482 0.672836
O -6.573599 3.765883 -0.404480
O -7.975368 2.688616 0.943818
H -8.456928 2.472787 0.118035
C -1.820161 7.463798 2.573112
H -1.745374 8.458468 2.115265
H -0.837758 7.194056 2.974060
C -2.784606 7.491464 3.723115
O -2.616380 6.949444 4.785712
O -3.899792 8.155580 3.457983
H -4.491035 8.085557 4.214162
C -4.950677 4.481634 -3.096047
H -4.682284 5.009814 -2.171784
H -4.487652 5.057627 -3.913769
C -6.439937 4.579824 -3.282392
O -7.160616 3.709067 -3.699960
O -6.902466 5.784624 -3.003991
H -7.856535 5.784620 -3.126744
C -3.292848 -5.979212 -2.166180
H -4.125260 -6.431226 -1.610054
H -3.578735 -5.952484 -3.223132
C -2.068771 -6.847543 -1.945933
O -1.744257 -7.247863 -0.866214
O -1.333536 -7.132570 -3.015400
H -1.643180 -6.696197 -3.838654
C 3.290342 -7.229762 -0.817990
H 4.270199 -7.404873 -1.286530
H 3.211413 -7.986026 -0.023111
C 2.260251 -7.606843 -1.858552
O 2.273092 -8.665494 -2.426935
O 1.365292 -6.669458 -2.102389
H 0.620793 -7.004480 -2.631996
C 2.551037 -3.397325 -5.165523
H 1.782593 -3.397862 -5.948498
H 3.204124 -2.546724 -5.403146
C 3.379498 -4.669368 -5.221954
H 3.941806 -4.716817 -6.168079

H 4.138936 -4.671610 -4.428487
C 2.587947 -5.947243 -5.137497
O 1.420329 -6.070601 -5.420522
O 3.322549 -6.968894 -4.749184
H 2.783778 -7.763601 -4.640143
C 7.169391 0.951967 -2.168013
H 7.528221 0.618393 -3.155424
H 6.765873 0.054951 -1.679023
C 8.368608 1.439578 -1.400063
O 8.682959 2.587682 -1.250031
O 9.099301 0.440903 -0.916127
H 9.854995 0.806282 -0.445922
C 6.799306 -1.375100 1.672228
H 7.598156 -0.902013 1.087698
H 6.856359 -0.925160 2.676809
C 7.085561 -2.842953 1.850753
O 6.253189 -3.701104 1.954481
O 8.386470 -3.104733 1.901502
H 8.501380 -4.043157 2.076333
C 4.845917 -3.419637 5.113445
H 4.678627 -4.217143 4.372135
H 4.287216 -3.730089 6.006623
C 6.320159 -3.407147 5.410948
O 7.105181 -2.594631 5.011337
O 6.689254 -4.436871 6.169723
H 7.639658 -4.388634 6.306636
C -7.010608 -2.478504 3.355135
H -6.415969 -3.337480 3.006147
H -7.173704 -2.664146 4.426592
C -8.334471 -2.524730 2.640377
O -8.743391 -1.699392 1.876466
O -9.028017 -3.621199 2.944677
H -9.849063 -3.610187 2.444502
C -0.702233 -2.512325 6.803636
H -1.205804 -2.116110 7.694397
H 0.360463 -2.249601 6.859498
C -0.873962 -4.011629 6.742685
O -1.936732 -4.561987 6.854454
O 0.251862 -4.646914 6.466759
H 0.064705 -5.573132 6.227714
C -2.232792 -6.136626 3.805769
H -2.980296 -5.483886 4.284052
H -2.782701 -6.715848 3.051057
C -1.736064 -7.072346 4.871860
O -0.643860 -7.050540 5.379114
O -2.648463 -7.963198 5.224398
H -2.296218 -8.496698 5.942918

C 2.859853 6.503300 -3.131907
H 3.600936 5.755783 -3.450387
H 2.287880 6.747758 -4.038741
C 3.624359 7.719156 -2.683315
O 3.587809 8.201066 -1.587501
O 4.368536 8.228958 -3.662090
H 4.865346 8.970663 -3.306425
C 4.928658 5.479768 0.543193
H 5.404335 5.735001 1.497711
H 4.258325 6.300168 0.261964
C 5.964976 5.276243 -0.531724
O 5.777766 5.459827 -1.704168
O 7.087424 4.773733 -0.042456
H 7.664495 4.442523 -0.743385
C 0.749390 3.354274 5.396824
H 0.346952 2.979871 6.345132
H 0.402251 2.641563 4.631889
C 0.072913 4.646549 5.000362
O 0.464619 5.345122 4.095059
O -1.012755 4.896581 5.686491
H -1.501619 5.668382 5.330624

[Ag₂₅(MPA)₁₈]⁻ PBEh-3c T₁ (gas)

Ag 0.087996 0.189803 0.270161
Ag 1.429616 2.093387 1.871524
Ag -1.827263 1.240919 -1.467090
Ag 2.061014 -0.786238 2.038963
Ag -1.208012 -1.605278 -1.412668
Ag 0.669685 2.729003 -0.777889
Ag 1.552803 -2.048665 -0.679916
Ag -1.275272 2.432112 1.278840
Ag -0.371640 -2.311945 1.418870
Ag 2.822247 0.673735 -0.573965
Ag -0.566310 0.120896 2.926677
Ag 0.732386 0.350346 -2.502147
Ag -2.683209 -0.398015 0.955519
Ag 2.228660 -3.705489 2.340910
S 1.838197 -5.527640 0.838348
Ag -0.055916 -4.679853 -0.488691
C 3.246310 -5.751210 -0.307749
H 3.228668 -4.982323 -1.089440
H 4.168629 -5.597084 0.264065
Ag 0.798344 5.016791 1.459227
S -0.966750 6.168813 0.222016
Ag -1.533486 4.502982 -1.473174

C -2.352358 6.362422 1.388730
H -2.560102 5.404665 1.881948
H -3.243427 6.645215 0.814200
Ag -3.291878 0.767332 3.715999
S -4.681018 -1.257992 4.076101
Ag -3.232725 -2.685206 2.791315
C -6.221163 -1.162578 3.104310
H -5.989628 -0.994095 2.048172
H -6.792264 -0.294624 3.456627
Ag 2.810261 2.521826 -2.791972
S 4.864868 1.541039 -3.772988
Ag 3.637306 -0.466727 -3.138981
C 6.129983 1.780013 -2.477750
H 5.661680 1.863120 -1.488565
H 6.608391 2.743724 -2.686633
Ag -1.805691 0.902334 -4.390593
S -3.407083 -0.927394 -5.063844
Ag -3.805456 -1.065943 -2.706964
C -2.185822 -2.241604 -5.427839
H -1.414117 -2.254219 -4.651697
H -1.685667 -1.970123 -6.364739
Ag 3.766365 1.580507 3.532204
S 2.905648 2.001331 5.763064
Ag 1.444286 0.096738 5.067830
C 1.952588 3.561017 5.584980
H 2.377041 4.138227 4.756138
H 2.151535 4.135148 6.499628
S 1.122595 4.355935 -2.645398
S -3.179619 3.037161 2.723511
S 2.991709 -2.734963 -2.595000
S -1.774278 -4.357511 1.855951
S 2.979642 4.061544 2.163279
S -2.654872 3.017838 -3.101546
S 2.517439 -2.174781 4.224928
S -1.640056 -3.900690 -2.214955
S 0.591711 0.347373 -4.988414
S -4.652338 -1.146828 -0.439379
S 4.375532 0.439060 1.410707
S -1.102098 -0.038259 5.380697
C -5.919855 0.169188 -0.507548
H -5.467345 1.069273 -0.939854
H -6.208770 0.420506 0.519228
C 1.269677 1.872993 -5.735450
H 0.989844 2.756114 -5.150046
H 2.365421 1.809955 -5.730740
C -1.358747 -1.834062 5.593331
H -0.971081 -2.363591 4.712811

H -2.437933 -2.019608 5.648648
C 5.554283 -0.952025 1.378259
H 5.140999 -1.811961 1.915252
H 5.658662 -1.258067 0.330037
C -1.077072 -5.335548 3.232601
H -0.574445 -4.678797 3.949461
H -0.308502 -5.984967 2.794165
C 1.778658 -3.160252 -3.904775
H 1.075096 -2.333443 -4.048055
H 1.193351 -4.015062 -3.542900
C -4.445252 3.137465 1.411363
H -4.484563 2.186819 0.866758
H -4.128634 3.898289 0.686673
C 2.056095 5.810954 -2.048240
H 2.432199 5.637161 -1.034823
H 1.342875 6.641287 -1.971894
C -3.191408 -4.631719 -1.569184
H -3.172904 -4.636608 -0.473558
H -4.040644 -4.007537 -1.872342
C -4.479450 3.117588 -3.052638
H -4.863335 2.567254 -2.188829
H -4.846638 2.612635 -3.953054
C 4.282038 -2.048622 4.674593
H 4.756497 -1.250955 4.093338
H 4.309077 -1.724530 5.722224
C 4.120367 4.006644 0.738841
H 3.559528 4.008322 -0.202676
H 4.659976 3.054434 0.788445
C 0.771326 2.019322 -7.160382
H 1.011070 1.124519 -7.753968
H -0.327164 2.087317 -7.184780
C 1.333057 3.226767 -7.863671
O 2.090189 4.022363 -7.392044
O 0.883305 3.325453 -9.117663
H 1.267344 4.113133 -9.512666
C -2.839742 -3.611412 -5.525821
H -3.450916 -3.686540 -6.439081
H -3.537237 -3.765153 -4.692877
C -1.879569 -4.774452 -5.504693
O -2.203950 -5.884808 -5.140315
O -0.683029 -4.485877 -5.934886
H -0.024029 -5.201628 -5.792352
C -7.170587 -0.253898 -1.295794
H -6.899043 -0.949495 -2.098986
H -7.877694 -0.754501 -0.626647
C -7.796206 0.979521 -1.895063
O -8.602319 1.681269 -1.330896

O -7.308587 1.257339 -3.079772
H -7.467643 2.191613 -3.333210
C -5.828904 3.487648 1.940485
H -5.821972 4.506695 2.352901
H -6.120855 2.809303 2.750890
C -6.813915 3.411571 0.795376
O -6.618883 3.952654 -0.263019
O -7.855974 2.654448 1.053262
H -8.339336 2.428434 0.229216
C -2.037024 7.428054 2.440288
H -1.993712 8.418659 1.969684
H -1.067143 7.221778 2.903497
C -3.074984 7.410900 3.523770
O -2.947656 6.892407 4.604192
O -4.208770 8.001039 3.175011
H -4.842842 7.906459 3.892837
C -4.950691 4.556550 -2.996672
H -4.642541 5.032291 -2.056046
H -4.477043 5.146561 -3.797812
C -6.438658 4.726963 -3.143016
O -7.211695 3.894207 -3.544676
O -6.834285 5.949537 -2.842827
H -7.791254 5.994403 -2.928347
C -3.393475 -6.048347 -2.105513
H -4.221720 -6.514194 -1.554433
H -3.677011 -6.016949 -3.163144
C -2.157959 -6.902401 -1.887506
O -1.821541 -7.287469 -0.805440
O -1.427003 -7.190140 -2.957940
H -1.742145 -6.761545 -3.783338
C 3.297031 -7.149385 -0.899947
H 4.247738 -7.272438 -1.440722
H 3.318666 -7.904586 -0.101268
C 2.216373 -7.584939 -1.863723
O 2.209063 -8.670739 -2.377032
O 1.307946 -6.661839 -2.115636
H 0.550690 -7.023045 -2.608342
C 2.454346 -3.464520 -5.232795
H 1.684776 -3.514297 -6.012741
H 3.092775 -2.615632 -5.512007
C 3.302495 -4.724522 -5.234177
H 3.886478 -4.791503 -6.165859
H 4.046363 -4.692008 -4.426311
C 2.529581 -6.012141 -5.130803
O 1.362789 -6.156777 -5.405815
O 3.281340 -7.019568 -4.736035
H 2.753725 -7.821080 -4.623758

C 7.152790 0.659100 -2.469579
H 7.625219 0.566187 -3.460623
H 6.675042 -0.312575 -2.285098
C 8.249299 0.872887 -1.461188
O 8.604485 1.938327 -1.034768
O 8.817945 -0.262665 -1.077203
H 9.487467 -0.074826 -0.410309
C 6.895453 -0.543810 1.957292
H 7.293025 0.343263 1.448197
H 6.784731 -0.249406 3.013610
C 7.894017 -1.668443 1.933350
O 7.621379 -2.833361 1.914724
O 9.156975 -1.234707 1.957785
H 9.735175 -2.001163 2.018796
C 5.031905 -3.354759 4.509560
H 5.014067 -3.692976 3.460160
H 4.555201 -4.160549 5.083884
C 6.486249 -3.248371 4.886740
O 7.094129 -2.224176 5.018921
O 7.048612 -4.441474 5.045392
H 7.984717 -4.317465 5.224680
C -7.028698 -2.435413 3.266551
H -6.444461 -3.305764 2.927404
H -7.241825 -2.634769 4.326415
C -8.319679 -2.431317 2.493973
O -8.652055 -1.603354 1.696158
O -9.080185 -3.486314 2.784573
H -9.875912 -3.444854 2.246420
C -0.695417 -2.402772 6.845884
H -1.183940 -2.001214 7.742942
H 0.367143 -2.136908 6.882573
C -0.862087 -3.903837 6.800157
O -1.927369 -4.454258 6.886460
O 0.271933 -4.541405 6.570224
H 0.093580 -5.473226 6.346494
C -2.154778 -6.166161 3.903293
H -2.918734 -5.517915 4.361399
H -2.687452 -6.775109 3.159869
C -1.644784 -7.060931 4.997546
O -0.564753 -6.986905 5.525721
O -2.530540 -7.977122 5.352723
H -2.173739 -8.481244 6.090006
C 3.197626 6.159109 -2.983667
H 3.898107 5.316006 -3.087191
H 2.832053 6.351565 -4.002206
C 4.011317 7.331586 -2.506069
O 3.900503 7.866214 -1.439616

O 4.897132 7.726726 -3.415655
H 5.435627 8.422484 -3.029283
C 5.115788 5.166385 0.757026
H 5.547192 5.265472 1.760737
H 4.626357 6.110329 0.491705
C 6.193653 4.843954 -0.246492
O 6.176987 5.174764 -1.400711
O 7.129573 4.066715 0.277207
H 7.713864 3.696478 -0.399820
C 0.451407 3.386517 5.407750
H -0.016712 2.984560 6.313145
H 0.250246 2.652538 4.612425
C -0.256990 4.635033 4.938739
O 0.132883 5.294358 4.001193
O -1.346106 4.908153 5.605991
H -1.841395 5.657954 5.211276

[Ag₂₅(MPA)₁₈]⁻ PBEh-3c S₀ (acetonitrile)

Ag 0.098791 0.260992 0.317114
Ag 1.427719 2.139986 1.925948
Ag -1.781132 1.297266 -1.454917
Ag 1.897640 -0.782428 2.147728
Ag -1.146636 -1.552547 -1.425744
Ag 0.698007 2.794358 -0.723177
Ag 1.655285 -1.914109 -0.611884
Ag -1.394487 2.401558 1.301913
Ag -0.420624 -2.307543 1.358575
Ag 2.819834 0.732833 -0.249418
Ag -0.773537 0.127536 2.960893
Ag 0.901459 0.430747 -2.394966
Ag -2.632000 -0.343083 0.736671
Ag 2.248817 -3.772670 2.284666
S 1.899425 -5.649467 0.845009
Ag 0.113031 -4.676086 -0.516066
C 3.338350 -5.836195 -0.273487
H 3.315040 -5.049796 -1.035494
H 4.252847 -5.690115 0.311851
Ag 0.816405 5.130034 1.345806
S -1.024050 6.236913 0.245749
Ag -1.662730 4.512118 -1.352756
C -2.302832 6.504157 1.515954
H -2.561244 5.544370 1.978388
H -3.197051 6.889691 1.010442
Ag -3.774458 0.955021 3.269445
S -4.640598 -1.180714 3.968109

Ag -3.231513 -2.654680 2.693506
C -6.284467 -1.336876 3.181154
H -6.174089 -1.278657 2.092923
H -6.890063 -0.482091 3.505188
Ag 2.854597 2.815950 -2.850159
S 4.788883 1.522614 -3.440493
Ag 3.832738 -0.589593 -2.815301
C 6.108691 2.014212 -2.277130
H 5.682845 2.233658 -1.291836
H 6.530552 2.940833 -2.681618
Ag -1.719478 0.956321 -4.342588
S -3.369984 -0.879858 -4.897388
Ag -3.857855 -1.078032 -2.550087
C -2.123303 -2.149913 -5.335938
H -1.333231 -2.154782 -4.579494
H -1.659640 -1.825762 -6.274700
Ag 3.941185 1.335006 3.213924
S 3.093764 1.780786 5.454880
Ag 1.434649 -0.018770 5.067249
C 2.212352 3.392736 5.477112
H 2.611635 4.003196 4.661815
H 2.506388 3.883295 6.413493
S 1.046983 4.420879 -2.614364
S -3.378660 3.227412 2.560418
S 3.097702 -2.842947 -2.411750
S -1.800029 -4.358781 1.783466
S 2.911507 4.217863 2.150305
S -2.614909 3.059380 -3.093027
S 2.540747 -2.247994 4.155517
S -1.425164 -3.866807 -2.251263
S 0.664728 0.340645 -4.856960
S -4.743566 -1.238610 -0.283764
S 4.956939 0.711028 1.075151
S -1.032218 -0.227926 5.418213
C -5.925554 0.157678 -0.277261
H -5.455969 1.016814 -0.770371
H -6.098657 0.456284 0.764608
C 1.371620 1.793816 -5.711648
H 1.083812 2.721111 -5.203214
H 2.465665 1.716925 -5.673184
C -1.247518 -2.035165 5.559456
H -0.808476 -2.525179 4.679993
H -2.324745 -2.242326 5.554732
C 5.465917 -1.045701 1.067191
H 4.702023 -1.671602 1.541493
H 5.514050 -1.367466 0.019001
C -1.148663 -5.367848 3.160419

H -0.635863 -4.731708 3.887885
H -0.391351 -6.030002 2.722242
C 1.962418 -3.179269 -3.815083
H 1.305006 -2.318740 -3.979257
H 1.323356 -4.017723 -3.513044
C -4.545067 3.525028 1.183676
H -4.445216 2.739608 0.424837
H -4.234652 4.460902 0.701836
C 1.899591 5.945951 -2.071577
H 2.498841 5.741178 -1.179569
H 1.125303 6.665870 -1.781100
C -2.999790 -4.602065 -1.665789
H -3.022035 -4.608820 -0.570900
H -3.838899 -3.981754 -2.001294
C -4.443739 3.105798 -3.089370
H -4.823245 2.727553 -2.135930
H -4.778644 2.424614 -3.879262
C 4.325710 -2.189539 4.541993
H 4.876494 -1.798743 3.683275
H 4.451252 -1.473062 5.362558
C 4.077358 4.177766 0.750515
H 3.558703 3.907998 -0.177982
H 4.804339 3.382241 0.951066
C 0.910018 1.828745 -7.155178
H 1.163274 0.890269 -7.670193
H -0.186733 1.903704 -7.214360
C 1.499628 2.972495 -7.937051
O 2.251896 3.796522 -7.492121
O 1.091345 2.974244 -9.196751
H 1.482042 3.714799 -9.676113
C -2.717583 -3.541933 -5.470449
H -3.334478 -3.620556 -6.379540
H -3.395195 -3.761274 -4.635147
C -1.698857 -4.653053 -5.509558
O -1.978500 -5.803909 -5.226128
O -0.513201 -4.287038 -5.894211
H 0.174057 -4.995302 -5.810997
C -7.259559 -0.203928 -0.945517
H -7.103563 -0.985866 -1.700031
H -7.964653 -0.594383 -0.204164
C -7.832507 1.014548 -1.626344
O -8.725307 1.690545 -1.186910
O -7.192820 1.272247 -2.748360
H -7.348511 2.177641 -3.102515
C -5.980985 3.634260 1.652410
H -6.081580 4.405041 2.431348
H -6.318587 2.701519 2.129187

C -6.927198 3.968838 0.527633
O -6.580833 4.195414 -0.600384
O -8.186827 3.990874 0.918807
H -8.767427 4.152875 0.165050
C -1.827304 7.488521 2.584592
H -1.718977 8.493610 2.160176
H -0.855077 7.177597 2.982507
C -2.797873 7.500361 3.732284
O -2.724653 6.761378 4.688542
O -3.775035 8.362475 3.586915
H -4.394518 8.316565 4.327097
C -4.935408 4.517951 -3.334131
H -4.620208 5.188289 -2.523160
H -4.479229 4.927311 -4.249554
C -6.424465 4.651616 -3.504773
O -7.199161 3.743113 -3.694222
O -6.810487 5.906405 -3.490459
H -7.762509 5.974154 -3.635531
C -3.197533 -6.014811 -2.213363
H -4.029887 -6.483975 -1.672082
H -3.479717 -5.977905 -3.270388
C -1.967566 -6.869018 -2.005648
O -1.636427 -7.288278 -0.929951
O -1.222355 -7.128745 -3.070419
H -1.529197 -6.679057 -3.892246
C 3.376906 -7.222177 -0.896323
H 4.199686 -7.251724 -1.629277
H 3.607540 -7.985301 -0.144181
C 2.125292 -7.663343 -1.612948
O 1.687390 -8.780982 -1.559451
O 1.568146 -6.709233 -2.339375
H 0.716819 -7.005026 -2.705697
C 2.717919 -3.486067 -5.098316
H 2.015490 -3.442315 -5.940444
H 3.442795 -2.683710 -5.291076
C 3.460368 -4.809861 -5.095890
H 4.174360 -4.849522 -5.932836
H 4.077825 -4.914297 -4.191992
C 2.599650 -6.032747 -5.234261
O 1.432410 -6.044321 -5.558711
O 3.263196 -7.144115 -5.009846
H 2.704568 -7.916367 -5.162209
C 7.175563 0.949088 -2.145594
H 7.540011 0.633330 -3.136236
H 6.772207 0.040740 -1.676710
C 8.375133 1.416872 -1.363213
O 8.649039 2.567894 -1.143390

O 9.127851 0.411812 -0.957281
H 9.907614 0.734952 -0.488612
C 6.812437 -1.241251 1.736206
H 7.603595 -0.708570 1.193524
H 6.811170 -0.812331 2.751597
C 7.181499 -2.695599 1.884213
O 6.391592 -3.602451 1.878163
O 8.480301 -2.868411 2.046050
H 8.684110 -3.802792 2.174178
C 4.845927 -3.555056 4.938890
H 4.680060 -4.289463 4.136048
H 4.301721 -3.945134 5.810723
C 6.319980 -3.554518 5.243455
O 7.051238 -2.611672 5.098632
O 6.734602 -4.729164 5.685635
H 7.681347 -4.706672 5.870386
C -6.949680 -2.640528 3.572611
H -6.336701 -3.502338 3.264568
H -7.042944 -2.725137 4.664803
C -8.313236 -2.813802 2.955902
O -8.803104 -2.069323 2.150044
O -8.921357 -3.901212 3.398487
H -9.784900 -4.000499 2.979348
C -0.628698 -2.623091 6.826523
H -1.124600 -2.212609 7.714969
H 0.439503 -2.383575 6.882180
C -0.835225 -4.115843 6.777792
O -1.902860 -4.643691 6.963455
O 0.248140 -4.777962 6.424352
H 0.028111 -5.703223 6.199460
C -2.255360 -6.181986 3.804928
H -2.988636 -5.525478 4.299833
H -2.823345 -6.730501 3.041200
C -1.775925 -7.160500 4.843266
O -0.681434 -7.150688 5.356030
O -2.693132 -8.047792 5.153561
H -2.375465 -8.643918 5.843723
C 2.771059 6.512344 -3.173517
H 3.504674 5.771937 -3.521794
H 2.166826 6.765905 -4.057351
C 3.526015 7.742359 -2.745363
O 3.410824 8.284464 -1.678766
O 4.334924 8.181382 -3.694376
H 4.802497 8.972000 -3.399646
C 4.815850 5.503050 0.570611
H 5.291891 5.795674 1.514652
H 4.129186 6.303895 0.273125

C 5.853199 5.306939 -0.504851
O 5.677151 5.538934 -1.672045
O 6.957786 4.762977 -0.026939
H 7.558705 4.476418 -0.729121
C 0.697213 3.306638 5.398933
H 0.265406 2.930024 6.334193
H 0.386855 2.581988 4.628546
C 0.012063 4.586979 4.979707
O 0.522268 5.408825 4.254636
O -1.216920 4.676937 5.421549
H -1.690425 5.472762 5.076209

[Ag₂₅(MPA)₁₈]⁻ PBEh-3c T₁ (acetonitrile)

Ag 0.142718 -0.007970 0.110001
Ag 1.374023 1.923772 1.779336
Ag -1.767336 0.937172 -1.778102
Ag 1.965214 -0.993220 2.032841
Ag -1.045196 -1.854877 -1.649936
Ag 0.781685 2.569650 -0.888471
Ag 1.670311 -2.240973 -0.727637
Ag -1.305627 2.234350 1.006466
Ag -0.353709 -2.546755 1.284800
Ag 2.908613 0.509785 -0.670002
Ag -0.727756 -0.036162 2.715300
Ag 0.852412 0.229293 -2.602780
Ag -2.590071 -0.736765 0.650343
Ag 2.036594 -3.899845 2.570886
S 1.817636 -5.782928 1.115606
Ag 0.281194 -5.041022 -0.608640
C 3.494702 -6.184764 0.516495
H 3.896984 -5.357774 -0.082775
H 4.129850 -6.269209 1.404543
Ag 0.989278 4.880531 1.387855
S -0.728953 6.141907 0.213906
Ag -1.421691 4.455821 -1.401870
C -2.071707 6.424382 1.415315
H -2.255529 5.504076 1.983458
H -2.983923 6.655222 0.850175
Ag -3.633148 0.712532 3.073174
S -4.868276 -1.327040 3.617531
Ag -3.313059 -2.865131 2.611134
C -6.377672 -1.383491 2.588973
H -6.103836 -1.329321 1.530181
H -6.974837 -0.494935 2.826430
Ag 2.828295 2.383415 -3.019267

S 4.838222 1.439940 -4.113465
Ag 3.816202 -0.591003 -3.269144
C 6.230826 1.893339 -3.018755
H 5.961019 1.717484 -1.970565
H 6.386741 2.971961 -3.137568
Ag -1.293762 -0.256119 -4.551911
S -3.081120 -1.757609 -5.306183
Ag -3.655481 -1.614381 -2.973771
C -1.976542 -3.197844 -5.571829
H -1.191815 -3.200398 -4.809408
H -1.497752 -3.041555 -6.545489
Ag 3.650402 1.343443 3.516966
S 2.752309 1.854860 5.728694
Ag 1.213969 0.027168 4.980451
C 1.892745 3.463277 5.513220
H 2.377791 4.006790 4.695648
H 2.084792 4.035635 6.429990
S 1.361907 4.355602 -2.547006
S -3.213439 3.004295 2.351722
S 3.034905 -2.812870 -2.743566
S -1.739138 -4.541448 1.916641
S 3.080337 3.793642 2.136910
S -2.601354 2.968526 -2.924639
S 2.270972 -2.272261 4.349316
S -1.375475 -4.265227 -2.218713
S 0.817484 0.885697 -5.087688
S -4.553957 -1.419711 -0.744021
S 4.280419 0.131510 1.434065
S -1.325306 -0.012546 5.139830
C -5.482389 0.153556 -0.779016
H -4.901232 0.898598 -1.335627
H -5.565529 0.521009 0.251932
C 0.200309 2.597436 -5.310697
H -0.112049 3.011525 -4.347420
H 1.049883 3.200423 -5.651098
C -1.640963 -1.779338 5.474684
H -1.163244 -2.387381 4.694904
H -2.723412 -1.944071 5.412540
C 5.386205 -1.320960 1.520304
H 4.894067 -2.128182 2.072730
H 5.528358 -1.679787 0.494280
C -1.171117 -5.430322 3.408507
H -0.752722 -4.728758 4.136791
H -0.354609 -6.086532 3.081413
C 1.742225 -3.146085 -4.004971
H 0.981199 -2.358475 -3.987384
H 1.236728 -4.065870 -3.692810

C -4.402857 3.495658 1.053697
H -4.505630 2.696748 0.311100
H -3.958986 4.352518 0.533401
C 2.387590 5.697207 -1.853237
H 2.861178 5.383059 -0.918170
H 1.708765 6.521901 -1.603846
C -2.911360 -4.942757 -1.480396
H -2.858221 -4.880417 -0.388751
H -3.763961 -4.332397 -1.799399
C -4.393829 3.310903 -2.835912
H -4.765499 3.144833 -1.819658
H -4.883588 2.590940 -3.500361
C 4.021146 -2.180596 4.866528
H 4.551237 -1.451088 4.245053
H 4.015546 -1.780064 5.887400
C 4.259817 3.670653 0.745681
H 3.716569 3.629778 -0.206590
H 4.790455 2.718989 0.851497
C -0.948649 2.699082 -6.294596
H -0.673733 2.275475 -7.273663
H -1.822424 2.129270 -5.951517
C -1.388941 4.122926 -6.521373
O -0.719250 5.094930 -6.302137
O -2.615280 4.190999 -7.019622
H -2.853453 5.108516 -7.199351
C -2.705867 -4.528137 -5.530462
H -3.374850 -4.642962 -6.397585
H -3.349401 -4.594381 -4.644064
C -1.788739 -5.723229 -5.500294
O -2.120326 -6.807682 -5.076766
O -0.596350 -5.490958 -5.992525
H -0.016089 -6.258986 -5.912281
C -6.879412 0.007145 -1.378555
H -6.843694 -0.561562 -2.315063
H -7.535155 -0.522502 -0.676740
C -7.386485 1.406690 -1.620145
O -7.705158 2.152394 -0.729828
O -7.343477 1.750759 -2.888576
H -7.375506 2.729093 -3.016964
C -5.756473 3.873732 1.618793
H -5.635347 4.507288 2.512021
H -6.310779 2.988796 1.959922
C -6.601660 4.650383 0.639202
O -6.188270 5.147877 -0.373518
O -7.849501 4.780108 1.050949
H -8.359747 5.291619 0.412062
C -1.728296 7.581965 2.351111

H -1.656952 8.519614 1.789226
H -0.760090 7.393633 2.830095
C -2.756213 7.692026 3.441107
O -2.829557 6.925217 4.376899
O -3.604696 8.677133 3.279930
H -4.256777 8.695941 3.993071
C -4.683194 4.734450 -3.269194
H -4.182776 5.451929 -2.605257
H -4.262532 4.916115 -4.271254
C -6.141426 5.100427 -3.340167
O -7.068569 4.324874 -3.370810
O -6.319057 6.397996 -3.430805
H -7.257157 6.610723 -3.512110
C -3.155848 -6.379220 -1.920926
H -4.012163 -6.773497 -1.355002
H -3.437601 -6.414494 -2.978595
C -1.970865 -7.276629 -1.631870
O -1.563621 -7.469938 -0.516755
O -1.379116 -7.854248 -2.657119
H -1.727567 -7.561301 -3.518147
C 3.567508 -7.515162 -0.243049
H 4.548267 -7.969772 -0.068711
H 2.810834 -8.213509 0.140237
C 3.411472 -7.343898 -1.726037
O 4.332988 -7.528333 -2.497932
O 2.228980 -6.944834 -2.107689
H 2.210807 -6.740277 -3.075742
C 2.265656 -3.273582 -5.427836
H 1.435087 -3.650311 -6.038964
H 2.502201 -2.276867 -5.825804
C 3.500997 -4.145529 -5.615506
H 3.627779 -4.378030 -6.683981
H 4.410582 -3.607444 -5.322561
C 3.464036 -5.447207 -4.869815
O 2.430817 -6.038316 -4.606928
O 4.639432 -5.890811 -4.522464
H 4.560164 -6.662803 -3.907811
C 7.486236 1.131032 -3.392647
H 7.687537 1.223076 -4.470310
H 7.363482 0.051587 -3.215225
C 8.717924 1.586905 -2.660609
O 8.748294 2.449233 -1.813519
O 9.795733 0.943138 -3.043094
H 10.572833 1.248678 -2.557805
C 6.710809 -0.956530 2.158720
H 7.241603 -0.200010 1.565404
H 6.555665 -0.494585 3.146988

C 7.603189 -2.152459 2.370459
O 7.240887 -3.295250 2.286713
O 8.837607 -1.801594 2.679720
H 9.382376 -2.581854 2.839383
C 4.717919 -3.524942 4.833723
H 4.734659 -3.941845 3.813748
H 4.182054 -4.262925 5.446366
C 6.154185 -3.451850 5.284349
O 6.764907 -2.431298 5.457657
O 6.680054 -4.650499 5.456350
H 7.605907 -4.580056 5.718568
C -7.163082 -2.649466 2.866664
H -6.555740 -3.540963 2.643669
H -7.416355 -2.731086 3.933495
C -8.431334 -2.755981 2.061851
O -8.766929 -1.991497 1.197870
O -9.148611 -3.811866 2.408758
H -9.946635 -3.870287 1.869468
C -1.146929 -2.240135 6.844751
H -1.709933 -1.736391 7.640338
H -0.083104 -2.009002 6.972776
C -1.379478 -3.728867 6.917093
O -2.472213 -4.221507 7.047536
O -0.284033 -4.433766 6.728878
H -0.496770 -5.377013 6.550204
C -2.300323 -6.254723 4.004483
H -3.093305 -5.598197 4.398455
H -2.776567 -6.866351 3.228221
C -1.876400 -7.140250 5.145238
O -0.970712 -6.899955 5.911609
O -2.613217 -8.219843 5.251270
H -2.350817 -8.743211 6.019820
C 3.435450 6.147643 -2.850879
H 4.118233 5.323866 -3.104573
H 2.965083 6.442575 -3.800664
C 4.269288 7.298991 -2.355801
O 4.134119 7.840323 -1.290843
O 5.170401 7.676204 -3.246703
H 5.694536 8.409514 -2.903588
C 5.261792 4.821386 0.735508
H 5.761642 4.886264 1.711275
H 4.766338 5.779664 0.543579
C 6.285092 4.565044 -0.345169
O 6.317607 5.146930 -1.399211
O 7.106225 3.586863 -0.025806
H 7.686197 3.306724 -0.768110
C 0.395109 3.362004 5.278221

H -0.126728 2.993796 6.168918
H 0.179409 2.630401 4.482362
C -0.236263 4.638666 4.778572
O 0.304652 5.368738 3.976760
O -1.437412 4.845924 5.245267
H -1.878134 5.636690 4.842840

[Au₂₅(MPA)₁₈]⁻ B3LYP S₀ (gas)

Au -0.051904 0.245460 0.231163
Au 0.919888 2.110354 2.177852
Au -2.113685 0.838181 -1.829625
Au 1.836487 -0.995130 2.217984
Au -1.085552 -1.787004 -1.582528
Au 0.652197 2.841020 -0.823333
Au 1.829738 -2.154949 -0.382476
Au -1.715705 2.438718 1.045140
Au -0.281917 -2.579810 1.435398
Au 2.689165 0.771128 -0.377367
Au -1.224325 0.142361 2.803998
Au 0.790808 0.484913 -2.512410
Au -2.806247 -0.735567 0.499805
Au 2.289551 -4.322363 2.663561
S 1.899690 -6.122629 1.180301
Au 0.487357 -5.109495 -0.444426
C 3.575797 -6.370180 0.440639
H 3.873681 -5.468563 -0.113117
H 4.262219 -6.449576 1.293026
Au 0.312916 5.376756 1.111942
S -1.354245 6.341473 -0.289140
Au -2.037006 4.509534 -1.657901
C -2.815706 6.525357 0.823246
H -3.004785 5.565862 1.318164
H -3.679266 6.753207 0.182584
Au -4.476632 1.154592 2.884296
S -5.215509 -0.940356 3.762535
Au -3.539562 -2.484561 3.057473
C -6.650436 -1.278380 2.632068
H -6.482923 -0.760603 1.684276
H -7.527488 -0.816152 3.108220
Au 3.143412 2.962781 -3.197576
S 4.888470 1.434910 -3.730068
Au 3.900992 -0.646574 -3.071851
C 6.048511 1.885306 -2.360497
H 5.469139 2.050899 -1.446513
H 6.505491 2.845935 -2.635176

Au -1.548697 -0.453793 -4.971553
S -3.319430 -2.091044 -5.037360
Au -4.082535 -1.922699 -2.781277
C -2.072269 -3.462900 -5.150257
H -1.293919 -3.253707 -4.412163
H -1.625248 -3.356701 -6.147000
Au 4.237714 0.800817 2.860465
S 3.648427 1.245859 5.131070
Au 1.347550 0.591959 5.175445
C 3.763338 3.095042 5.246988
H 3.972082 3.490098 4.246601
H 4.640835 3.311447 5.872561
S 1.415368 4.460892 -2.570240
S -3.783529 3.271540 2.048152
S 3.015714 -2.771725 -2.479638
S -2.072787 -4.058286 2.097719
S 1.969743 4.355335 2.486271
S -2.820071 2.794963 -3.095775
S 2.629869 -2.491171 4.136578
S -1.132851 -4.234804 -1.935416
S 0.501791 0.736651 -4.996665
S -4.923074 -1.594798 -0.557035
S 4.935623 0.417352 0.625956
S -0.920447 -0.121219 5.247005
C -5.709336 0.059957 -0.764271
H -4.979695 0.709248 -1.266864
H -5.867355 0.478765 0.239464
C 0.043063 2.522190 -5.111732
H -0.280357 2.865883 -4.122910
H 0.965515 3.066466 -5.356013
C -0.813017 -1.962503 5.293348
H -0.240627 -2.304318 4.420175
H -1.850677 -2.305189 5.166706
C 5.147054 -1.414834 0.524173
H 4.310072 -1.906970 1.035904
H 5.067711 -1.673570 -0.541173
C -1.296389 -5.239352 3.268108
H -0.639414 -4.699610 3.956286
H -0.667252 -5.872426 2.626176
C 1.586155 -2.991124 -3.634979
H 0.838010 -2.218138 -3.416005
H 1.153075 -3.958524 -3.353461
C -4.840242 3.611334 0.572180
H -5.087416 2.669464 0.072864
H -4.214087 4.193825 -0.116131
C 2.275053 5.857809 -1.734855
H 2.701489 5.505693 -0.793730

H 1.494591 6.593251 -1.491934
C -2.744968 -4.774035 -1.211519
H -2.759206 -4.475705 -0.157989
H -3.514288 -4.193794 -1.742399
C -4.641236 3.098601 -3.205886
H -5.089456 3.103612 -2.206589
H -5.068171 2.263646 -3.779260
C 4.459458 -2.371090 4.273069
H 4.874788 -2.145286 3.288488
H 4.667345 -1.516399 4.933344
C 3.408549 4.029934 1.378524
H 3.033743 3.724804 0.391173
H 3.907844 3.149405 1.806715
C -1.047380 2.814005 -6.132570
H -0.735764 2.523229 -7.151896
H -1.960608 2.243130 -5.909288
C -1.401839 4.283292 -6.152043
O -0.708080 5.188748 -5.764290
O -2.630888 4.499631 -6.690735
H -2.765844 5.463275 -6.677741
C -2.561040 -4.893559 -4.937486
H -3.158813 -5.251541 -5.794147
H -3.195682 -4.978483 -4.045332
C -1.368583 -5.826821 -4.744768
O -1.386397 -6.848295 -4.082971
O -0.296672 -5.393604 -5.397420
H 0.553778 -5.807494 -5.102260
C -7.029495 0.022036 -1.536059
H -6.932783 -0.575295 -2.453746
H -7.819003 -0.421039 -0.908524
C -7.371793 1.451257 -1.893653
O -7.373700 2.356878 -1.081730
O -7.572352 1.631286 -3.196094
H -7.583413 2.604401 -3.396429
C -6.100282 4.395025 0.914868
H -5.857419 5.233849 1.592202
H -6.854321 3.765870 1.407252
C -6.698038 5.016438 -0.324816
O -6.063988 5.374385 -1.297037
O -8.021164 5.203099 -0.229099
H -8.312913 5.559021 -1.085551
C -2.603162 7.604613 1.871812
H -2.350974 8.578826 1.417456
H -1.755791 7.354181 2.532769
C -3.834657 7.795052 2.728080
O -4.911319 7.278382 2.545066
O -3.605783 8.642279 3.752249

H -4.436957 8.705247 4.253976
C -4.867647 4.438841 -3.896965
H -4.407481 5.247859 -3.307775
H -4.374368 4.458004 -4.884377
C -6.300246 4.845218 -4.104896
O -7.306758 4.184791 -3.923126
O -6.383876 6.093976 -4.586349
H -7.329364 6.289902 -4.701617
C -3.047822 -6.269582 -1.344442
H -4.016766 -6.447191 -0.850662
H -3.133450 -6.558739 -2.401009
C -2.027570 -7.154343 -0.635102
O -1.999766 -7.295220 0.564951
O -1.135310 -7.766019 -1.426291
H -1.217180 -7.474726 -2.359588
C 3.662114 -7.648067 -0.425121
H 4.664659 -8.087711 -0.327957
H 2.912296 -8.382726 -0.093238
C 3.469619 -7.332395 -1.883974
O 4.423287 -7.238655 -2.653980
O 2.222484 -7.114586 -2.236055
H 2.177092 -6.770279 -3.171789
C 1.919254 -2.957527 -5.122994
H 1.005733 -3.271788 -5.651081
H 2.123744 -1.918444 -5.428925
C 3.112873 -3.824711 -5.560212
H 3.052419 -4.022957 -6.645057
H 4.062369 -3.302135 -5.380053
C 3.210917 -5.158377 -4.859677
O 2.227644 -5.873568 -4.600371
O 4.425029 -5.500770 -4.538662
H 4.427827 -6.301819 -3.916823
C 7.092964 0.810587 -2.114639
H 7.718784 0.628306 -3.006277
H 6.617473 -0.155966 -1.881337
C 8.009640 1.159694 -0.970905
O 8.083906 2.233065 -0.410925
O 8.798357 0.130014 -0.621225
H 9.336799 0.420905 0.135884
C 6.481552 -1.873162 1.102619
H 7.334383 -1.539186 0.496241
H 6.629388 -1.466422 2.118719
C 6.528454 -3.372794 1.276654
O 5.586480 -4.073831 1.578320
O 7.761204 -3.874786 1.087356
H 7.705939 -4.828264 1.272819
C 5.093375 -3.646547 4.812761

H 4.844716 -4.491988 4.145790
H 4.715104 -3.912959 5.811020
C 6.598785 -3.562424 4.837862
O 7.280630 -2.837030 4.148500
O 7.146999 -4.436782 5.706834
H 8.111681 -4.336243 5.628341
C -6.889557 -2.752058 2.347826
H -5.985225 -3.211003 1.911908
H -7.120803 -3.331791 3.256375
C -7.992869 -2.947529 1.334468
O -8.570933 -2.070074 0.737026
O -8.262989 -4.253446 1.139301
H -8.942761 -4.297112 0.444943
C -0.232676 -2.555327 6.580072
H -0.758893 -2.143978 7.454236
H 0.843821 -2.345185 6.647218
C -0.499161 -4.047211 6.509550
O -1.605303 -4.527736 6.655730
O 0.573293 -4.760451 6.159777
H 0.277942 -5.675456 5.921547
C -2.328648 -6.083480 3.995508
H -2.973333 -5.450719 4.630405
H -2.974019 -6.610551 3.275528
C -1.700571 -7.098320 4.914519
O -0.551752 -7.100429 5.316829
O -2.565340 -8.051955 5.284979
H -2.092398 -8.633605 5.905360
C 3.369729 6.478730 -2.587870
H 4.133416 5.726235 -2.842010
H 2.981534 6.873728 -3.541105
C 4.092139 7.578868 -1.851263
O 3.898365 7.918762 -0.707062
O 5.025255 8.170376 -2.626239
H 5.467443 8.830283 -2.065370
C 4.414008 5.177966 1.255557
H 4.844661 5.405023 2.242469
H 3.956488 6.084968 0.839728
C 5.489097 4.682586 0.307810
O 5.530264 4.929804 -0.881121
O 6.333070 3.849636 0.918512
H 6.939384 3.416299 0.272776
C 2.518627 3.770005 5.802889
H 2.339351 3.494480 6.856665
H 1.619978 3.464504 5.247462
C 2.637000 5.275360 5.708846
O 3.662033 5.889480 5.533580
O 1.440631 5.879067 5.854175

H 1.594996 6.833630 5.749741

[Au₂₅(MPA)₁₈]⁻ B3LYP T₁ (gas)

Au 0.067381 0.110786 0.115346
Au 1.089956 1.941685 2.009190
Au -2.204083 0.770629 -1.699733
Au 1.800655 -0.954169 2.234066
Au -1.301057 -1.826846 -1.520359
Au 0.575143 2.832194 -0.846597
Au 1.824688 -2.134268 -0.361260
Au -1.657021 2.297093 0.845804
Au -0.343515 -2.564611 1.407604
Au 2.896897 0.803667 -0.521467
Au -1.597273 -0.101063 2.580509
Au 1.068325 0.631201 -2.590845
Au -3.167746 -0.936177 0.541516
Au 2.265557 -4.325199 2.646118
S 1.810534 -6.150650 1.213824
Au 0.455343 -5.123650 -0.448621
C 3.478781 -6.548127 0.529867
H 3.911745 -5.659197 0.050820
H 4.101563 -6.761621 1.408804
Au 0.280926 5.283116 1.038142
S -1.386221 6.281310 -0.347252
Au -2.083636 4.457108 -1.725725
C -2.841082 6.429282 0.781911
H -2.996820 5.468775 1.286818
H -3.719510 6.625370 0.150871
Au -4.446943 0.993071 2.898660
S -5.319513 -1.083038 3.766408
Au -3.617079 -2.638428 3.087546
C -6.683429 -1.354582 2.539529
H -6.408291 -0.864814 1.602303
H -7.565228 -0.832125 2.937433
Au 3.262810 3.002530 -3.196748
S 5.011897 1.459154 -3.738727
Au 3.973298 -0.608368 -3.055251
C 6.162230 1.902355 -2.358679
H 5.573750 2.078430 -1.452184
H 6.632630 2.857284 -2.631294
Au -1.549663 -0.391439 -4.895084
S -3.264932 -2.070059 -5.108136
Au -4.162862 -1.978104 -2.907998
C -1.997627 -3.422009 -5.188562
H -1.253869 -3.218639 -4.413401

H -1.510948 -3.294941 -6.163883
Au 4.380644 0.769815 2.810483
S 3.681049 1.287543 5.029719
Au 1.350382 0.742390 4.881227
C 3.900895 3.127467 5.076355
H 4.041034 3.486216 4.051919
H 4.842449 3.309445 5.613778
S 1.495829 4.446787 -2.562522
S -3.666953 3.067343 2.036235
S 3.012789 -2.705594 -2.445702
S -2.044828 -4.144006 2.158578
S 1.940789 4.254708 2.399287
S -2.948164 2.693834 -3.065743
S 2.623910 -2.487815 4.102395
S -1.171143 -4.249085 -1.933482
S 0.446721 0.859311 -4.967918
S -5.160922 -1.718392 -0.763790
S 5.077765 0.340679 0.603444
S -0.903025 0.057631 4.952467
C -5.887285 -0.030796 -0.932259
H -5.123734 0.613282 -1.388147
H -6.065381 0.354820 0.081017
C -0.061130 2.635481 -4.997382
H -0.415116 2.913793 -3.999793
H 0.853789 3.212985 -5.185881
C -0.805448 -1.770056 5.196395
H -0.238337 -2.201744 4.360865
H -1.845192 -2.116164 5.104568
C 5.186681 -1.499693 0.508866
H 4.328335 -1.943833 1.028963
H 5.088008 -1.759333 -0.554343
C -1.236114 -5.230439 3.399459
H -0.567652 -4.635834 4.030386
H -0.614779 -5.914072 2.803216
C 1.583892 -2.902044 -3.609581
H 0.844383 -2.119700 -3.396634
H 1.137828 -3.865811 -3.333697
C -4.766706 3.431500 0.596157
H -5.022614 2.495689 0.087863
H -4.159317 4.025164 -0.099303
C 2.289769 5.867772 -1.704561
H 2.665148 5.543971 -0.731697
H 1.485981 6.595573 -1.521685
C -2.765057 -4.865056 -1.221260
H -2.771449 -4.629721 -0.150627
H -3.553692 -4.274138 -1.709410
C -4.757733 3.066373 -3.175121

H -5.204240 3.077329 -2.175752
H -5.216519 2.255034 -3.757864
C 4.454158 -2.390923 4.239949
H 4.876459 -2.190020 3.252962
H 4.674902 -1.529077 4.886563
C 3.423008 4.010836 1.320882
H 3.082230 3.763840 0.306087
H 3.913857 3.108355 1.710192
C -1.135937 2.951650 -6.025691
H -0.784090 2.787644 -7.059330
H -2.014278 2.302018 -5.889570
C -1.611997 4.380901 -5.901961
O -1.104843 5.250225 -5.240105
O -2.727598 4.602401 -6.646735
H -2.958284 5.538548 -6.515565
C -2.483771 -4.859333 -5.019779
H -3.064178 -5.198496 -5.895959
H -3.132094 -4.967297 -4.139613
C -1.288150 -5.787396 -4.828914
O -1.302422 -6.814912 -4.176796
O -0.213703 -5.339572 -5.466977
H 0.637395 -5.742126 -5.155167
C -7.184918 0.007256 -1.736503
H -7.075450 -0.520100 -2.695031
H -7.993401 -0.470783 -1.160450
C -7.503522 1.464645 -1.989351
O -7.442468 2.317323 -1.124243
O -7.762670 1.732480 -3.266402
H -7.745144 2.716733 -3.399396
C -6.016265 4.210316 0.986748
H -5.760827 5.011979 1.702906
H -6.774839 3.566635 1.452588
C -6.617143 4.909576 -0.209575
O -5.989549 5.307238 -1.170915
O -7.933610 5.119062 -0.082414
H -8.231461 5.524518 -0.914378
C -2.642409 7.524640 1.816447
H -2.422867 8.499927 1.348118
H -1.777624 7.304325 2.465993
C -3.861495 7.692221 2.694021
O -4.916107 7.118165 2.559933
O -3.649846 8.590356 3.678058
H -4.470988 8.633215 4.198095
C -4.938834 4.421871 -3.850046
H -4.414074 5.199864 -3.272851
H -4.479331 4.425057 -4.853423
C -6.350545 4.915957 -4.006990

O -7.391871 4.316312 -3.810987
O -6.369538 6.179552 -4.457702
H -7.303806 6.435706 -4.542586
C -3.023539 -6.357652 -1.443469
H -3.995557 -6.591017 -0.979776
H -3.081292 -6.588969 -2.516025
C -1.990645 -7.248617 -0.758427
O -1.974905 -7.432359 0.435084
O -1.076187 -7.812215 -1.560343
H -1.150668 -7.488987 -2.483364
C 3.463058 -7.772844 -0.413413
H 4.415911 -8.312511 -0.314478
H 2.632642 -8.446942 -0.155523
C 3.362166 -7.339278 -1.850980
O 4.369363 -7.128203 -2.525142
O 2.138096 -7.157350 -2.287733
H 2.148905 -6.745832 -3.197915
C 1.944590 -2.873046 -5.091904
H 1.043254 -3.190413 -5.638130
H 2.155793 -1.834562 -5.395470
C 3.150675 -3.739515 -5.503984
H 3.102413 -3.950495 -6.586838
H 4.094168 -3.208512 -5.317732
C 3.244503 -5.064186 -4.785563
O 2.262161 -5.797753 -4.574770
O 4.443975 -5.378287 -4.394687
H 4.427367 -6.173027 -3.761228
C 7.193099 0.818537 -2.094110
H 7.854897 0.655508 -2.963340
H 6.705702 -0.150620 -1.901409
C 8.058030 1.141071 -0.902539
O 8.126242 2.210574 -0.334243
O 8.806116 0.093074 -0.520299
H 9.306226 0.367458 0.268615
C 6.501644 -2.022148 1.077419
H 7.363512 -1.723734 0.465074
H 6.675558 -1.624973 2.092930
C 6.477479 -3.522315 1.246831
O 5.505363 -4.177059 1.557316
O 7.681232 -4.084970 1.041861
H 7.577450 -5.036633 1.216067
C 5.062080 -3.668864 4.804723
H 4.802807 -4.520037 4.148954
H 4.671508 -3.912143 5.804144
C 6.568442 -3.611461 4.839250
O 7.268151 -2.920224 4.132877
O 7.094406 -4.467744 5.739241

H 8.061353 -4.387723 5.664569
C -6.989649 -2.814709 2.252313
H -6.090011 -3.334473 1.881041
H -7.313188 -3.366555 3.150765
C -8.045684 -2.952163 1.180214
O -8.605748 -2.041010 0.617120
O -8.302554 -4.244479 0.897409
H -8.955569 -4.247737 0.176677
C -0.225641 -2.241545 6.531444
H -0.760856 -1.765414 7.366379
H 0.848504 -2.016074 6.584749
C -0.474768 -3.738084 6.577106
O -1.577164 -4.218842 6.749150
O 0.609134 -4.462740 6.295521
H 0.327508 -5.397120 6.126086
C -2.252771 -6.005371 4.222394
H -2.883653 -5.312248 4.807081
H -2.920510 -6.592381 3.572645
C -1.612271 -6.928404 5.225301
O -0.465182 -6.877152 5.629697
O -2.463769 -7.858969 5.676330
H -1.986522 -8.372837 6.351039
C 3.423083 6.490643 -2.504758
H 4.212591 5.745892 -2.697992
H 3.086516 6.860533 -3.486881
C 4.089602 7.612485 -1.748833
O 3.861265 7.937734 -0.606670
O 5.018720 8.239340 -2.500251
H 5.431250 8.904984 -1.923965
C 4.430935 5.163069 1.299515
H 4.811095 5.348831 2.315664
H 3.995365 6.087298 0.898389
C 5.547909 4.700356 0.382800
O 5.663365 5.017106 -0.784032
O 6.337997 3.809146 0.986526
H 6.969845 3.399904 0.349857
C 2.748221 3.885717 5.714713
H 2.664778 3.685806 6.796861
H 1.784996 3.590085 5.271686
C 2.908039 5.375309 5.501224
O 3.898380 5.922409 5.077996
O 1.793475 6.050452 5.843663
H 1.960715 6.986469 5.638608
[Au₂₅(MPA)₁₈]⁻ B3LYP S₀ (acetonitrile)

Au -0.046915 0.235528 0.212830
Au 0.918290 2.114730 2.155690

Au -2.116109 0.844305 -1.839264
Au 1.840989 -0.997280 2.205768
Au -1.064810 -1.789153 -1.606290
Au 0.635115 2.850240 -0.830145
Au 1.833507 -2.156503 -0.398290
Au -1.710328 2.438224 1.018178
Au -0.274068 -2.592712 1.431063
Au 2.691081 0.773623 -0.376970
Au -1.228617 0.129841 2.766943
Au 0.794551 0.492227 -2.515954
Au -2.794147 -0.764064 0.475650
Au 2.281256 -4.316360 2.656861
S 1.894457 -6.120148 1.176116
Au 0.501352 -5.109914 -0.466481
C 3.587728 -6.406172 0.484983
H 3.921994 -5.503386 -0.044762
H 4.238993 -6.512497 1.361215
Au 0.307177 5.383999 1.103914
S -1.372046 6.340953 -0.286588
Au -2.049673 4.513137 -1.661792
C -2.832597 6.537817 0.828604
H -3.008249 5.585977 1.342593
H -3.696639 6.742131 0.180920
Au -4.486029 1.118283 2.844327
S -5.221844 -0.974782 3.723828
Au -3.535733 -2.511757 3.031825
C -6.665833 -1.327902 2.607521
H -6.497998 -0.819513 1.654578
H -7.537536 -0.862394 3.088915
Au 3.150728 2.980244 -3.174983
S 4.881382 1.445818 -3.723193
Au 3.891327 -0.637276 -3.078253
C 6.074110 1.874678 -2.373092
H 5.505876 2.048618 -1.453819
H 6.544123 2.823982 -2.663698
Au -1.522187 -0.443922 -4.981645
S -3.292608 -2.076156 -5.058444
Au -4.065891 -1.915242 -2.806708
C -2.057993 -3.460083 -5.188081
H -1.272789 -3.251269 -4.457337
H -1.625679 -3.353756 -6.191017
Au 4.239027 0.818110 2.847749
S 3.644150 1.271080 5.115678
Au 1.346524 0.614505 5.147355
C 3.750847 3.121242 5.244573
H 3.956403 3.519635 4.244647
H 4.626494 3.330291 5.874661

S 1.425153 4.485850 -2.557520
S -3.791607 3.239624 2.027277
S 3.016214 -2.765961 -2.496271
S -2.050008 -4.087777 2.105505
S 1.979984 4.364769 2.465067
S -2.829214 2.799936 -3.101316
S 2.622666 -2.485119 4.130280
S -1.118990 -4.235231 -1.959692
S 0.517534 0.767604 -4.997535
S -4.913432 -1.606454 -0.582412
S 4.935939 0.435041 0.614212
S -0.925130 -0.089259 5.217991
C -5.702142 0.049559 -0.772534
H -4.980252 0.701430 -1.283065
H -5.845944 0.462857 0.235742
C 0.036022 2.549566 -5.099139
H -0.289045 2.878228 -4.105907
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C -0.826596 -1.928900 5.301696
H -0.252596 -2.285847 4.435654
H -1.865378 -2.269018 5.177500
C 5.159235 -1.395913 0.509161
H 4.318226 -1.892883 1.008999
H 5.095368 -1.650496 -0.557905
C -1.284290 -5.232540 3.319509
H -0.636758 -4.670576 3.998989
H -0.640051 -5.876762 2.703953
C 1.592272 -2.993610 -3.658494
H 0.848022 -2.214464 -3.448642
H 1.155304 -3.955954 -3.366709
C -4.844635 3.604542 0.554786
H -5.097810 2.668251 0.047869
H -4.208280 4.186112 -0.124600
C 2.275871 5.880423 -1.705958
H 2.663476 5.531231 -0.746639
H 1.494851 6.625292 -1.496512
C -2.729351 -4.769319 -1.227153
H -2.732027 -4.485893 -0.169633
H -3.499331 -4.178752 -1.744345
C -4.651233 3.100815 -3.208888
H -5.092343 3.111344 -2.206365
H -5.074909 2.259506 -3.773959
C 4.454484 -2.353351 4.253427
H 4.852589 -2.105945 3.267191
H 4.659229 -1.507612 4.925263
C 3.412233 4.018547 1.352336
H 3.031622 3.737944 0.360094

H 3.884347 3.118405 1.768861
C -1.056318 2.833831 -6.118337
H -0.730587 2.594252 -7.145834
H -1.949133 2.221156 -5.921923
C -1.481623 4.283252 -6.091020
O -0.865958 5.190057 -5.579129
O -2.654991 4.467986 -6.728035
H -2.858839 5.421547 -6.724536
C -2.557509 -4.885532 -4.970348
H -3.155361 -5.245822 -5.825139
H -3.192966 -4.967622 -4.078157
C -1.372267 -5.823239 -4.779557
O -1.408434 -6.862439 -4.138480
O -0.286759 -5.386016 -5.395768
H 0.556548 -5.824595 -5.109824
C -7.034010 0.010852 -1.524526
H -6.950236 -0.586029 -2.443675
H -7.814230 -0.431916 -0.885999
C -7.380653 1.440749 -1.874826
O -7.425184 2.334821 -1.048408
O -7.529975 1.637136 -3.179098
H -7.536273 2.617285 -3.381653
C -6.095494 4.399455 0.899621
H -5.845376 5.219674 1.596930
H -6.865719 3.774287 1.371821
C -6.666687 5.066631 -0.331048
O -6.005740 5.432508 -1.283181
O -7.981033 5.283089 -0.239034
H -8.273637 5.735033 -1.052009
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H -2.420203 8.618019 1.360307
H -1.748714 7.439368 2.486057
C -3.827142 7.817016 2.742724
O -4.863626 7.194557 2.649231
O -3.619194 8.754017 3.675791
H -4.419209 8.828482 4.228929
C -4.889188 4.432994 -3.911831
H -4.391121 5.247124 -3.363220
H -4.446979 4.425581 -4.923001
C -6.329248 4.848551 -4.064309
O -7.321032 4.159450 -3.881778
O -6.427400 6.106821 -4.481282
H -7.369730 6.331212 -4.597032
C -3.049173 -6.258918 -1.385954
H -4.010853 -6.440404 -0.880720
H -3.159437 -6.523511 -2.446057
C -2.025268 -7.168775 -0.727123

O -1.979941 -7.368803 0.467904
O -1.138082 -7.746678 -1.545344
H -1.236869 -7.437938 -2.475537
C 3.682291 -7.675986 -0.386338
H 4.689726 -8.102041 -0.284929
H 2.947165 -8.426389 -0.057995
C 3.486432 -7.358610 -1.843173
O 4.439304 -7.245260 -2.612954
O 2.237309 -7.157416 -2.202713
H 2.192016 -6.817680 -3.141498
C 1.929010 -2.979680 -5.145461
H 1.007071 -3.273699 -5.670317
H 2.159311 -1.948687 -5.459785
C 3.098847 -3.878874 -5.583796
H 3.008396 -4.109637 -6.659286
H 4.060693 -3.365753 -5.447904
C 3.194296 -5.191838 -4.849931
O 2.212703 -5.897372 -4.561161
O 4.410716 -5.529839 -4.523265
H 4.415035 -6.332598 -3.906584
C 7.104788 0.783548 -2.146940
H 7.718431 0.599846 -3.045355
H 6.621353 -0.179031 -1.911702
C 8.042060 1.110763 -1.012593
O 8.082760 2.166941 -0.406579
O 8.862277 0.099240 -0.733203
H 9.452971 0.356010 0.000234
C 6.487028 -1.849455 1.102537
H 7.345714 -1.532455 0.494336
H 6.636082 -1.421627 2.109815
C 6.523310 -3.348122 1.307599
O 5.554052 -4.039097 1.545578
O 7.766253 -3.838639 1.240200
H 7.732309 -4.795087 1.428812
C 5.109929 -3.626483 4.766218
H 4.876691 -4.470853 4.093816
H 4.747046 -3.910655 5.766116
C 6.615253 -3.513004 4.793271
O 7.261789 -2.652677 4.231603
O 7.181658 -4.507825 5.488112
H 8.150843 -4.404894 5.446131
C -6.900026 -2.806164 2.347673
H -5.993455 -3.275245 1.927504
H -7.142790 -3.364906 3.265797
C -7.998912 -3.023895 1.332032
O -8.581155 -2.146724 0.729995
O -8.246005 -4.325938 1.147476

H -8.938804 -4.420042 0.467343
C -0.248673 -2.493262 6.602529
H -0.763366 -2.055187 7.470171
H 0.830680 -2.295798 6.659367
C -0.532350 -3.980708 6.571962
O -1.640851 -4.445996 6.766257
O 0.512837 -4.716154 6.200202
H 0.198131 -5.636082 5.991362
C -2.325893 -6.059034 4.056589
H -2.956761 -5.411302 4.690388
H -2.992275 -6.571864 3.346106
C -1.715946 -7.088081 4.976344
O -0.579695 -7.059121 5.424464
O -2.566656 -8.063198 5.277073
H -2.139439 -8.677623 5.904187
C 3.401846 6.486970 -2.527129
H 4.167104 5.728265 -2.756019
H 3.044504 6.882977 -3.491802
C 4.108649 7.591536 -1.779893
O 3.849434 7.956866 -0.651864
O 5.086868 8.138099 -2.513329
H 5.521864 8.831185 -1.982926
C 4.452128 5.136832 1.251665
H 4.879886 5.342322 2.245041
H 4.026775 6.061995 0.842337
C 5.533570 4.635497 0.313632
O 5.659634 4.983098 -0.844808
O 6.281776 3.694251 0.886890
H 6.906119 3.270949 0.244056
C 2.501019 3.777774 5.808792
H 2.330024 3.491716 6.860647
H 1.604348 3.468522 5.251437
C 2.589406 5.285525 5.738243
O 3.603977 5.918125 5.541175
O 1.393205 5.858464 5.929904
H 1.501778 6.826715 5.889711

[Au₂₅(MPA)₁₈]⁻ B3LYP T₁ (acetonitrile)

Au 0.079490 0.093808 0.077136
Au 1.088770 1.924274 1.972727
Au -2.193121 0.772666 -1.743165
Au 1.794267 -0.970257 2.224851
Au -1.281108 -1.830595 -1.570151
Au 0.576571 2.831102 -0.881097
Au 1.842291 -2.149009 -0.374685

Au -1.654970 2.284394 0.794135
Au -0.343958 -2.583862 1.381853
Au 2.908988 0.785927 -0.522388
Au -1.582668 -0.106407 2.537670
Au 1.099846 0.628660 -2.606690
Au -3.133263 -0.959156 0.501011
Au 2.255286 -4.326676 2.626659
S 1.855325 -6.138255 1.157029
Au 0.459984 -5.127013 -0.483636
C 3.545804 -6.445095 0.469648
H 3.903033 -5.538828 -0.038414
H 4.188288 -6.581473 1.348161
Au 0.276983 5.270761 1.020079
S -1.389173 6.274589 -0.360719
Au -2.087461 4.458483 -1.747885
C -2.845542 6.445061 0.767450
H -2.991952 5.494533 1.293364
H -3.722520 6.619303 0.128426
Au -4.454513 0.966879 2.831581
S -5.314538 -1.095532 3.726724
Au -3.622684 -2.662630 3.055719
C -6.686261 -1.398067 2.519870
H -6.338559 -1.098843 1.527730
H -7.507305 -0.728443 2.812236
Au 3.283587 3.005434 -3.189007
S 5.022716 1.451712 -3.723726
Au 3.982278 -0.618666 -3.054178
C 6.193557 1.885185 -2.355903
H 5.609165 2.076169 -1.449774
H 6.678077 2.826719 -2.648865
Au -1.512423 -0.383192 -4.919948
S -3.242943 -2.040340 -5.146209
Au -4.144688 -1.956402 -2.949066
C -1.992020 -3.408611 -5.241013
H -1.244480 -3.210418 -4.468421
H -1.513661 -3.279986 -6.219951
Au 4.374261 0.773335 2.810160
S 3.671684 1.298794 5.025884
Au 1.343584 0.762410 4.864497
C 3.894586 3.139222 5.076725
H 4.018598 3.497222 4.049897
H 4.842732 3.311012 5.605470
S 1.520699 4.466623 -2.571554
S -3.669595 3.044889 1.988905
S 3.028822 -2.720114 -2.460375
S -2.038216 -4.171329 2.151216
S 1.937550 4.238598 2.379984

S -2.943374 2.699345 -3.095854
S 2.587073 -2.499394 4.103240
S -1.165697 -4.254447 -1.972694
S 0.482795 0.869635 -4.982611
S -5.128180 -1.726217 -0.794798
S 5.079036 0.344841 0.606915
S -0.918257 0.099005 4.917296
C -5.868134 -0.040434 -0.926418
H -5.131811 0.605350 -1.423030
H -5.993739 0.344474 0.095314
C -0.041528 2.642023 -5.014124
H -0.400843 2.913787 -4.016540
H 0.869557 3.225192 -5.203373
C -0.847114 -1.724819 5.194134
H -0.281755 -2.174866 4.367017
H -1.891405 -2.057000 5.102498
C 5.211404 -1.495429 0.521560
H 4.346867 -1.946293 1.025201
H 5.140872 -1.759676 -0.542758
C -1.230556 -5.227183 3.420863
H -0.582327 -4.613158 4.054449
H -0.583709 -5.902210 2.841361
C 1.595069 -2.916344 -3.621125
H 0.856127 -2.137117 -3.395327
H 1.156192 -3.883127 -3.345117
C -4.765296 3.438478 0.554501
H -5.023370 2.510216 0.033619
H -4.150220 4.037642 -0.129151
C 2.310880 5.875281 -1.685561
H 2.641901 5.541954 -0.699558
H 1.513127 6.615968 -1.530982
C -2.766020 -4.853379 -1.261248
H -2.764552 -4.632301 -0.187720
H -3.548709 -4.247546 -1.739171
C -4.757329 3.054965 -3.194913
H -5.192609 3.071961 -2.190273
H -5.208743 2.230540 -3.763696
C 4.417563 -2.377951 4.248648
H 4.833347 -2.149615 3.264984
H 4.620386 -1.524742 4.911446
C 3.423285 3.985317 1.306945
H 3.087086 3.757587 0.286148
H 3.894505 3.069708 1.687817
C -1.112162 2.940152 -6.051376
H -0.743371 2.791386 -7.080926
H -1.978104 2.271202 -5.929318
C -1.623986 4.356780 -5.934648

O -1.129626 5.235865 -5.266966
O -2.730717 4.543310 -6.681083
H -2.997285 5.478148 -6.606644
C -2.494171 -4.839531 -5.073911
H -3.071038 -5.176867 -5.952192
H -3.148383 -4.944798 -4.197378
C -1.308585 -5.775167 -4.881965
O -1.345813 -6.821324 -4.252757
O -0.218625 -5.324287 -5.479503
H 0.625158 -5.754577 -5.180420
C -7.208707 -0.016684 -1.660714
H -7.152719 -0.571810 -2.607714
H -7.986706 -0.471197 -1.027705
C -7.522275 1.437362 -1.935513
O -7.512991 2.293423 -1.068685
O -7.702677 1.698235 -3.224575
H -7.676514 2.686859 -3.380264
C -6.009289 4.219783 0.951886
H -5.748529 5.006268 1.683022
H -6.776389 3.576129 1.404032
C -6.595724 4.954015 -0.232766
O -5.952617 5.347454 -1.186511
O -7.900296 5.199209 -0.091903
H -8.205006 5.692549 -0.875932
C -2.650118 7.572601 1.766560
H -2.473681 8.540057 1.267398
H -1.765191 7.392289 2.401841
C -3.847048 7.727683 2.677614
O -4.854198 7.053614 2.632261
O -3.668775 8.715467 3.563314
H -4.460953 8.775634 4.129381
C -4.963798 4.398615 -3.886958
H -4.407448 5.187042 -3.357283
H -4.561744 4.375137 -4.914336
C -6.386402 4.885756 -3.983948
O -7.406134 4.239518 -3.798560
O -6.435267 6.161892 -4.353856
H -7.368921 6.432331 -4.437983
C -3.051669 -6.336701 -1.511227
H -4.020801 -6.567507 -1.041408
H -3.130748 -6.543295 -2.586918
C -2.021990 -7.255564 -0.872982
O -1.996431 -7.497430 0.314625
O -1.110740 -7.787105 -1.694718
H -1.199118 -7.447603 -2.614973
C 3.621256 -7.696655 -0.430101
H 4.616261 -8.150054 -0.323836

H 2.861615 -8.435290 -0.133596
C 3.459205 -7.331236 -1.879409
O 4.431569 -7.173037 -2.616776
O 2.217338 -7.137176 -2.266268
H 2.193605 -6.766962 -3.194428
C 1.939391 -2.878956 -5.106166
H 1.024053 -3.172448 -5.642011
H 2.164966 -1.841965 -5.403939
C 3.120824 -3.761893 -5.549688
H 3.038582 -3.976483 -6.628994
H 4.076524 -3.241457 -5.399125
C 3.222432 -5.084962 -4.834978
O 2.245102 -5.810181 -4.581743
O 4.434752 -5.410059 -4.483630
H 4.434264 -6.224633 -3.881417
C 7.211653 0.790292 -2.093033
H 7.864405 0.613271 -2.964940
H 6.717150 -0.172560 -1.884965
C 8.095194 1.111520 -0.914136
O 8.125572 2.174495 -0.319115
O 8.881179 0.088738 -0.583097
H 9.436346 0.343153 0.178260
C 6.518635 -1.995479 1.123166
H 7.389313 -1.708859 0.516857
H 6.678129 -1.567343 2.128696
C 6.501406 -3.492009 1.338959
O 5.506983 -4.145976 1.578283
O 7.726256 -4.027453 1.282287
H 7.657012 -4.981015 1.475547
C 5.050628 -3.650164 4.791656
H 4.823993 -4.500794 4.124813
H 4.663091 -3.917686 5.786803
C 6.556002 -3.550709 4.849998
O 7.224325 -2.714476 4.277376
O 7.095566 -4.529200 5.587673
H 8.066715 -4.438323 5.564095
C -7.143189 -2.845101 2.469576
H -6.303379 -3.514022 2.212297
H -7.531278 -3.198178 3.439173
C -8.211991 -3.046983 1.418303
O -8.653269 -2.181480 0.693123
O -8.618575 -4.321777 1.367955
H -9.296495 -4.406602 0.671804
C -0.277155 -2.179787 6.538979
H -0.799947 -1.679641 7.367331
H 0.801336 -1.976284 6.588616
C -0.554597 -3.668030 6.610467

O -1.666636 -4.124071 6.807631
O 0.502796 -4.421082 6.321816
H 0.201561 -5.358159 6.175381
C -2.248233 -6.012924 4.235947
H -2.864027 -5.323215 4.840461
H -2.932323 -6.574807 3.582529
C -1.609112 -6.968537 5.213026
O -0.498034 -6.843104 5.706169
O -2.401663 -7.990135 5.516821
H -1.961140 -8.548433 6.186059
C 3.479932 6.484037 -2.443144
H 4.266081 5.730753 -2.614141
H 3.180635 6.863223 -3.433751
C 4.131359 7.603293 -1.667728
O 3.821506 7.958239 -0.549089
O 5.123944 8.174056 -2.361851
H 5.525549 8.871938 -1.811655
C 4.452956 5.117219 1.313196
H 4.822138 5.284880 2.336875
H 4.041856 6.055162 0.918883
C 5.584620 4.658835 0.412194
O 5.786361 5.075611 -0.711907
O 6.284496 3.669471 0.967464
H 6.938562 3.275080 0.336310
C 2.750288 3.888093 5.737738
H 2.683264 3.676531 6.818021
H 1.781243 3.596880 5.302675
C 2.895477 5.381541 5.547515
O 3.863111 5.935648 5.072107
O 1.807846 6.039642 5.969017
H 1.946851 6.994438 5.827025

[Au₂₅(MPA)₁₈]⁻ TPSSh S₀ (gas)

Au -0.053423 0.091103 0.066518
Au 0.900050 1.910727 1.973870
Au -2.014466 0.750586 -1.893054
Au 1.708141 -0.832726 2.070855
Au -1.053069 -1.837828 -1.694362
Au 0.618027 2.700117 -0.838371
Au 1.667731 -2.132746 -0.548952
Au -1.752051 2.207741 0.649326
Au -0.382540 -2.509045 1.258269
Au 2.638193 0.629372 -0.359310
Au -1.233370 0.090389 2.594759
Au 0.821946 0.390817 -2.541802

Au -2.722391 -0.815934 0.444925
Au 2.148216 -4.014762 2.385776
S 1.875950 -5.880082 0.989595
Au 0.438641 -4.939703 -0.609957
C 3.529415 -6.119347 0.210643
H 3.764119 -5.245665 -0.414550
H 4.245062 -6.127987 1.040909
Au 0.193185 5.015986 1.049083
S -1.365720 6.049758 -0.387626
Au -2.061067 4.225973 -1.715775
C -2.827834 6.388052 0.675922
H -3.093597 5.461608 1.201969
H -3.656333 6.663164 0.008057
Au -4.161975 1.068076 2.716275
S -4.893364 -0.958407 3.685755
Au -3.309919 -2.515423 2.889732
C -6.353965 -1.323273 2.613667
H -6.091955 -1.069423 1.581501
H -7.160949 -0.653235 2.941653
Au 3.006849 2.916681 -2.901446
S 4.736833 1.453172 -3.540559
Au 3.759084 -0.624055 -2.941525
C 5.957307 1.856351 -2.217440
H 5.412066 1.986281 -1.275655
H 6.409009 2.821328 -2.484549
Au -1.337105 -0.319506 -4.860861
S -3.161027 -1.847885 -5.037503
Au -3.859019 -1.804532 -2.782954
C -1.987627 -3.263843 -5.263356
H -1.190866 -3.128945 -4.524303
H -1.557328 -3.118955 -6.262748
Au 4.150766 0.717664 2.725358
S 3.542148 1.253475 4.943004
Au 1.216562 0.799975 4.835690
C 3.837475 3.074953 5.023284
H 3.947631 3.448669 3.999822
H 4.802947 3.206770 5.531506
S 1.336164 4.494619 -2.409629
S -3.611379 3.194567 1.855169
S 2.968716 -2.815831 -2.537363
S -1.939160 -4.200561 2.012119
S 1.862983 4.118809 2.451702
S -2.872968 2.593676 -3.204477
S 2.378435 -2.293691 3.970291
S -1.199131 -4.228478 -2.130978
S 0.699978 0.865510 -4.978930
S -4.781572 -1.643459 -0.592170

S 4.889242 0.230738 0.550067
S -1.039166 0.117555 5.029160
C -5.618625 -0.009018 -0.755293
H -4.920554 0.659131 -1.279955
H -5.756309 0.396050 0.258182
C 0.132154 2.621212 -4.951495
H -0.273237 2.834069 -3.951715
H 1.025491 3.246284 -5.085324
C -0.888868 -1.711890 5.220299
H -0.343550 -2.102525 4.346644
H -1.923284 -2.086921 5.172319
C 5.024685 -1.609225 0.558842
H 4.165169 -2.035431 1.098787
H 4.949522 -1.933921 -0.489975
C -1.097598 -5.157196 3.333820
H -0.511152 -4.479498 3.963810
H -0.399432 -5.813392 2.794196
C 1.565615 -2.978600 -3.731193
H 0.817135 -2.207644 -3.483529
H 1.122782 -3.957589 -3.502921
C -4.801572 3.514787 0.483294
H -5.090044 2.564031 0.024255
H -4.237140 4.091152 -0.266285
C 2.201520 5.867946 -1.543779
H 2.545780 5.525916 -0.563574
H 1.434514 6.638105 -1.376503
C -2.768255 -4.780351 -1.331175
H -2.716514 -4.521116 -0.265956
H -3.567821 -4.184033 -1.798891
C -4.694775 2.890689 -3.241220
H -5.106224 2.868792 -2.226010
H -5.135534 2.071266 -3.825618
C 4.184444 -2.280814 4.305801
H 4.722263 -2.086967 3.372652
H 4.366857 -1.439156 4.989757
C 3.330702 3.870111 1.356640
H 2.976262 3.651237 0.336047
H 3.803983 2.944582 1.725604
C -0.913313 2.921573 -6.016286
H -0.508203 2.773012 -7.032578
H -1.777301 2.245305 -5.919894
C -1.413075 4.342856 -5.907669
O -0.879636 5.247398 -5.310389
O -2.574398 4.522998 -6.596061
H -2.802269 5.464839 -6.480182
C -2.547571 -4.676146 -5.114049
H -3.161466 -4.968226 -5.983413

H -3.181425 -4.768294 -4.220830
C -1.395907 -5.663901 -4.960535
O -1.460194 -6.722022 -4.355475
O -0.301604 -5.234167 -5.582314
H 0.536806 -5.690638 -5.301442
C -6.960524 -0.113184 -1.482771
H -6.863254 -0.713382 -2.398280
H -7.705037 -0.584835 -0.822678
C -7.374682 1.296248 -1.838248
O -7.402599 2.208199 -1.029286
O -7.606136 1.456503 -3.140924
H -7.638423 2.432600 -3.349176
C -6.025198 4.301163 0.932754
H -5.722869 5.148387 1.574630
H -6.730951 3.678212 1.498074
C -6.723989 4.904071 -0.261904
O -6.170595 5.267334 -1.283313
O -8.043074 5.065951 -0.069136
H -8.394999 5.421774 -0.906036
C -2.530762 7.483602 1.686808
H -2.204266 8.418613 1.201097
H -1.703514 7.184842 2.353820
C -3.739221 7.788521 2.540082
O -4.834600 7.282063 2.432265
O -3.469172 8.726648 3.475039
H -4.293679 8.848070 3.982336
C -4.929420 4.251273 -3.886199
H -4.462941 5.039963 -3.273625
H -4.441581 4.298376 -4.874960
C -6.364965 4.657773 -4.076950
O -7.374326 3.994262 -3.900332
O -6.452274 5.915371 -4.540014
H -7.403711 6.107610 -4.634216
C -3.045710 -6.273832 -1.521018
H -3.985470 -6.503499 -0.995196
H -3.167742 -6.507657 -2.589249
C -1.965244 -7.158766 -0.905648
O -1.892132 -7.383107 0.281952
O -1.076422 -7.679661 -1.766771
H -1.220902 -7.341739 -2.681403
C 3.607446 -7.448973 -0.577821
H 4.604188 -7.892861 -0.453809
H 2.848055 -8.153193 -0.204618
C 3.415825 -7.211817 -2.050552
O 4.364842 -7.219831 -2.838792
O 2.177803 -6.939758 -2.399521
H 2.143317 -6.646667 -3.358765

C 1.939253 -2.864725 -5.204482
H 1.037504 -3.133745 -5.775245
H 2.169614 -1.813067 -5.440335
C 3.133312 -3.724268 -5.655566
H 3.095438 -3.869752 -6.749176
H 4.083788 -3.223233 -5.426297
C 3.199333 -5.087394 -5.011873
O 2.202087 -5.805471 -4.797352
O 4.405046 -5.457202 -4.682003
H 4.381653 -6.284332 -4.082570
C 6.994924 0.758615 -2.059419
H 7.609799 0.636170 -2.968105
H 6.506890 -0.215744 -1.888375
C 7.919836 1.024747 -0.900633
O 8.016242 2.063660 -0.274720
O 8.697092 -0.036598 -0.615653
H 9.240725 0.214234 0.155489
C 6.351844 -2.027430 1.185636
H 7.209299 -1.730080 0.566506
H 6.479072 -1.539399 2.169524
C 6.413929 -3.505068 1.476036
O 5.473933 -4.198488 1.809080
O 7.662306 -3.997656 1.361383
H 7.613403 -4.931326 1.640177
C 4.650342 -3.599925 4.908868
H 4.401304 -4.423272 4.214593
H 4.149867 -3.823119 5.862200
C 6.147713 -3.625512 5.079907
O 6.950044 -2.996600 4.420190
O 6.541274 -4.476677 6.053950
H 7.516678 -4.444223 6.059935
C -6.776820 -2.781794 2.666957
H -5.939167 -3.433359 2.359143
H -7.059788 -3.105579 3.681662
C -7.925822 -3.048739 1.723311
O -8.430069 -2.245499 0.969523
O -8.345241 -4.331141 1.798010
H -9.058614 -4.421880 1.138804
C -0.228777 -2.183678 6.518119
H -0.744558 -1.744138 7.384448
H 0.835442 -1.911521 6.526905
C -0.412313 -3.688052 6.543852
O -1.499734 -4.218353 6.691202
O 0.708324 -4.367694 6.281903
H 0.453188 -5.310232 6.090757
C -2.098898 -5.971995 4.138179
H -2.775844 -5.305449 4.700070

H -2.719690 -6.593766 3.474391
C -1.438413 -6.863821 5.155868
O -0.288857 -6.787899 5.559612
O -2.269946 -7.811070 5.615981
H -1.772281 -8.303887 6.295580
C 3.369709 6.409345 -2.353891
H 4.114533 5.615333 -2.529830
H 3.051735 6.775741 -3.342867
C 4.089576 7.510489 -1.617332
O 3.877030 7.866514 -0.477919
O 5.045765 8.083981 -2.381458
H 5.486863 8.736809 -1.806718
C 4.351772 5.011345 1.374550
H 4.711852 5.176503 2.401152
H 3.933787 5.947476 0.982196
C 5.488383 4.559559 0.479600
O 5.663907 4.927672 -0.667537
O 6.233005 3.621982 1.076842
H 6.877288 3.222784 0.439454
C 2.726745 3.843275 5.720791
H 2.685542 3.628847 6.801992
H 1.742580 3.565822 5.309488
C 2.912014 5.329879 5.517260
O 3.896860 5.861027 5.052487
O 1.830929 6.030516 5.920485
H 2.022685 6.964363 5.713825

[Au₂₅(MPA)₁₈]⁻ TPSSh T₁ (gas)

Au -0.030209 0.093843 0.039639
Au 0.943234 1.867532 1.962195
Au -2.048918 0.713860 -1.867705
Au 1.778541 -0.842860 2.071512
Au -1.232790 -1.876258 -1.551191
Au 0.546318 2.749029 -0.796260
Au 1.658902 -2.130495 -0.481777
Au -1.775997 2.218774 0.608284
Au -0.398460 -2.425328 1.307408
Au 2.718838 0.636566 -0.407706
Au -1.371039 0.118985 2.575177
Au 1.035131 0.610962 -2.543611
Au -2.870426 -0.766418 0.535695
Au 2.167883 -4.031152 2.489897
S 1.818430 -5.918228 1.137059
Au 0.416621 -4.975426 -0.495892
C 3.468600 -6.263936 0.393629

H 3.806055 -5.386518 -0.175036
H 4.151522 -6.377064 1.244320
Au 0.226167 5.052030 1.055512
S -1.382332 6.114399 -0.315013
Au -2.052824 4.283964 -1.666349
C -2.833196 6.341793 0.796614
H -3.061337 5.376991 1.268486
H -3.682441 6.631528 0.161877
Au -4.301832 0.953530 2.685640
S -5.137341 -1.050014 3.660979
Au -3.441141 -2.529626 2.911592
C -6.564718 -1.416308 2.539190
H -6.387885 -0.916139 1.582133
H -7.446869 -0.953872 3.004399
Au 3.100635 2.919618 -2.937876
S 4.855738 1.454445 -3.559832
Au 3.808614 -0.594283 -2.928995
C 6.039069 1.844526 -2.200015
H 5.467100 1.955978 -1.271164
H 6.492314 2.816176 -2.438865
Au -1.486844 -0.327593 -4.736391
S -3.240028 -1.931479 -4.983040
Au -3.967451 -1.881282 -2.742627
C -2.011328 -3.303528 -5.180540
H -1.235401 -3.141557 -4.424557
H -1.565977 -3.147143 -6.171355
Au 4.260149 0.720257 2.731659
S 3.686290 1.319750 4.942334
Au 1.363381 0.865368 4.779314
C 3.971908 3.145171 4.948947
H 4.046569 3.481856 3.909792
H 4.952530 3.299611 5.420430
S 1.384517 4.442908 -2.433173
S -3.661828 3.075061 1.885569
S 2.907189 -2.736948 -2.489906
S -1.950412 -4.119872 2.052064
S 1.902593 4.086255 2.401640
S -2.870889 2.635913 -3.140682
S 2.475726 -2.269978 4.017768
S -1.215474 -4.255738 -2.023514
S 0.528038 0.855968 -4.915426
S -4.907642 -1.646776 -0.586181
S 4.953066 0.186271 0.565131
S -0.888726 0.230121 4.942175
C -5.709015 -0.001331 -0.804237
H -4.969649 0.654709 -1.287171
H -5.899299 0.406217 0.199986

C 0.032446 2.632031 -4.959406
H -0.351024 2.905850 -3.967402
H 0.953242 3.207576 -5.126266
C -0.811769 -1.604299 5.143493
H -0.236231 -2.015704 4.299746
H -1.855310 -1.940236 5.038266
C 5.054370 -1.655899 0.569040
H 4.205195 -2.069080 1.134741
H 4.938366 -1.973551 -0.478193
C -1.145465 -5.120774 3.362084
H -0.545594 -4.469196 4.006072
H -0.462538 -5.788101 2.816588
C 1.498493 -2.870083 -3.683311
H 0.775108 -2.072435 -3.452337
H 1.028432 -3.833254 -3.440254
C -4.816128 3.468362 0.501615
H -5.100178 2.540306 -0.004512
H -4.230398 4.071884 -0.208993
C 2.181843 5.867657 -1.585581
H 2.494116 5.570113 -0.579715
H 1.389647 6.622944 -1.476354
C -2.793411 -4.851656 -1.266569
H -2.765941 -4.610457 -0.195714
H -3.591562 -4.258044 -1.741181
C -4.686995 2.955192 -3.229264
H -5.128993 2.922670 -2.227261
H -5.119032 2.150173 -3.839788
C 4.290225 -2.263048 4.304549
H 4.803569 -2.065036 3.358374
H 4.492873 -1.424028 4.986308
C 3.358705 3.853330 1.285311
H 2.994595 3.655880 0.264320
H 3.830331 2.920074 1.635609
C -1.012172 2.921389 -6.027069
H -0.623913 2.714272 -7.039830
H -1.898918 2.283266 -5.889695
C -1.454993 4.365162 -5.977127
O -0.867347 5.276870 -5.445479
O -2.632074 4.554428 -6.635115
H -2.823493 5.508354 -6.559229
C -2.531510 -4.731807 -5.039006
H -3.131523 -5.037454 -5.913398
H -3.167945 -4.844031 -4.150047
C -1.351771 -5.685193 -4.883419
O -1.381632 -6.740013 -4.270066
O -0.273271 -5.227097 -5.511517
H 0.580350 -5.648496 -5.215947

C -7.007110 -0.071252 -1.609165
H -6.862733 -0.639896 -2.538718
H -7.790880 -0.561744 -1.010772
C -7.396867 1.352406 -1.936985
O -7.419082 2.245268 -1.106727
O -7.617355 1.547598 -3.236793
H -7.634971 2.529571 -3.417846
C -6.044147 4.243515 0.957761
H -5.751508 5.060832 1.641341
H -6.766327 3.602141 1.480651
C -6.713295 4.900307 -0.225851
O -6.138879 5.288449 -1.226286
O -8.032023 5.079124 -0.045629
H -8.365856 5.470371 -0.874024
C -2.550128 7.382867 1.867479
H -2.254773 8.352905 1.432437
H -1.706349 7.068360 2.505603
C -3.755032 7.608668 2.750281
O -4.850713 7.113180 2.601847
O -3.481904 8.461138 3.762935
H -4.304529 8.537739 4.281774
C -4.890637 4.328628 -3.857252
H -4.416384 5.099911 -3.227918
H -4.392759 4.382298 -4.840637
C -6.317636 4.761270 -4.055637
O -7.338507 4.107635 -3.909968
O -6.381908 6.031665 -4.486927
H -7.329296 6.239008 -4.589386
C -3.044256 -6.345053 -1.485658
H -3.997844 -6.592708 -0.993464
H -3.128751 -6.569514 -2.559395
C -1.974183 -7.222297 -0.841967
O -1.934325 -7.448354 0.346885
O -1.057323 -7.734434 -1.678195
H -1.175191 -7.390254 -2.593894
C 3.460184 -7.551971 -0.465548
H 4.416375 -8.077919 -0.338853
H 2.634908 -8.210831 -0.157612
C 3.341018 -7.205843 -1.924093
O 4.339778 -7.081414 -2.639307
O 2.113356 -6.990789 -2.337182
H 2.120188 -6.623505 -3.272819
C 1.896028 -2.798980 -5.153946
H 1.007333 -3.092925 -5.732673
H 2.123953 -1.753370 -5.417111
C 3.108441 -3.659320 -5.557976
H 3.084230 -3.845598 -6.645741

H 4.048014 -3.134282 -5.337474
C 3.190252 -4.997748 -4.865830
O 2.201073 -5.731636 -4.660606
O 4.391584 -5.331029 -4.491581
H 4.369509 -6.142093 -3.865815
C 7.076688 0.747380 -2.035074
H 7.704317 0.634720 -2.936470
H 6.587201 -0.228903 -1.880315
C 7.987335 1.003564 -0.862697
O 8.082445 2.040202 -0.232298
O 8.754202 -0.063360 -0.571178
H 9.288103 0.180665 0.208852
C 6.393583 -2.103965 1.146527
H 7.235495 -1.815475 0.502120
H 6.563838 -1.631167 2.131026
C 6.434488 -3.586421 1.416694
O 5.491464 -4.265937 1.769312
O 7.668445 -4.103231 1.256731
H 7.605404 -5.042030 1.514813
C 4.773307 -3.584358 4.888653
H 4.498493 -4.405455 4.201285
H 4.306073 -3.808982 5.858400
C 6.275372 -3.615562 5.010554
O 7.058136 -2.977626 4.336088
O 6.697439 -4.483579 5.957204
H 7.672537 -4.453406 5.932238
C -6.773349 -2.900274 2.286608
H -5.844913 -3.352202 1.893735
H -7.023567 -3.458200 3.203584
C -7.848288 -3.130995 1.251531
O -8.465437 -2.271002 0.660972
O -8.051082 -4.447442 1.027629
H -8.723541 -4.501274 0.323132
C -0.238724 -2.085675 6.477718
H -0.775520 -1.609952 7.311528
H 0.835441 -1.862379 6.535550
C -0.493055 -3.580127 6.517440
O -1.607692 -4.057989 6.635550
O 0.604129 -4.311484 6.303644
H 0.316036 -5.248978 6.129040
C -2.175928 -5.918777 4.146547
H -2.847464 -5.236097 4.696549
H -2.797096 -6.527595 3.471772
C -1.550469 -6.820389 5.177059
O -0.427556 -6.726702 5.647638
O -2.381705 -7.797020 5.571597
H -1.908416 -8.295290 6.264574

C 3.369904 6.409863 -2.365692
H 4.133197 5.622346 -2.490581
H 3.086051 6.744993 -3.375512
C 4.048673 7.536693 -1.628939
O 3.836161 7.871285 -0.482764
O 4.972890 8.155931 -2.396602
H 5.393959 8.819956 -1.819587
C 4.380777 4.992922 1.319410
H 4.724639 5.159745 2.351391
H 3.969391 5.929324 0.920938
C 5.534862 4.541253 0.446692
O 5.734151 4.909290 -0.696387
O 6.268564 3.606531 1.062242
H 6.929136 3.206140 0.442217
C 2.878536 3.931030 5.654416
H 2.873683 3.756246 6.743439
H 1.883763 3.632931 5.285194
C 3.044752 5.410771 5.391297
O 4.007546 5.930430 4.870589
O 1.974210 6.118793 5.808639
H 2.150187 7.045681 5.560575

[Au₂₅(MPA)₁₈]⁻ TPSSh S₀ (Acetonitrile)

Au -0.055917 0.085558 0.053058
Au 0.885994 1.910625 1.957031
Au -2.020533 0.749721 -1.910525
Au 1.716769 -0.830129 2.060787
Au -1.034464 -1.836765 -1.722958
Au 0.603950 2.703584 -0.850384
Au 1.671553 -2.132229 -0.564060
Au -1.762776 2.198928 0.629203
Au -0.371259 -2.513983 1.255674
Au 2.634461 0.635061 -0.356210
Au -1.245734 0.083008 2.569435
Au 0.820242 0.392457 -2.546880
Au -2.713462 -0.848945 0.419248
Au 2.131533 -4.005909 2.379036
S 1.869589 -5.875628 0.983740
Au 0.448117 -4.939926 -0.632410
C 3.544168 -6.140247 0.253560
H 3.802404 -5.271750 -0.368556
H 4.231657 -6.146719 1.106824
Au 0.178167 5.006720 1.057227
S -1.393608 6.035543 -0.366973
Au -2.081039 4.219831 -1.709359

C -2.852093 6.389499 0.700582
H -3.101214 5.473220 1.251601
H -3.684886 6.635280 0.027175
Au -4.190794 1.019985 2.676615
S -4.911734 -1.015721 3.631670
Au -3.298620 -2.552772 2.857973
C -6.387482 -1.401747 2.583078
H -6.171522 -1.070641 1.562465
H -7.214223 -0.798191 2.982104
Au 2.986028 2.945673 -2.877230
S 4.704517 1.477567 -3.530203
Au 3.739686 -0.608237 -2.945277
C 5.959775 1.871534 -2.235262
H 5.428563 2.014760 -1.287425
H 6.418349 2.825578 -2.527638
Au -1.298387 -0.308664 -4.869157
S -3.128269 -1.822879 -5.059111
Au -3.845754 -1.786518 -2.811615
C -1.976478 -3.256375 -5.297137
H -1.173523 -3.124824 -4.564509
H -1.558256 -3.115877 -6.302020
Au 4.152099 0.727435 2.714933
S 3.541335 1.268638 4.930878
Au 1.215942 0.827563 4.810688
C 3.842090 3.089519 5.024013
H 3.926412 3.469880 4.000408
H 4.817728 3.208406 5.515225
S 1.324341 4.537734 -2.391067
S -3.633400 3.156870 1.847258
S 2.973151 -2.807880 -2.551450
S -1.888519 -4.235594 2.037857
S 1.861822 4.116488 2.450783
S -2.884492 2.598479 -3.212954
S 2.366889 -2.285275 3.966592
S -1.191445 -4.225544 -2.151098
S 0.729012 0.897997 -4.978805
S -4.778217 -1.650861 -0.623263
S 4.887910 0.255776 0.537412
S -1.046722 0.162576 5.003022
C -5.615820 -0.014859 -0.764739
H -4.921385 0.658532 -1.287619
H -5.745634 0.379059 0.254360
C 0.130363 2.645012 -4.947379
H -0.279749 2.844850 -3.946681
H 1.015415 3.281841 -5.079838
C -0.909773 -1.662417 5.240016
H -0.370219 -2.073200 4.372243

H -1.947053 -2.030129 5.204341
C 5.040218 -1.583631 0.533324
H 4.178149 -2.019696 1.061018
H 4.980220 -1.898526 -0.519047
C -1.068361 -5.135217 3.414593
H -0.502955 -4.427585 4.030569
H -0.347066 -5.799883 2.917182
C 1.576157 -2.988931 -3.751489
H 0.833285 -2.207318 -3.521912
H 1.126875 -3.959681 -3.502106
C -4.817493 3.511719 0.478352
H -5.121187 2.568731 0.013283
H -4.237266 4.081423 -0.263951
C 2.192658 5.895633 -1.500473
H 2.501749 5.543341 -0.511646
H 1.434218 6.678118 -1.352968
C -2.760465 -4.756209 -1.335959
H -2.690247 -4.511104 -0.268492
H -3.555144 -4.142098 -1.786830
C -4.706978 2.898079 -3.249119
H -5.110468 2.881923 -2.230506
H -5.146533 2.073819 -3.826514
C 4.178642 -2.269960 4.282966
H 4.698363 -2.060393 3.342976
H 4.364708 -1.436954 4.975616
C 3.323279 3.855819 1.348254
H 2.963939 3.658252 0.325192
H 3.778189 2.916341 1.704005
C -0.914400 2.925825 -6.016581
H -0.498089 2.808900 -7.031832
H -1.756236 2.219178 -5.936845
C -1.474037 4.322882 -5.896125
O -1.006411 5.220545 -5.227955
O -2.585031 4.476340 -6.648100
H -2.873181 5.407278 -6.569855
C -2.557061 -4.658469 -5.138702
H -3.168582 -4.952800 -6.008035
H -3.196874 -4.738498 -4.248130
C -1.421001 -5.657714 -4.975548
O -1.518377 -6.730010 -4.390519
O -0.305692 -5.236706 -5.551850
H 0.519876 -5.723437 -5.276559
C -6.963334 -0.115366 -1.482619
H -6.873227 -0.711102 -2.401697
H -7.703663 -0.590285 -0.820872
C -7.380406 1.295755 -1.826806
O -7.439728 2.194124 -1.001382

O -7.574388 1.476104 -3.130038
H -7.598981 2.460402 -3.337804
C -6.025458 4.320519 0.926743
H -5.707847 5.145002 1.590771
H -6.757551 3.707857 1.469807
C -6.684743 4.978762 -0.263768
O -6.091291 5.354009 -1.259118
O -7.996862 5.173010 -0.087689
H -8.341659 5.625486 -0.883100
C -2.555627 7.522303 1.669204
H -2.281883 8.452705 1.146144
H -1.698537 7.269166 2.317744
C -3.739040 7.809947 2.564296
O -4.788681 7.195983 2.562948
O -3.497270 8.840864 3.387100
H -4.286367 8.976865 3.948747
C -4.950133 4.251677 -3.906160
H -4.442457 5.044984 -3.334851
H -4.516939 4.271650 -4.920335
C -6.391603 4.672042 -4.036841
O -7.388929 3.986650 -3.848440
O -6.488440 5.935641 -4.443458
H -7.435658 6.161280 -4.536795
C -3.074587 -6.239151 -1.550583
H -4.011543 -6.461487 -1.017713
H -3.220602 -6.446760 -2.620407
C -2.005158 -7.159097 -0.983564
O -1.925980 -7.444957 0.195076
O -1.122970 -7.652862 -1.861896
H -1.273509 -7.296190 -2.773489
C 3.648121 -7.475096 -0.516329
H 4.659916 -7.882754 -0.394845
H 2.923521 -8.203594 -0.121745
C 3.428071 -7.269786 -1.988787
O 4.359435 -7.297938 -2.798355
O 2.184809 -6.997801 -2.325175
H 2.136866 -6.720878 -3.289655
C 1.954968 -2.914127 -5.225244
H 1.042765 -3.158712 -5.789964
H 2.222702 -1.876165 -5.480369
C 3.115082 -3.822507 -5.669671
H 3.046764 -4.008771 -6.754769
H 4.084040 -3.338238 -5.487680
C 3.164884 -5.162487 -4.983156
O 2.163032 -5.859686 -4.727816
O 4.371251 -5.539982 -4.654356
H 4.346309 -6.371433 -4.065858

C 6.988384 0.764749 -2.092041
H 7.587945 0.635147 -3.008571
H 6.497456 -0.205918 -1.906606
C 7.938494 1.024976 -0.951225
O 7.998962 2.050930 -0.289588
O 8.755691 -0.006374 -0.734065
H 9.354826 0.217162 0.006770
C 6.362296 -2.000524 1.169343
H 7.223351 -1.718169 0.548284
H 6.491993 -1.499472 2.146154
C 6.406471 -3.478233 1.477868
O 5.443796 -4.148762 1.799436
O 7.648038 -3.975896 1.401469
H 7.616218 -4.917056 1.666252
C 4.661969 -3.590385 4.861984
H 4.405741 -4.416152 4.174734
H 4.188565 -3.820630 5.828358
C 6.163765 -3.609430 5.009240
O 6.931427 -2.828247 4.478546
O 6.580211 -4.626761 5.778978
H 7.557665 -4.606231 5.808639
C -6.726621 -2.882320 2.565777
H -5.856497 -3.471937 2.224293
H -6.990932 -3.267298 3.563231
C -7.861082 -3.171394 1.609265
O -8.397456 -2.354021 0.886724
O -8.205878 -4.466966 1.632028
H -8.924395 -4.604742 0.982933
C -0.242589 -2.100831 6.545775
H -0.741372 -1.631774 7.406178
H 0.825061 -1.842952 6.534191
C -0.440660 -3.599703 6.617840
O -1.529538 -4.113652 6.824836
O 0.654429 -4.299838 6.325787
H 0.384994 -5.249667 6.172933
C -2.082611 -5.932684 4.222798
H -2.755126 -5.253241 4.774358
H -2.714470 -6.548360 3.564580
C -1.441804 -6.833941 5.248853
O -0.304574 -6.725310 5.691305
O -2.263140 -7.800076 5.651724
H -1.811572 -8.326875 6.342317
C 3.387773 6.422964 -2.278965
H 4.127490 5.620994 -2.439209
H 3.097689 6.795543 -3.274066
C 4.100575 7.522609 -1.531016
O 3.835355 7.895911 -0.403417

O 5.092707 8.055797 -2.259065
H 5.531980 8.741641 -1.718031
C 4.367877 4.973890 1.383231
H 4.723698 5.123161 2.414020
H 3.972948 5.922501 0.997660
C 5.511772 4.521213 0.497554
O 5.753241 4.967869 -0.610480
O 6.184073 3.507045 1.047119
H 6.842711 3.114857 0.410649
C 2.746365 3.842955 5.757954
H 2.731481 3.610511 6.835415
H 1.753697 3.569988 5.362519
C 2.910862 5.335367 5.584550
O 3.862819 5.881222 5.061456
O 1.861642 6.008911 6.080057
H 2.018046 6.963759 5.938591

[Au₂₅(MPA)₁₈]- TPSSh T₁ (Acetonitrile).

Au -0.041918 0.058265 -0.046551
Au 0.878358 1.866218 1.898093
Au -2.103045 0.646532 -1.873033
Au 1.771675 -0.832324 1.953019
Au -1.128710 -1.936850 -1.684362
Au 0.594086 2.686686 -0.842933
Au 1.649168 -2.172633 -0.643833
Au -1.744483 2.222643 0.559002
Au -0.386959 -2.509440 1.149729
Au 2.765646 0.519448 -0.399994
Au -1.362996 0.085950 2.484581
Au 1.157272 0.508898 -2.567085
Au -2.805793 -0.900602 0.459596
Au 2.151144 -4.054385 2.162139
S 2.087064 -5.870845 0.667045
Au 0.509105 -5.004758 -0.846842
C 3.755973 -5.856205 -0.121489
H 3.861409 -4.926712 -0.700198
H 4.461260 -5.812380 0.716147
Au 0.233234 5.003336 1.007294
S -1.346188 6.010174 -0.436806
Au -2.034174 4.172179 -1.765209
C -2.809287 6.319696 0.641839
H -3.048038 5.386459 1.168599
H -3.646064 6.573631 -0.023740
Au -4.265441 0.914383 2.600869
S -4.999851 -1.098794 3.616695

Au -3.310865 -2.587135 2.875457
C -6.439494 -1.552227 2.554363
H -6.139128 -1.422912 1.508064
H -7.239046 -0.835916 2.787885
Au 3.216093 2.828811 -2.869114
S 5.006110 1.391911 -3.454275
Au 3.933691 -0.666624 -2.916569
C 6.166406 1.764411 -2.069112
H 5.569900 1.887093 -1.157495
H 6.640970 2.725490 -2.307913
Au -1.251118 -0.425349 -4.786953
S -3.134774 -1.823978 -5.047679
Au -3.896890 -1.820154 -2.818934
C -2.264148 -3.425832 -5.357991
H -1.379085 -3.459971 -4.710005
H -1.948859 -3.388539 -6.409348
Au 4.231870 0.663231 2.775855
S 3.626945 1.293294 4.965138
Au 1.298521 0.935607 4.717801
C 3.966072 3.109449 4.984140
H 3.993152 3.461996 3.948178
H 4.971605 3.221255 5.412932
S 1.491299 4.370677 -2.439767
S -3.678523 3.051528 1.799280
S 2.990123 -2.805760 -2.607160
S -1.794891 -4.220243 2.128039
S 1.877439 4.070486 2.428873
S -2.868100 2.509458 -3.219052
S 2.141370 -2.381667 3.827118
S -1.264040 -4.318168 -2.234852
S 0.710134 0.851068 -4.930732
S -4.850243 -1.728468 -0.657387
S 4.970560 0.107572 0.632513
S -0.979907 0.379283 4.860389
C -5.700410 -0.097062 -0.763842
H -5.005650 0.591759 -1.265685
H -5.837370 0.269724 0.264657
C 0.102952 2.593139 -4.931162
H -0.317226 2.806855 -3.939402
H 0.992343 3.224515 -5.058639
C -0.950792 -1.423180 5.255700
H -0.480654 -1.935671 4.403585
H -2.007316 -1.725319 5.302980
C 5.104601 -1.733041 0.689506
H 4.207162 -2.147316 1.173089
H 5.109360 -2.075978 -0.355918
C -0.941488 -4.995568 3.561958

H -0.397784 -4.232561 4.130791
H -0.198169 -5.669794 3.111668
C 1.602395 -2.891589 -3.838952
H 0.809979 -2.203483 -3.505207
H 1.230448 -3.920117 -3.737513
C -4.829255 3.437302 0.410783
H -5.142537 2.501755 -0.063535
H -4.228444 4.001643 -0.318509
C 2.272317 5.786920 -1.558840
H 2.517677 5.489275 -0.534146
H 1.491670 6.559388 -1.502303
C -2.745694 -4.808554 -1.237576
H -2.533859 -4.580474 -0.185922
H -3.569178 -4.162654 -1.576155
C -4.687872 2.815878 -3.286927
H -5.106557 2.817032 -2.274358
H -5.121608 1.983709 -3.857500
C 3.884967 -2.326917 4.404003
H 4.532469 -2.102561 3.549684
H 3.950970 -1.492185 5.116639
C 3.356123 3.788371 1.352407
H 3.014952 3.584700 0.324667
H 3.796310 2.848311 1.725195
C -0.927045 2.854453 -6.017967
H -0.493401 2.748468 -7.026873
H -1.759481 2.135173 -5.953015
C -1.511542 4.241629 -5.896583
O -1.095091 5.126920 -5.180097
O -2.582606 4.398692 -6.703687
H -2.890257 5.322534 -6.616700
C -3.152108 -4.639865 -5.087814
H -4.040007 -4.619027 -5.740966
H -3.487231 -4.650097 -4.042970
C -2.403403 -5.923964 -5.358682
O -2.255858 -6.844727 -4.569331
O -1.902208 -5.965880 -6.593573
H -1.430517 -6.814921 -6.714550
C -7.042114 -0.183609 -1.496285
H -6.950544 -0.789618 -2.408094
H -7.798211 -0.640087 -0.839545
C -7.427564 1.231770 -1.862053
O -7.505988 2.136377 -1.045426
O -7.563810 1.405262 -3.173704
H -7.573434 2.387741 -3.391354
C -6.029634 4.263930 0.847111
H -5.704573 5.085787 1.510664
H -6.773733 3.663390 1.387358

C -6.672089 4.926929 -0.349426
O -6.069325 5.280761 -1.347034
O -7.979940 5.152112 -0.177110
H -8.312939 5.606399 -0.976529
C -2.523183 7.431337 1.637602
H -2.259688 8.376210 1.135149
H -1.661164 7.172243 2.277165
C -3.705311 7.689549 2.542616
O -4.762269 7.089128 2.511149
O -3.453679 8.678592 3.412957
H -4.243256 8.798565 3.977535
C -4.917042 4.159459 -3.967901
H -4.403906 4.958232 -3.409052
H -4.481905 4.157991 -4.981329
C -6.355200 4.586437 -4.110787
O -7.356649 3.907890 -3.919154
O -6.443377 5.844960 -4.534684
H -7.388776 6.074110 -4.637311
C -3.140094 -6.277263 -1.416910
H -3.958258 -6.492555 -0.713571
H -3.498594 -6.453612 -2.441302
C -1.996758 -7.225252 -1.098563
O -1.697752 -7.566923 0.027918
O -1.293402 -7.663122 -2.151541
H -1.642667 -7.285359 -2.995752
C 4.021126 -7.116904 -0.973873
H 5.062892 -7.434819 -0.838872
H 3.361296 -7.939928 -0.658545
C 3.829980 -6.838558 -2.440418
O 4.784341 -6.764387 -3.218659
O 2.580296 -6.632087 -2.799023
H 2.548305 -6.294861 -3.751660
C 1.986100 -2.573265 -5.282726
H 1.142812 -2.904286 -5.911132
H 2.064362 -1.480856 -5.401874
C 3.299722 -3.194974 -5.781689
H 3.310860 -3.217076 -6.884355
H 4.164249 -2.593615 -5.464730
C 3.509368 -4.598456 -5.278265
O 2.578575 -5.390840 -5.100753
O 4.766188 -4.894915 -5.014858
H 4.797557 -5.758821 -4.491243
C 7.185509 0.655712 -1.878614
H 7.839797 0.541077 -2.759305
H 6.685550 -0.317444 -1.737524
C 8.066203 0.901682 -0.680653
O 8.103008 1.928641 -0.018373

O 8.853054 -0.141293 -0.412229
H 9.410557 0.076682 0.362046
C 6.381694 -2.127678 1.425284
H 7.280865 -1.866195 0.850705
H 6.447343 -1.583557 2.385592
C 6.414940 -3.588118 1.804128
O 5.437534 -4.257016 2.083759
O 7.663524 -4.071156 1.847971
H 7.623202 -4.997314 2.160127
C 4.303620 -3.640001 5.045848
H 4.128199 -4.472051 4.340680
H 3.723488 -3.862569 5.953628
C 5.780532 -3.652746 5.356162
O 6.603529 -2.889688 4.885611
O 6.107768 -4.644058 6.199831
H 7.076558 -4.623537 6.333115
C -6.890661 -2.986048 2.774308
H -6.061577 -3.690270 2.583019
H -7.217742 -3.167596 3.810629
C -8.023042 -3.346447 1.839159
O -8.498318 -2.610953 0.996109
O -8.449512 -4.602370 2.040830
H -9.170155 -4.787165 1.405966
C -0.235529 -1.788449 6.557715
H -0.698002 -1.269252 7.410192
H 0.830940 -1.532118 6.495294
C -0.419745 -3.282264 6.718936
O -1.513480 -3.798015 6.893424
O 0.700513 -3.981749 6.549204
H 0.452734 -4.942240 6.425977
C -1.940399 -5.766076 4.416660
H -2.616630 -5.064999 4.936109
H -2.570332 -6.419090 3.794074
C -1.291828 -6.609400 5.485775
O -0.175922 -6.439465 5.962270
O -2.083312 -7.599770 5.890817
H -1.633045 -8.085026 6.612084
C 3.510546 6.300342 -2.276495
H 4.270038 5.502712 -2.346121
H 3.287910 6.622298 -3.305746
C 4.159392 7.439083 -1.529344
O 3.852683 7.816486 -0.413647
O 5.152080 7.996894 -2.238151
H 5.554532 8.702635 -1.693964
C 4.405023 4.902396 1.398020
H 4.718323 5.081099 2.438247
H 4.027806 5.840754 0.972030

C 5.586217 4.427150 0.576266
O 5.888042 4.855522 -0.524382
O 6.223386 3.418835 1.176418
H 6.914235 3.012653 0.584297
C 2.930352 3.899080 5.764714
H 2.952464 3.668597 6.842014
H 1.912709 3.659500 5.411307
C 3.130598 5.385309 5.577748
O 4.017285 5.898841 4.923590
O 2.191180 6.093824 6.221755
H 2.359581 7.043483 6.059906

[Au₂₅(MPA)₁₈]⁻ PBEh-3c S₀ (gas)

Au 0.032341 0.077941 0.091779
Au 1.077018 1.923425 1.924884
Au -1.654978 0.965923 -1.971717
Au 1.681474 -0.908919 2.165364
Au -1.030404 -1.801037 -1.739811
Au 0.724425 2.603886 -0.949063
Au 1.714421 -2.124965 -0.661688
Au -1.623823 2.238058 0.772579
Au -0.471186 -2.522928 1.082215
Au 2.781388 0.570096 -0.121965
Au -1.071274 0.045161 2.675200
Au 1.154740 0.187951 -2.491455
Au -2.709002 -0.489865 0.358420
Au 2.152008 -4.145418 2.046968
S 1.819716 -5.880938 0.529182
Au 0.309178 -4.898958 -0.967006
C 3.362361 -6.099928 -0.418490
H 3.515450 -5.222469 -1.059466
H 4.200727 -6.113595 0.286172
Au 0.161805 5.000923 1.045419
S -1.344148 6.025275 -0.432854
Au -1.989416 4.275009 -1.854199
C -2.818163 6.496770 0.525912
H -3.199377 5.628792 1.073760
H -3.582465 6.801831 -0.198687
Au -4.002929 1.150359 2.828515
S -4.574032 -0.853263 3.899257
Au -3.197942 -2.459349 2.887673
C -6.233044 -1.265873 3.255962
H -6.187474 -1.386902 2.168920
H -6.887765 -0.412468 3.470301
Au 3.199849 2.910958 -2.945584

S 5.123122 1.632334 -3.289993
Au 4.222564 -0.441775 -2.648909
C 6.174537 2.237382 -1.923152
H 5.581191 2.308947 -1.006243
H 6.484774 3.252875 -2.196548
Au -1.150050 -0.605438 -4.750208
S -3.446816 -1.019256 -4.816207
Au -4.066302 -1.199963 -2.569662
C -3.651857 -2.696321 -5.502931
H -3.111494 -3.422211 -4.883528
H -3.176933 -2.696447 -6.492006
Au 4.228820 0.772863 2.939210
S 3.556017 1.207679 5.132295
Au 1.267532 0.731143 4.983147
C 3.755890 3.008426 5.343430
H 3.274991 3.537531 4.513323
H 4.831883 3.212375 5.294577
S 1.347255 4.290906 -2.629491
S -3.559570 3.248429 1.866684
S 3.561875 -2.654939 -2.192056
S -1.939059 -4.224862 2.018085
S 1.811089 4.182491 2.499084
S -2.553239 2.660215 -3.456088
S 2.290296 -2.602245 3.803790
S -1.356978 -4.114034 -2.425342
S 1.116933 -0.053026 -4.918436
S -4.869622 -1.375464 -0.372481
S 5.056036 0.345144 0.800584
S -0.989959 0.105589 5.119032
C -6.149065 -0.071964 -0.299915
H -5.762695 0.828029 -0.789168
H -6.278894 0.186273 0.757437
C 1.095690 1.645176 -5.595580
H 0.574115 2.322206 -4.909010
H 2.142486 1.968740 -5.637381
C -0.916146 -1.672252 5.528291
H -0.421787 -2.208686 4.709246
H -1.959465 -2.008320 5.576073
C 5.379952 -1.455756 0.800200
H 4.514708 -1.992174 1.204871
H 5.474390 -1.765017 -0.247985
C -1.115077 -5.032090 3.435291
H -0.495717 -4.313224 3.981502
H -0.431561 -5.773280 3.001999
C 2.795513 -3.245244 -3.748044
H 1.790868 -2.817527 -3.848225
H 2.658538 -4.327365 -3.615263

C -4.760069 3.346000 0.497838
H -4.673228 2.438673 -0.109763
H -4.453210 4.177916 -0.147051
C 2.036895 5.797414 -1.860173
H 2.494495 5.547171 -0.900260
H 1.183669 6.454723 -1.654431
C -2.889186 -4.702627 -1.587929
H -2.628807 -5.327147 -0.728246
H -3.447977 -3.845648 -1.199414
C -4.369853 2.492853 -3.496276
H -4.748558 2.189844 -2.515170
H -4.573614 1.674267 -4.197351
C 4.036857 -2.553833 4.314362
H 4.668658 -2.317499 3.456469
H 4.131014 -1.728816 5.032257
C 3.368725 4.179565 1.540526
H 3.177497 3.783374 0.534358
H 4.019645 3.454792 2.043353
C 0.468647 1.693846 -6.974179
H 0.893953 0.913518 -7.624806
H -0.607763 1.476027 -6.926000
C 0.665297 3.020334 -7.661610
O 1.402431 3.890209 -7.305032
O -0.081150 3.121352 -8.764174
H 0.091884 3.977230 -9.166230
C -5.133798 -3.016642 -5.620255
H -5.651346 -2.246365 -6.204532
H -5.603395 -2.994015 -4.622115
C -5.408665 -4.376529 -6.197491
O -4.753268 -5.362620 -5.987421
O -6.487105 -4.407353 -6.963315
H -6.630015 -5.310045 -7.265980
C -7.495668 -0.516020 -0.901958
H -7.415827 -1.542907 -1.284189
H -8.273407 -0.523658 -0.131684
C -7.921015 0.394257 -2.028634
O -8.864641 1.143328 -1.976448
O -7.120486 0.306909 -3.065740
H -7.221801 1.069827 -3.675704
C -6.186007 3.554556 0.982536
H -6.302113 4.571939 1.386843
H -6.433689 2.868298 1.802100
C -7.160202 3.357043 -0.153119
O -6.916698 3.645867 -1.294478
O -8.292897 2.798901 0.230510
H -8.802696 2.510288 -0.545185
C -2.506930 7.623656 1.487745

H -2.060357 8.483589 0.966124
H -1.751638 7.311857 2.224979
C -3.730591 8.093781 2.229434
O -4.841980 7.682358 2.066468
O -3.442060 9.050213 3.111046
H -4.253509 9.306136 3.558525
C -5.034472 3.776603 -3.950034
H -4.914266 4.568292 -3.199248
H -4.546745 4.156920 -4.862359
C -6.496766 3.629463 -4.264438
O -7.078156 2.590345 -4.454376
O -7.106851 4.793087 -4.388921
H -8.039313 4.635127 -4.564424
C -3.736953 -5.480104 -2.570990
H -4.678297 -5.769580 -2.076312
H -4.022459 -4.842529 -3.417558
C -3.062124 -6.765590 -3.030568
O -2.440557 -7.459676 -2.285260
O -3.239695 -7.110514 -4.295424
H -3.707078 -6.437968 -4.806317
C 3.290129 -7.407601 -1.220317
H 3.630935 -8.246768 -0.601078
H 2.260346 -7.619583 -1.530676
C 4.166554 -7.268645 -2.433734
O 5.364720 -7.095030 -2.358170
O 3.499506 -7.262501 -3.556315
H 4.042349 -6.889420 -4.291682
C 3.589800 -2.940500 -5.012564
H 3.103582 -3.488180 -5.831462
H 3.481371 -1.875503 -5.257593
C 5.081270 -3.280832 -4.992663
H 5.487327 -3.122092 -6.001841
H 5.633826 -2.617093 -4.318601
C 5.323045 -4.714337 -4.611606
O 4.748132 -5.631160 -5.162858
O 6.163318 -4.878430 -3.626243
H 6.114753 -5.794134 -3.270356
C 7.367748 1.336756 -1.692725
H 7.999510 1.274286 -2.593082
H 7.046106 0.306849 -1.485757
C 8.228576 1.808673 -0.553624
O 8.194797 2.901426 -0.056707
O 9.085738 0.880300 -0.149386
H 9.602253 1.229822 0.583192
C 6.652227 -1.792198 1.558114
H 7.525544 -1.315421 1.096301
H 6.609215 -1.407064 2.590281

C 6.869761 -3.279222 1.678811
O 5.998110 -4.099799 1.738215
O 8.157167 -3.601695 1.739262
H 8.224841 -4.552545 1.866141
C 4.457227 -3.866365 4.943537
H 4.311665 -4.693319 4.229880
H 3.827696 -4.109569 5.809989
C 5.908568 -3.885003 5.335278
O 6.749029 -3.128316 4.939097
O 6.190815 -4.879170 6.176311
H 7.133646 -4.858669 6.363070
C -6.767582 -2.527061 3.901800
H -6.097528 -3.379190 3.706628
H -6.799498 -2.432759 4.996941
C -8.139092 -2.893059 3.399280
O -8.735954 -2.322379 2.533545
O -8.634272 -3.955634 4.031633
H -9.498904 -4.155674 3.661833
C -0.217213 -1.998415 6.844087
H -0.718660 -1.488722 7.676583
H 0.830355 -1.677501 6.814666
C -0.319056 -3.492891 7.035643
O -1.349263 -4.056399 7.290206
O 0.821160 -4.126700 6.816731
H 0.652486 -5.075367 6.718524
C -2.125210 -5.699762 4.347461
H -2.775535 -4.950801 4.825400
H -2.802075 -6.348098 3.772196
C -1.503494 -6.510097 5.451691
O -0.329295 -6.572372 5.701755
O -2.410534 -7.182171 6.145485
H -1.970883 -7.628955 6.874353
C 3.045062 6.493641 -2.749707
H 3.905417 5.843490 -2.959767
H 2.609340 6.733804 -3.731366
C 3.568112 7.760582 -2.127093
O 3.178612 8.249008 -1.106008
O 4.529213 8.316466 -2.863060
H 4.844163 9.098201 -2.401552
C 4.085555 5.523541 1.458481
H 4.362057 5.862668 2.465998
H 3.456039 6.293742 0.998204
C 5.318111 5.317056 0.605677
O 5.438015 5.692711 -0.528335
O 6.230603 4.593951 1.233421
H 6.934209 4.298117 0.635250
C 3.173850 3.469208 6.662883

H 3.580931 2.886812 7.503899
H 2.087452 3.298376 6.692262
C 3.438317 4.928434 6.927949
O 4.120909 5.643446 6.255865
O 2.821969 5.352396 8.031423
H 3.018613 6.286099 8.148607

[Au₂₅(MPA)₁₈]⁻ PBEh-3c T₁ (gas)

Au -0.037278 0.064606 0.008191
Au 0.999230 1.887927 1.853260
Au -1.944025 0.769741 -1.985555
Au 1.804406 -0.956620 1.921788
Au -1.259339 -1.923656 -1.641523
Au 0.579597 2.732190 -0.806031
Au 1.575486 -2.100368 -0.786111
Au -1.765642 2.160320 0.661703
Au -0.420099 -2.552732 1.100967
Au 2.752352 0.559438 -0.410798
Au -1.392457 -0.012929 2.568235
Au 1.124435 0.600152 -2.624937
Au -2.879801 -0.661995 0.403642
Au 2.095283 -4.208470 2.206921
S 1.791615 -6.052590 0.815136
Au 0.349635 -5.091050 -0.750859
C 3.439345 -6.384930 0.104931
H 3.797517 -5.519102 -0.465450
H 4.115940 -6.482350 0.959498
Au 0.253077 5.068544 1.242967
S -1.313794 6.156328 -0.126437
Au -1.939089 4.397850 -1.564764
C -2.780729 6.480952 0.907028
H -3.109554 5.552739 1.386877
H -3.577814 6.810332 0.229597
Au -4.352398 0.984766 2.612987
S -5.135499 -1.003900 3.591702
Au -3.451855 -2.468046 2.850859
C -6.589390 -1.455643 2.581555
H -6.310875 -1.493931 1.522645
H -7.325905 -0.652512 2.705118
Au 3.156491 2.889127 -2.970314
S 4.968810 1.507989 -3.558855
Au 3.934035 -0.552544 -3.016830
C 6.130915 1.988067 -2.233194
H 5.590508 2.095133 -1.288014
H 6.509958 2.979753 -2.508809

Au -1.474379 -0.243264 -4.885797
S -3.229126 -1.794830 -5.159224
Au -3.946356 -1.692326 -2.929181
C -2.091211 -3.214100 -5.397809
H -1.293141 -3.151744 -4.653829
H -1.638338 -3.057577 -6.383529
Au 4.345456 0.634735 2.716484
S 3.755275 1.147522 4.920771
Au 1.448428 0.757458 4.713425
C 4.090247 2.935352 5.090276
H 4.022612 3.419182 4.113258
H 5.132502 3.015952 5.421165
S 1.408316 4.351440 -2.460478
S -3.708383 3.087646 1.809340
S 3.000300 -2.692536 -2.683746
S -1.961011 -4.109241 2.121958
S 1.919649 4.077382 2.563291
S -2.625725 2.806106 -3.149683
S 2.356264 -2.488994 3.771896
S -1.350605 -4.326587 -2.173921
S 0.577034 0.838395 -4.982072
S -4.886079 -1.509088 -0.784364
S 5.025674 0.192278 0.543021
S -0.809850 0.208625 4.891626
C -5.918267 -0.013275 -0.940179
H -5.341729 0.745470 -1.482414
H -6.085284 0.378926 0.071471
C 0.243311 2.610702 -5.263823
H -0.095319 3.076118 -4.333562
H 1.205766 3.066733 -5.523778
C -0.815189 -1.556701 5.358898
H -0.314713 -2.133652 4.572740
H -1.872004 -1.851587 5.373001
C 5.299210 -1.616363 0.502562
H 4.445401 -2.140236 0.946158
H 5.328040 -1.909774 -0.555054
C -1.209076 -4.962660 3.546114
H -0.589029 -4.268840 4.120874
H -0.538252 -5.715972 3.114710
C 1.734583 -2.910235 -3.992752
H 0.979464 -2.121503 -3.912824
H 1.232203 -3.852189 -3.744886
C -4.873972 3.474817 0.461702
H -4.962553 2.613207 -0.208145
H -4.419485 4.283880 -0.121549
C 2.142705 5.812952 -1.655518
H 2.610861 5.528886 -0.710800

H 1.307746 6.483484 -1.418714
C -2.869586 -4.939552 -1.347479
H -2.776516 -4.805325 -0.264223
H -3.699153 -4.306161 -1.682750
C -4.433498 2.980167 -3.333315
H -4.934811 2.800560 -2.377738
H -4.749648 2.195342 -4.030661
C 4.128017 -2.538355 4.196757
H 4.730588 -2.426194 3.293010
H 4.325927 -1.671364 4.839560
C 3.419252 4.045810 1.512984
H 3.143536 3.781658 0.484061
H 4.024406 3.212701 1.887287
C -0.781245 2.847407 -6.356395
H -0.493058 2.325182 -7.282803
H -1.759726 2.448552 -6.063053
C -0.917117 4.312676 -6.687147
O -0.032560 5.115128 -6.655260
O -2.159163 4.634573 -7.059926
H -2.173236 5.571458 -7.277248
C -2.733559 -4.585422 -5.313065
H -3.395957 -4.774618 -6.171984
H -3.363192 -4.674561 -4.419035
C -1.706431 -5.695338 -5.247864
O -1.912225 -6.781441 -4.772479
O -0.554864 -5.359144 -5.795003
H 0.135461 -6.011965 -5.628127
C -7.260070 -0.284028 -1.623919
H -7.128209 -0.987022 -2.454884
H -7.967651 -0.719876 -0.909032
C -7.763668 1.040957 -2.142296
O -8.359955 1.842429 -1.475843
O -7.380251 1.244877 -3.387491
H -7.450700 2.182036 -3.661363
C -6.229811 3.909592 0.977115
H -6.117167 4.740348 1.692222
H -6.729347 3.100729 1.527297
C -7.126426 4.381298 -0.139447
O -6.746097 4.700725 -1.232252
O -8.396487 4.442535 0.226180
H -8.931596 4.632289 -0.549676
C -2.492196 7.537794 1.951857
H -2.103569 8.459310 1.492349
H -1.699930 7.204218 2.638872
C -3.711650 7.886355 2.764317
O -4.813035 7.455039 2.585322
O -3.432592 8.758790 3.731983

H -4.240028 8.937711 4.222210
C -4.769859 4.363742 -3.854810
H -4.457726 5.131780 -3.133890
H -4.196981 4.572763 -4.772695
C -6.220008 4.597563 -4.170875
O -7.083234 3.763718 -4.261788
O -6.471437 5.874495 -4.410844
H -7.409987 5.972378 -4.594621
C -3.194642 -6.388594 -1.680504
H -4.119055 -6.643994 -1.144658
H -3.402519 -6.499995 -2.751414
C -2.129092 -7.366645 -1.210609
O -1.968454 -7.631788 -0.057084
O -1.378480 -7.921999 -2.149561
H -1.572812 -7.575296 -3.029974
C 3.476528 -7.684261 -0.717267
H 4.426700 -8.197807 -0.536890
H 2.664023 -8.354682 -0.406715
C 3.393857 -7.393188 -2.187081
O 4.377308 -7.412667 -2.902952
O 2.205895 -7.063194 -2.600885
H 2.228502 -6.712053 -3.524810
C 2.269395 -2.933919 -5.415963
H 1.448722 -3.286890 -6.055164
H 2.484616 -1.906398 -5.739757
C 3.523515 -3.765873 -5.650633
H 3.695195 -3.876835 -6.732648
H 4.410367 -3.250608 -5.261817
C 3.489369 -5.144493 -5.051158
O 2.456599 -5.781449 -4.904480
O 4.655965 -5.594750 -4.708523
H 4.586817 -6.417885 -4.150451
C 7.259806 0.998422 -2.059287
H 7.853837 0.898222 -2.981269
H 6.868553 -0.007220 -1.850735
C 8.186089 1.393630 -0.941108
O 8.204585 2.459931 -0.391466
O 9.034565 0.422323 -0.621691
H 9.591186 0.721649 0.103622
C 6.601147 -1.981687 1.194457
H 7.462564 -1.541665 0.676968
H 6.627736 -1.568772 2.216650
C 6.793809 -3.467103 1.352023
O 5.911515 -4.275978 1.414956
O 8.076280 -3.800922 1.447012
H 8.132748 -4.744283 1.623328
C 4.487763 -3.822444 4.917781

H 4.230490 -4.694869 4.295226
H 3.903616 -3.939512 5.840106
C 5.959579 -3.925038 5.210560
O 6.825525 -3.313501 4.651697
O 6.224446 -4.818474 6.162182
H 7.177703 -4.863294 6.279133
C -7.162572 -2.786540 3.021567
H -6.421422 -3.591015 2.894729
H -7.401129 -2.782751 4.095486
C -8.400071 -3.165027 2.251438
O -8.889638 -2.528566 1.365079
O -8.912478 -4.321502 2.670948
H -9.687522 -4.521621 2.138452
C -0.177544 -1.859929 6.709949
H -0.677050 -1.289033 7.502352
H 0.886869 -1.597378 6.698259
C -0.371747 -3.337751 6.958179
O -1.425349 -3.819326 7.275340
O 0.711220 -4.053451 6.704677
H 0.474200 -4.992102 6.633403
C -2.264985 -5.619183 4.411774
H -2.928749 -4.864336 4.861758
H -2.918428 -6.261569 3.804013
C -1.698193 -6.435145 5.540495
O -0.538917 -6.493366 5.856455
O -2.635191 -7.116882 6.181677
H -2.228570 -7.574902 6.922794
C 3.149580 6.505688 -2.548884
H 3.986510 5.836731 -2.792870
H 2.698167 6.781201 -3.514083
C 3.719706 7.742304 -1.907168
O 3.373395 8.207910 -0.860298
O 4.668182 8.299213 -2.658164
H 5.015939 9.059550 -2.184644
C 4.257594 5.320172 1.534850
H 4.589460 5.536197 2.560070
H 3.691071 6.185302 1.171349
C 5.446750 5.094092 0.626123
O 5.589425 5.592012 -0.456168
O 6.293007 4.212025 1.136480
H 6.963004 3.942473 0.491709
C 3.149331 3.616267 6.058412
H 3.165385 3.138683 7.049294
H 2.110152 3.534190 5.705604
C 3.461285 5.081624 6.213441
O 4.343506 5.666500 5.655812
O 2.625887 5.680310 7.059924

H 2.847723 6.615002 7.096500

[Au₂₅(MPA)₁₈]⁻ PBEh-3c S₀ (acetonitrile)

Au 0.027320 0.028228 0.029664
Au 1.006720 1.891948 1.869212
Au -1.725582 0.846538 -2.047812
Au 1.674942 -0.975522 2.099886
Au -0.970113 -1.873478 -1.827965
Au 0.692945 2.592595 -0.970608
Au 1.760555 -2.137564 -0.682562
Au -1.697066 2.124267 0.667361
Au -0.425566 -2.610735 1.025507
Au 2.761602 0.559218 -0.208735
Au -1.112582 -0.035114 2.582838
Au 1.128080 0.219704 -2.553334
Au -2.678682 -0.681505 0.253535
Au 2.133368 -4.168763 2.161329
S 2.028156 -5.936268 0.640129
Au 0.651419 -4.985812 -0.989641
C 3.763394 -6.131799 0.097337
H 4.064757 -5.264481 -0.503630
H 4.362521 -6.093404 1.011431
Au 0.236286 4.989935 1.037468
S -1.264977 6.033740 -0.425929
Au -1.892579 4.267220 -1.837059
C -2.736119 6.495492 0.548054
H -3.084136 5.627705 1.117891
H -3.516291 6.766892 -0.173104
Au -4.137725 1.086015 2.632864
S -4.727435 -0.908279 3.704095
Au -3.278947 -2.499775 2.776374
C -6.362715 -1.333030 3.004152
H -6.273873 -1.440679 1.917997
H -7.027094 -0.485025 3.208642
Au 3.175283 2.840140 -3.014265
S 5.069912 1.529178 -3.401683
Au 4.168562 -0.552901 -2.787172
C 6.164981 2.149845 -2.074539
H 5.589239 2.255607 -1.150241
H 6.483797 3.149385 -2.393326
Au -1.177657 -0.746730 -4.798734
S -3.369248 -1.542022 -4.925468
Au -4.012851 -1.594973 -2.685664
C -3.265287 -3.269335 -5.508649
H -2.645109 -3.854490 -4.819459

H -2.744384 -3.237936 -6.473320
Au 4.125726 0.764271 2.898154
S 3.416319 1.104323 5.094296
Au 1.127176 0.662177 4.907098
C 3.641068 2.879769 5.450932
H 3.150464 3.477182 4.674173
H 4.719275 3.072181 5.399518
S 1.380590 4.280463 -2.636408
S -3.621599 3.175822 1.711255
S 3.422428 -2.744134 -2.393266
S -1.959067 -4.241666 1.951363
S 1.853569 4.114629 2.487823
S -2.544182 2.667179 -3.420136
S 2.270261 -2.571503 3.868796
S -1.037123 -4.234990 -2.444856
S 0.946177 0.229779 -4.999961
S -4.835839 -1.560424 -0.481285
S 5.004171 0.425972 0.762268
S -1.134109 0.033138 5.019302
C -5.923465 -0.097793 -0.561734
H -5.386419 0.688528 -1.104389
H -6.065458 0.271044 0.462011
C 0.563495 1.977185 -5.398913
H 0.185640 2.482320 -4.503524
H 1.522594 2.442496 -5.654597
C -1.057128 -1.728920 5.505464
H -0.628000 -2.308211 4.679541
H -2.097967 -2.048652 5.634572
C 5.431347 -1.354252 0.745582
H 4.581612 -1.946847 1.103098
H 5.590393 -1.632971 -0.303962
C -1.171843 -5.053359 3.385788
H -0.555697 -4.336955 3.938818
H -0.491663 -5.803068 2.963932
C 2.370582 -3.149846 -3.841415
H 1.456185 -2.547535 -3.813954
H 2.060663 -4.188617 -3.681296
C -4.801721 3.465317 0.350500
H -4.878811 2.566166 -0.268771
H -4.353835 4.243339 -0.278083
C 2.126637 5.753604 -1.857310
H 2.598766 5.474207 -0.912532
H 1.294532 6.428047 -1.624073
C -2.540625 -4.955978 -1.660847
H -2.276832 -5.434447 -0.713446
H -3.239401 -4.149981 -1.416186
C -4.369285 2.734557 -3.497080

H -4.796429 2.571811 -2.502901
H -4.677981 1.899907 -4.137647
C 4.039455 -2.535315 4.314200
H 4.636486 -2.319224 3.425369
H 4.167674 -1.699586 5.013165
C 3.414098 4.080794 1.537002
H 3.220911 3.656189 0.542764
H 4.057142 3.367827 2.063559
C -0.428692 2.135743 -6.532453
H -0.080425 1.623105 -7.443134
H -1.395207 1.681663 -6.278033
C -0.668559 3.581536 -6.882848
O 0.070606 4.487903 -6.612386
O -1.800158 3.747583 -7.551097
H -1.912590 4.674402 -7.794647
C -4.664141 -3.837515 -5.675403
H -5.274653 -3.181210 -6.307287
H -5.184579 -3.882682 -4.703616
C -4.680775 -5.233313 -6.236228
O -3.826943 -6.064123 -6.028558
O -5.740650 -5.479300 -6.965276
H -5.748637 -6.396742 -7.269184
C -7.279848 -0.396172 -1.210925
H -7.185656 -1.192129 -1.959131
H -8.003275 -0.723813 -0.455904
C -7.737561 0.877280 -1.875777
O -8.375346 1.735617 -1.323362
O -7.269781 0.972326 -3.101270
H -7.325197 1.879676 -3.485374
C -6.159525 3.915328 0.845637
H -6.048389 4.733092 1.575414
H -6.684894 3.110472 1.378740
C -7.031541 4.430270 -0.273326
O -6.640644 4.672207 -1.382954
O -8.275740 4.633484 0.118076
H -8.807568 4.961609 -0.616715
C -2.426601 7.654923 1.470965
H -2.051924 8.522892 0.909310
H -1.623140 7.392893 2.176788
C -3.624623 8.084528 2.276830
O -4.701269 7.553428 2.241805
O -3.354204 9.126385 3.045157
H -4.130984 9.378836 3.558885
C -4.812853 4.067950 -4.067112
H -4.504733 4.892518 -3.409430
H -4.309064 4.255586 -5.028632
C -6.289670 4.207064 -4.313071

O -7.107102 3.318189 -4.260473
O -6.616270 5.432017 -4.654278
H -7.563512 5.498995 -4.827658
C -3.204607 -5.935722 -2.605523
H -4.075132 -6.384726 -2.102601
H -3.598529 -5.410788 -3.482115
C -2.279907 -7.067174 -3.004213
O -1.617393 -7.667975 -2.203175
O -2.238209 -7.394900 -4.279111
H -2.800151 -6.835790 -4.846837
C 4.028058 -7.470242 -0.610274
H 4.973884 -7.884812 -0.247379
H 3.240861 -8.198505 -0.374859
C 4.147326 -7.282845 -2.093172
O 5.219719 -7.288875 -2.664922
O 3.012226 -7.052314 -2.693962
H 3.157585 -6.760830 -3.625427
C 3.035496 -2.979250 -5.199434
H 2.356823 -3.423312 -5.940920
H 3.091217 -1.911154 -5.448946
C 4.430748 -3.571818 -5.350006
H 4.725200 -3.550286 -6.410415
H 5.180464 -2.969675 -4.822309
C 4.526834 -4.992311 -4.878590
O 3.596073 -5.772848 -4.950162
O 5.686411 -5.315624 -4.373954
H 5.637185 -6.194561 -3.930850
C 7.353423 1.245469 -1.843957
H 7.956778 1.134569 -2.758160
H 7.030476 0.228347 -1.579080
C 8.258883 1.755723 -0.755707
O 8.180675 2.844368 -0.241989
O 9.182486 0.879201 -0.422991
H 9.762346 1.231935 0.263881
C 6.686503 -1.617660 1.557255
H 7.549688 -1.090122 1.132154
H 6.579607 -1.229020 2.583503
C 6.998768 -3.085919 1.699438
O 6.186374 -3.966926 1.617109
O 8.277144 -3.300938 1.957669
H 8.439995 -4.242456 2.091911
C 4.480092 -3.836260 4.951712
H 4.315130 -4.682762 4.266972
H 3.882058 -4.062239 5.845927
C 5.940630 -3.840151 5.316580
O 6.728941 -2.986773 5.009237
O 6.275618 -4.916021 6.009400

H 7.218445 -4.906283 6.214397
C -6.905168 -2.603853 3.623004
H -6.217825 -3.448317 3.457297
H -6.995024 -2.508593 4.714618
C -8.246579 -2.992534 3.058119
O -8.803888 -2.421678 2.160082
O -8.747630 -4.055750 3.663187
H -9.598506 -4.296091 3.276609
C -0.261373 -1.974472 6.772329
H -0.616850 -1.326982 7.589695
H 0.798938 -1.736799 6.622342
C -0.392600 -3.400805 7.244289
O -1.374074 -4.077720 7.091169
O 0.686253 -3.828914 7.874203
H 0.557406 -4.734963 8.180616
C -2.193855 -5.705706 4.292287
H -2.847177 -4.953808 4.757108
H -2.861660 -6.364854 3.716753
C -1.562789 -6.527425 5.386189
O -0.388034 -6.753497 5.486854
O -2.467495 -7.010427 6.222908
H -2.039677 -7.532424 6.911536
C 3.126119 6.440214 -2.763848
H 3.969096 5.777917 -3.002875
H 2.666049 6.698652 -3.730092
C 3.674636 7.705345 -2.158378
O 3.240989 8.243053 -1.175096
O 4.687802 8.188903 -2.857577
H 5.009239 9.007477 -2.461105
C 4.145162 5.413002 1.418570
H 4.449702 5.770234 2.412211
H 3.517129 6.188268 0.965401
C 5.364665 5.202495 0.547185
O 5.533160 5.712897 -0.528492
O 6.205300 4.337096 1.081370
H 6.910661 4.060463 0.468889
C 3.093943 3.214067 6.822799
H 3.548801 2.577830 7.596688
H 2.013201 3.012283 6.875957
C 3.316572 4.653416 7.205243
O 3.882358 5.464837 6.524872
O 2.809835 4.930063 8.395426
H 2.961170 5.855971 8.620471

[Au₂₅(MPA)₁₈]⁻ PBEh-3c T₁ (acetonitrile)

Au -0.054958 0.035992 -0.024630
Au 0.953363 1.860661 1.836259
Au -1.964452 0.740868 -2.026881
Au 1.776864 -0.988022 1.908737
Au -1.244571 -1.951551 -1.707068
Au 0.568584 2.708352 -0.827445
Au 1.568438 -2.123655 -0.816094
Au -1.792244 2.124829 0.620353
Au -0.440503 -2.591910 1.050016
Au 2.735094 0.533222 -0.402685
Au -1.418193 -0.049171 2.529282
Au 1.130389 0.566527 -2.631506
Au -2.877129 -0.714518 0.357252
Au 2.060297 -4.242824 2.163214
S 1.781435 -6.075669 0.750623
Au 0.370896 -5.115801 -0.845086
C 3.457287 -6.439859 0.123703
H 3.871667 -5.564084 -0.389981
H 4.072277 -6.590677 1.016313
Au 0.236834 5.041184 1.207341
S -1.323177 6.124417 -0.170863
Au -1.964603 4.361951 -1.595423
C -2.781330 6.493589 0.863728
H -3.106368 5.581366 1.375592
H -3.579811 6.802146 0.178194
Au -4.383420 0.959273 2.555063
S -5.150638 -1.024231 3.551334
Au -3.459379 -2.485661 2.822103
C -6.620162 -1.495629 2.570506
H -6.345375 -1.564000 1.512045
H -7.347795 -0.682838 2.681718
Au 3.157112 2.871450 -2.955205
S 4.987632 1.507061 -3.519505
Au 3.959309 -0.558878 -2.992511
C 6.143580 2.012195 -2.195807
H 5.594758 2.107859 -1.254452
H 6.501852 3.008630 -2.481411
Au -1.405320 -0.302213 -4.897889
S -3.205066 -1.784802 -5.187676
Au -3.941187 -1.707502 -2.965940
C -2.167421 -3.269608 -5.477479
H -1.337128 -3.259956 -4.765943
H -1.754092 -3.134713 -6.483358
Au 4.308355 0.628517 2.739899
S 3.712044 1.130338 4.942873
Au 1.410851 0.756234 4.688236

C 4.039938 2.916981 5.136789
H 3.879951 3.422960 4.181623
H 5.103883 2.999773 5.388520
S 1.415827 4.348324 -2.460332
S -3.742312 3.062866 1.755183
S 3.025309 -2.699754 -2.689958
S -1.963364 -4.136507 2.122316
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S -2.662745 2.777378 -3.178537
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O 2.682883 5.554369 7.308872
H 2.865845 6.498001 7.393505

Table S2. Average bond-length data for the $[M_{25}(MPA)_{18}]^-$ clusters in gas phase. The distances are given in Ångström (Å). The standard deviation is given within parenthesis.

Cluster	Level	State	$\langle d(M_o-M_c) \rangle^a$	$\langle d(M_c-M_e) \rangle^b$	$\langle d(M_c-S) \rangle^c$	$\langle d(M_e-S) \rangle^d$
$[Au_{25}(MPA)_{18}]^-$	B3LYP	S_0	2.935 (0.091)	3.467 (0.182)	2.484 (0.039)	2.381 (0.012)
	TPSSh	S_0	2.819 (0.039)	3.278 (0.181)	2.454 (0.026)	2.359 (0.011)
	PBEh-3c	S_0	2.820 (0.019)	3.299 (0.130)	2.444 (0.012)	2.342 (0.006)
$[Au_{25}(MPA)_{18}]^-$	B3LYP	T_1	2.971 (0.153)	3.441 (0.245)	2.486 (0.032)	2.382 (0.017)
	TPSSh	T_1	2.851 (0.056)	3.299 (0.228)	2.454 (0.033)	2.360 (0.014)
	PBEh-3c	T_1	2.860 (0.050)	3.334 (0.229)	2.452 (0.026)	2.344 (0.012)
$[Ag_{25}(MPA)_{18}]^-$	B3LYP	S_0	2.858 (0.040)	3.448 (0.196)	2.534 (0.026)	2.438 (0.013)
	TPSSh	S_0	2.764 (0.025)	3.112 (0.246)	2.517 (0.039)	2.439 (0.038)
	PBEh-3c	S_0	2.807 (0.027)	3.247 (0.265)	2.519 (0.029)	2.441 (0.037)
$[Ag_{25}(MPA)_{18}]^-$	B3LYP	T_1	2.916 (0.087)	3.414 (0.306)	2.542 (0.038)	2.448 (0.018)
	TPSSh	T_1	2.779 (0.055)	3.103 (0.333)	2.524 (0.046)	2.472 (0.046)
	PBEh-3c	T_1	2.823 (0.050)	3.249 (0.355)	2.525 (0.043)	2.461 (0.045)

^a The average distance from the central M atom (M_o) to its 12 neighbour atoms (M_c).

^b The average distance from a metal atom in the shell (M_e) to its neighbour metal atoms from the core (M_c).

^c The average distance from a metal atom in the core to the sulphur atom in the shell.

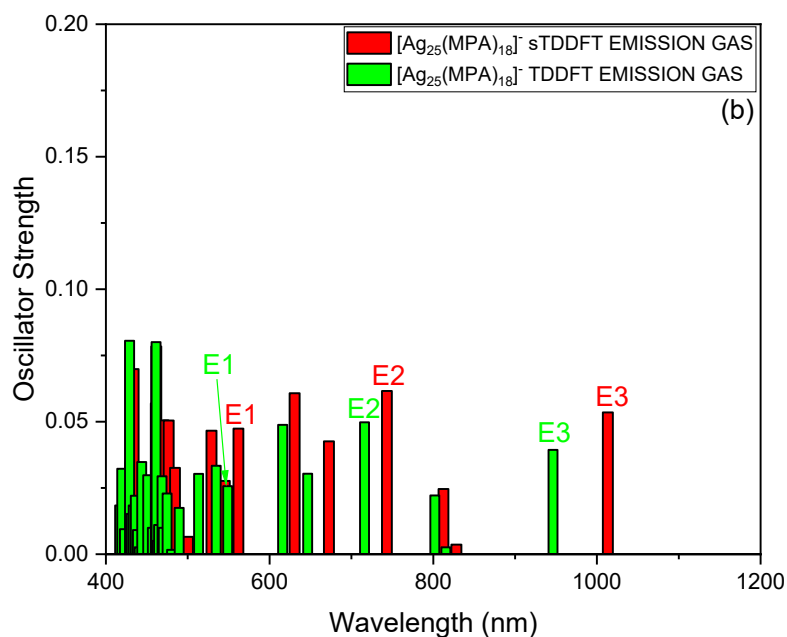
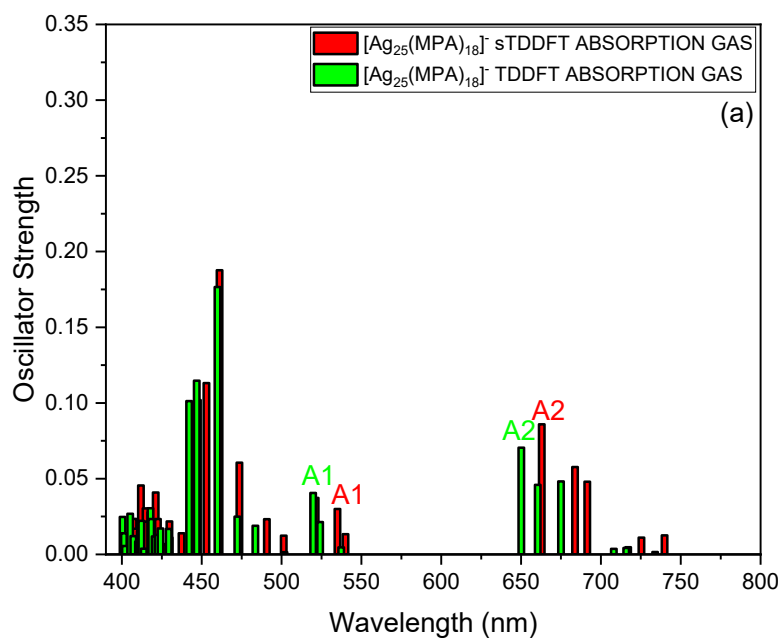
^d The average distance from a metal atom in the shell to the sulphur atom in the shell.

Table S3. Computational wall time in minutes for carrying out calculations of excitation energies of $[M_{25}(\text{MPA})_{18}]^-$ (M= Au, Ag; MPA = $\text{SCH}_2\text{CH}_2\text{COOH}$) at the conventional TDDFT and the sTDDFT level in gas phase, respectively. The number of states (# States) and number of cores (# Cores) are also reported.

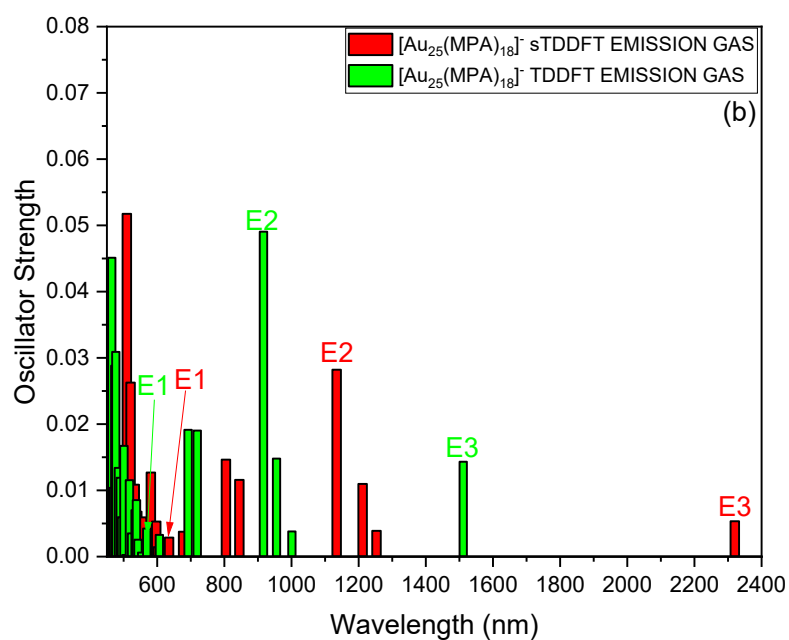
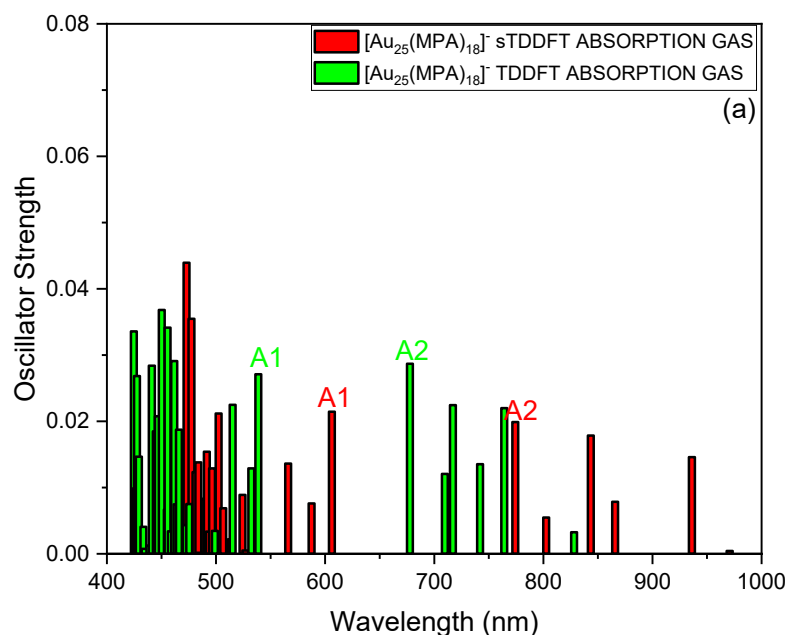
System	Functional	Structure	Method	# States	Time	# Cores
$[\text{Au}_{25}(\text{MPA})_{18}]^-$	B3LYP	S_0	TDDFT	30	2043	24
			sTDDFT	1057	19	1
			TDDFT	30	1008	24
		T_1	sTDDFT	2243	52	1
			TDDFT	30	1025	24
			sTDDFT	2720	49	1
	TPSSh	S_0	TDDFT	30	1253	24
			sTDDFT	1170	15	1
			TDDFT	30	1025	24
		T_1	sTDDFT	443	3	1
			TDDFT	30	1370	24
			sTDDFT	418	2	1
$[\text{Ag}_{25}(\text{MPA})_{18}]^-$	B3LYP	S_0	TDDFT	30	2275	24
			sTDDFT	895	5	1
			TDDFT	30	1366	24
		T_1	sTDDFT	1717	7	1
			TDDFT	30	1283	24
			sTDDFT	2211	8	1
	TPSSh	S_0	TDDFT	30	2372	24
			sTDDFT	1089	6	1
			TDDFT	30	1283	24
		T_1	sTDDFT	366	2	1
			TDDFT	30	1629	24
			sTDDFT	348	2	1

Figures.

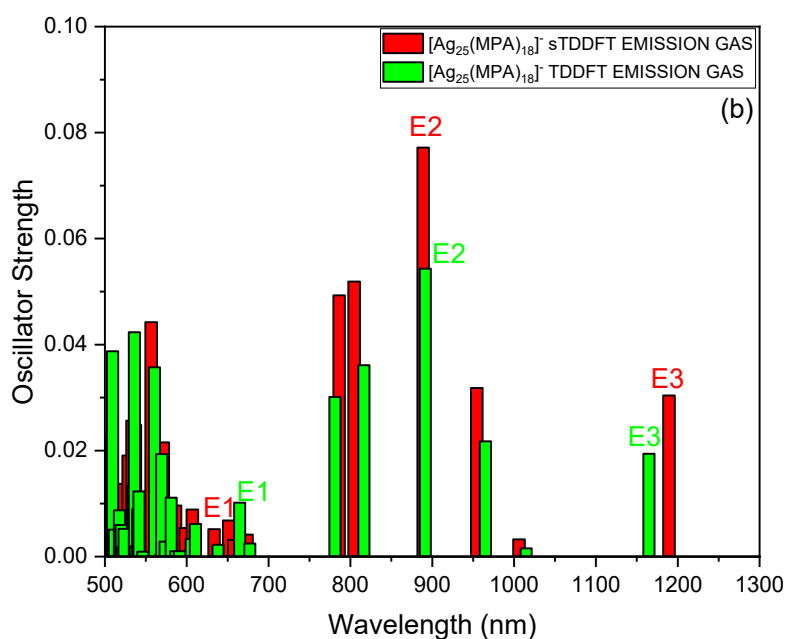
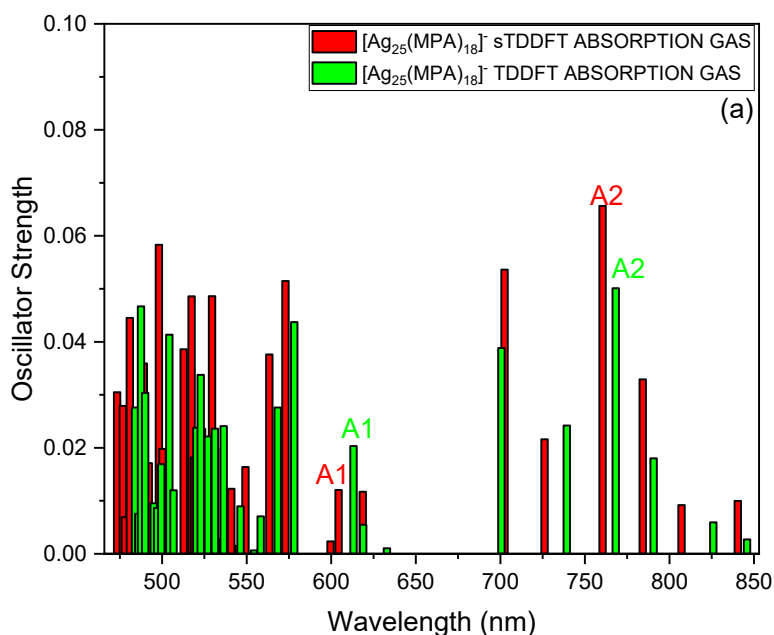
S1. Comparison of results between methodologies for the absorption (a) and emission (b) spectra of the complexes $[\text{Ag}_{25}(\text{MPA})_{18}]^-$ in gas phase using the functional B3LYP. The red bars represent the transition energies obtained by the sTDDFT approach and the green bars represent the transition energies obtained by TDDFT approach.



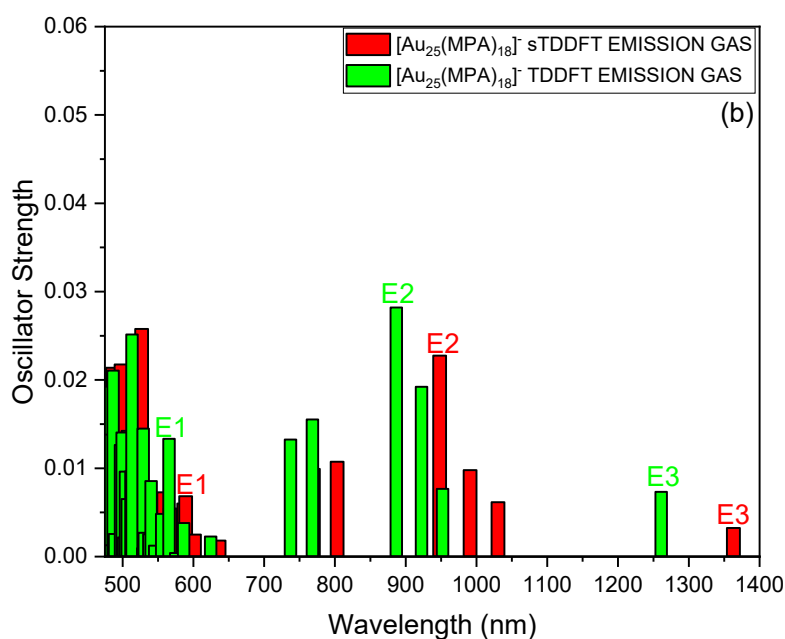
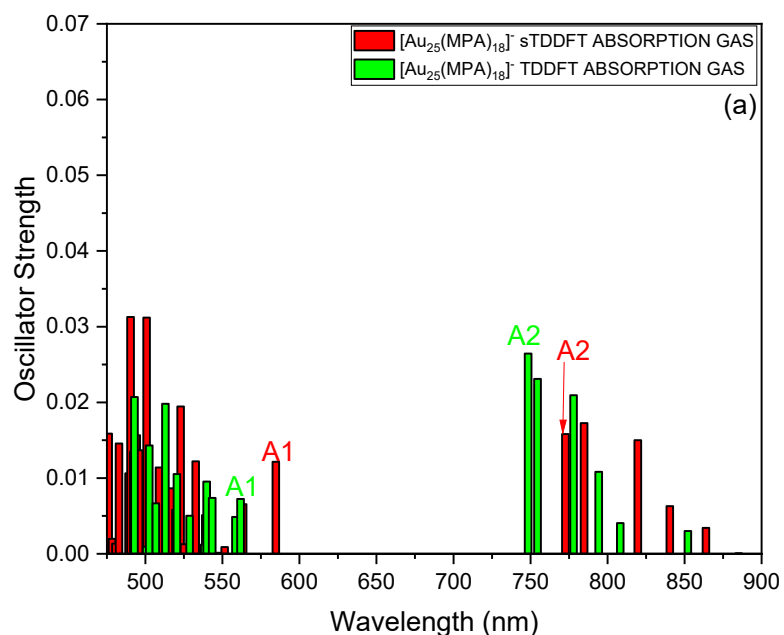
S2. Comparison of results between methodologies for the absorption (a) and emission (b) spectra of the complexes $[\text{Au}_{25}(\text{MPA})_{18}]^-$ in gas phase using the functional B3LYP. The red bars represent the transition energies obtained by the sTDDFT approach and the green bars represent the transition energies obtained by TDDFT approach.



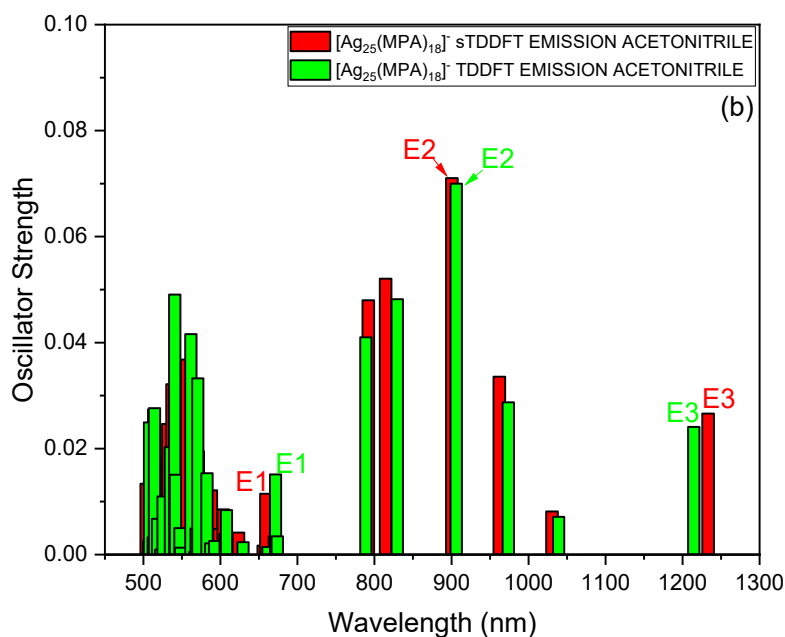
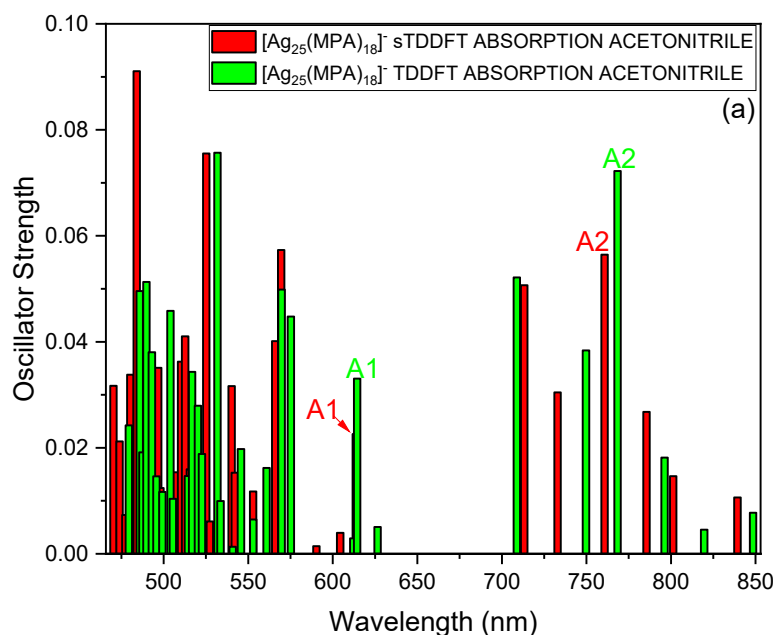
S3. Comparison of results between methodologies for the absorption (a) and emission (b) spectra of the complexes $[\text{Ag}_{25}(\text{MPA})_{18}]^-$ in gas phase using the functional TPSSh. The red bars represent the transition energies obtained by the sTDDFT approach and the green bars represent the transition energies obtained by TDDFT approach.



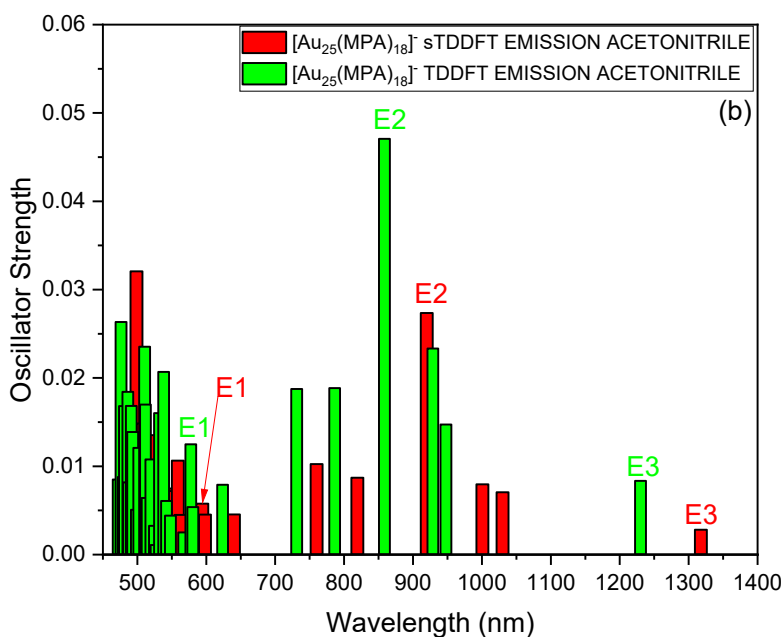
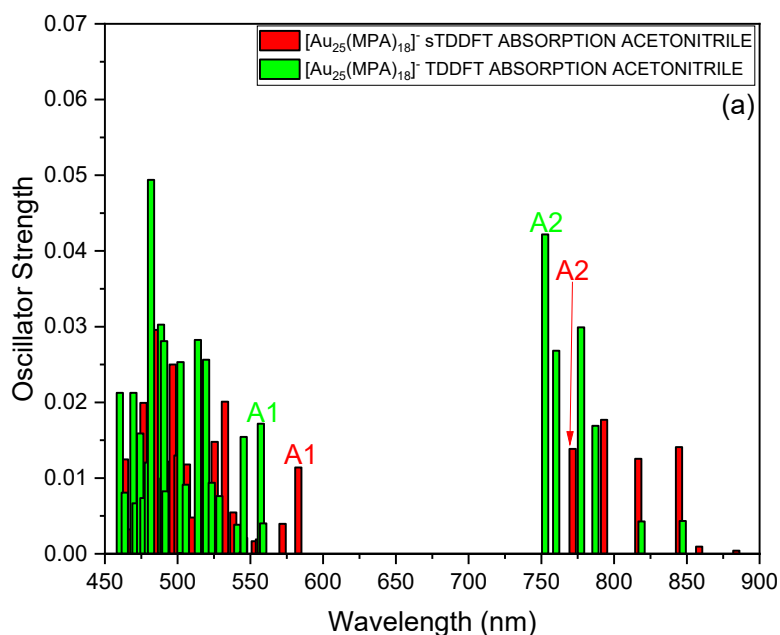
S4. Comparison of results between methodologies for the absorption (a) and emission (b) spectra of the complexes $[\text{Au}_{25}(\text{MPA})_{18}]^-$ in gas phase using the functional TPSSh. The red bars represent the transition energies obtained by the sTDDFT approach and the green bars represent the transition energies obtained by TDDFT approach.



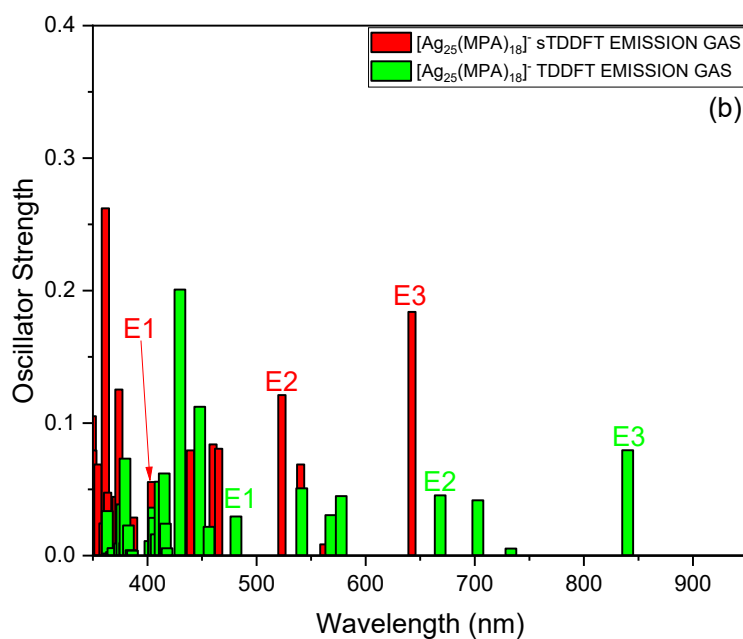
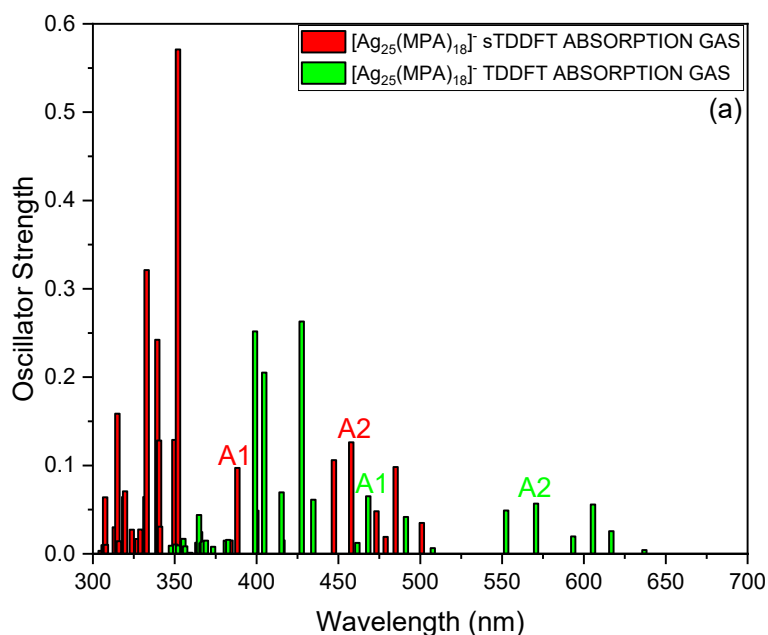
S5. Comparison of results between methodologies for the absorption (a) and emission (b) spectra of the complexes $[\text{Ag}_{25}(\text{MPA})_{18}]^-$ in acetonitrile phase using the functional TPSSH. The red bars represent the transition energies obtained by the sTDDFT approach and the green bars represent the transition energies obtained by TDDFT approach.



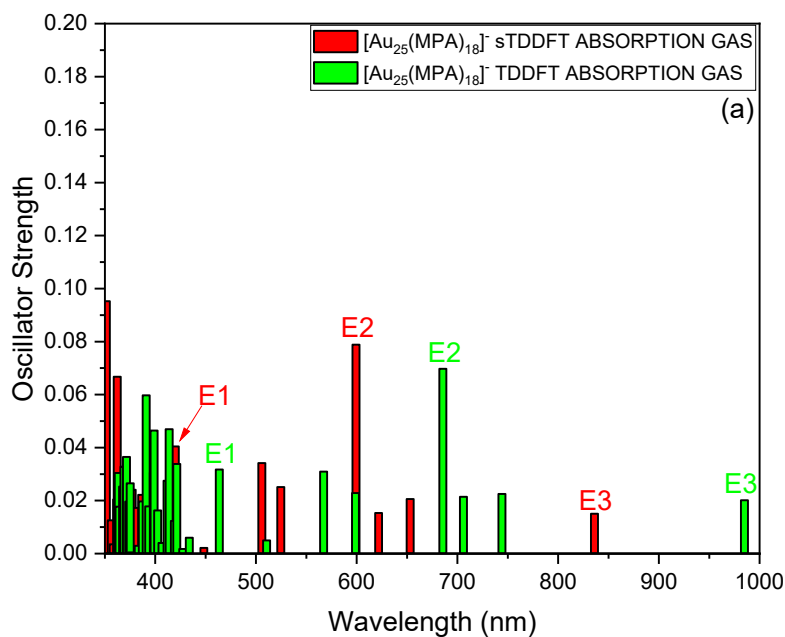
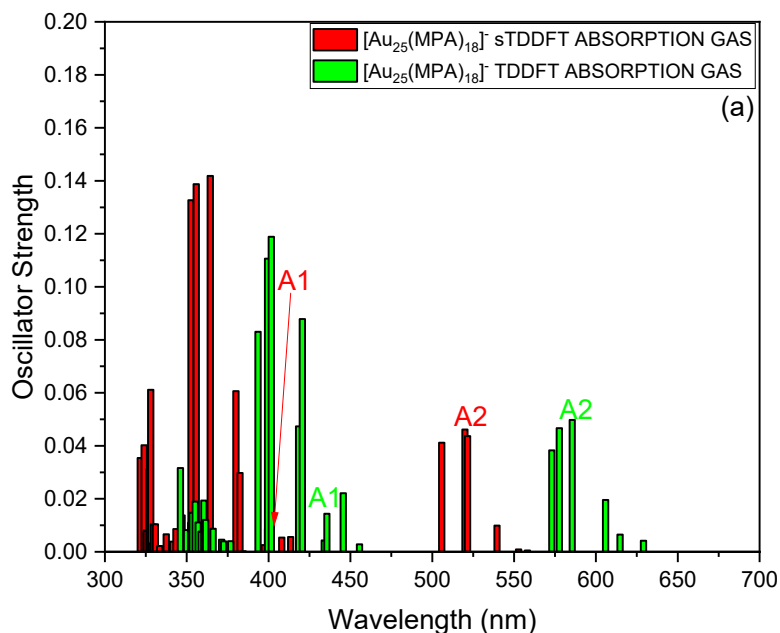
S6. Comparison of results between methodologies for the absorption (a) and emission (b) spectra of the complexes $[\text{Au}_{25}(\text{MPA})_{18}]^-$ in acetonitrile phase using the functional TPSSH. The red bars represent the transition energies obtained by the sTDDFT approach and the green bars represent the transition energies obtained by TDDFT approach.



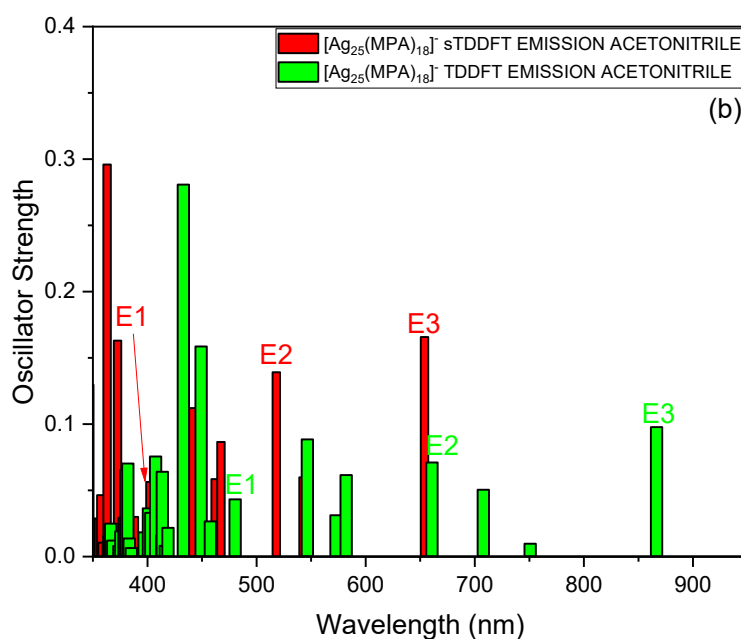
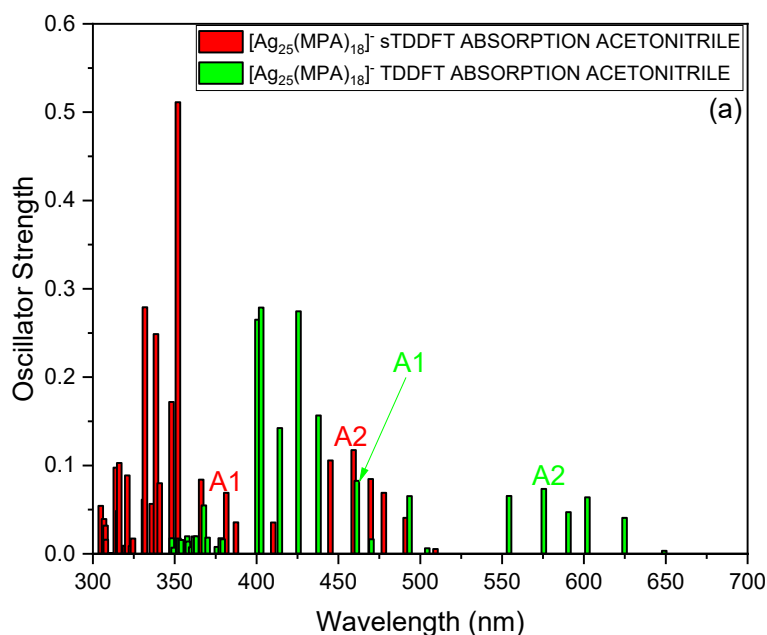
S7. Comparison of results between methodologies for the absorption (a) and emission (b) spectra of the complexes $[\text{Ag}_{25}(\text{MPA})_{18}]^-$ in gas phase using the functional PBEh-3c. The red bars represent the transition energies obtained by the sTDDFT approach and the green bars represent the transition energies obtained by TDDFT approach.



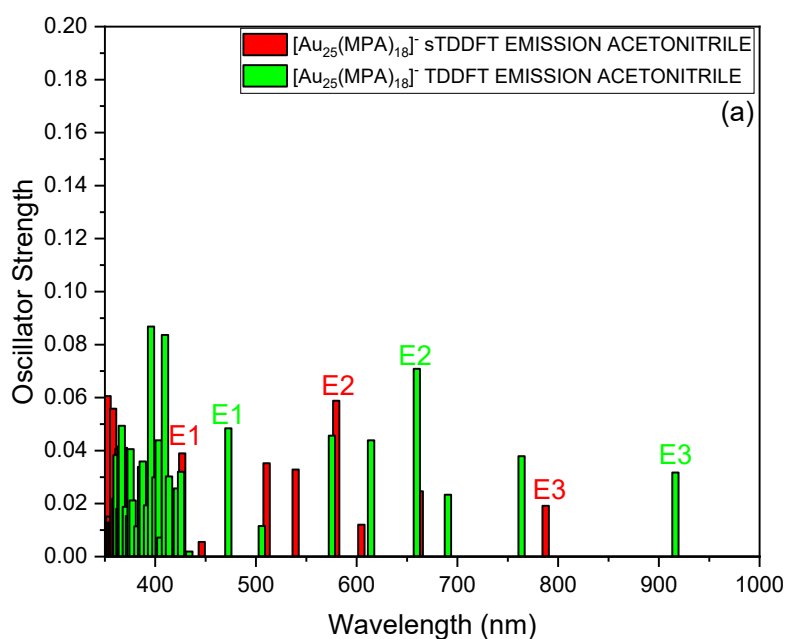
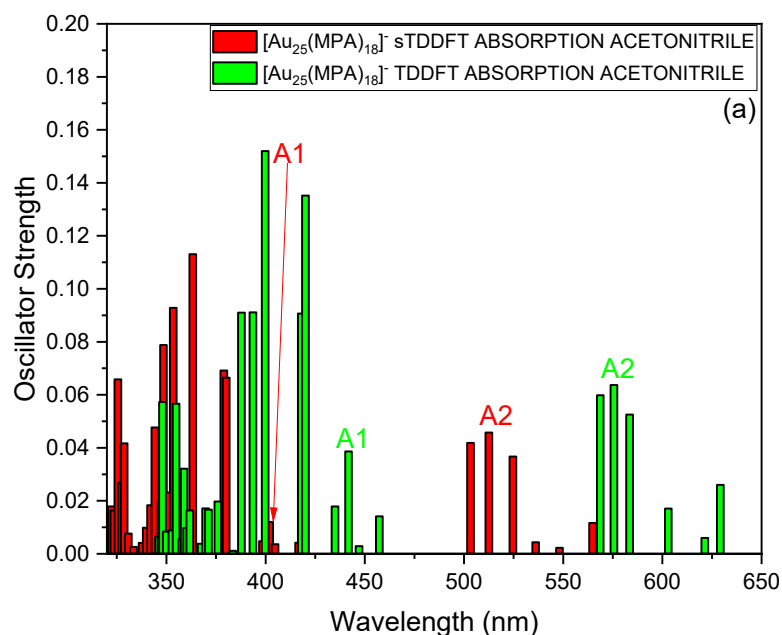
S8. Comparison of results between methodologies for the absorption (a) and emission (b) spectra of the complexes $[\text{Au}_{25}(\text{MPA})_{18}]^-$ in gas phase using the functional PBEh-3c. The red bars represent the transition energies obtained by the sTDDFT approach and the green bars represent the transition energies obtained by TDDFT approach.



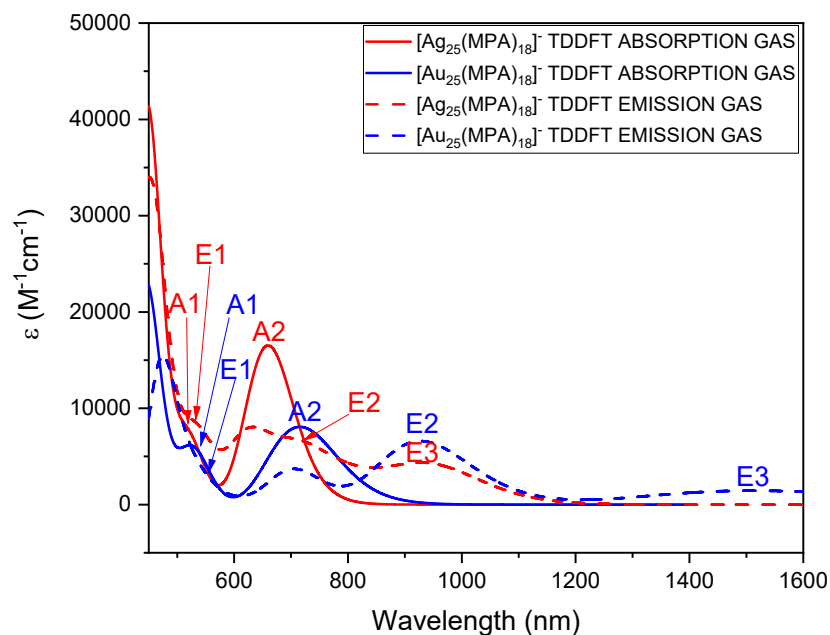
S9. Comparison of results between methodologies for the absorption (a) and emission (b) spectra of the complexes $[\text{Ag}_{25}(\text{MPA})_{18}]^-$ in acetonitrile phase using the functional PBEh-3c. The red bars represent the transition energies obtained by the sTDDFT approach and the green bars represent the transition energies obtained by TDDFT approach.



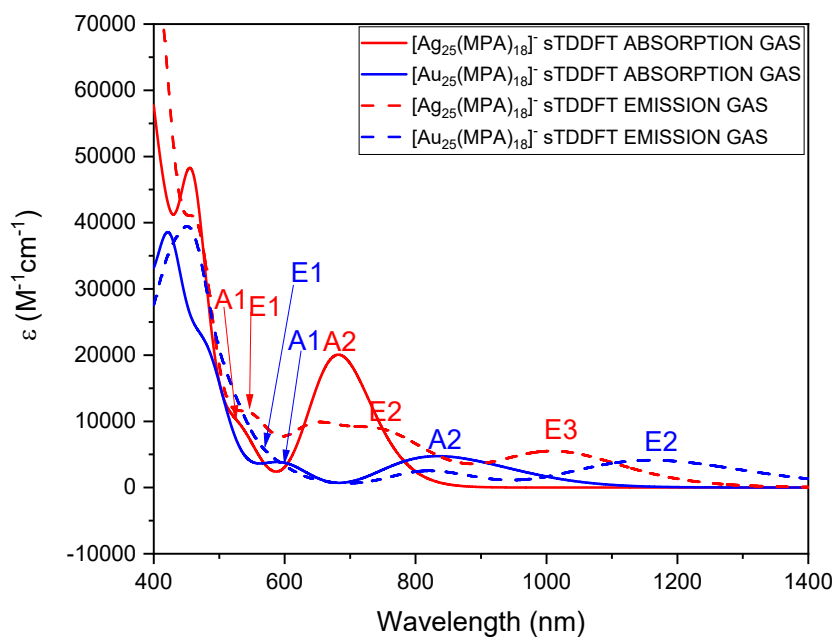
S10. Comparison of results between methodologies for the absorption (a) and emission (b) spectra of the complexes $[\text{Au}_{25}(\text{MPA})_{18}]^-$ in acetonitrile phase using the functional PBEh-3c. The red bars represent the transition energies obtained by the sTDDFT approach and the green bars represent the transition energies obtained by TDDFT approach.

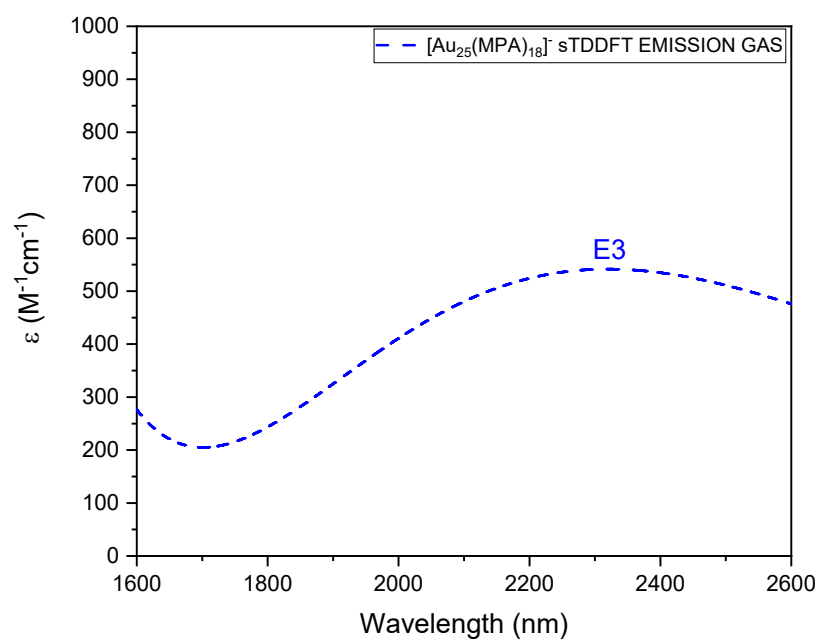


S11. Gaussian absorption and emission spectra obtained using the TDDFT methodology and B3LYP functional, for the complexes $[M_{25}(MPA)_{18}]^-$ (M = Au, Ag) in gas phase.

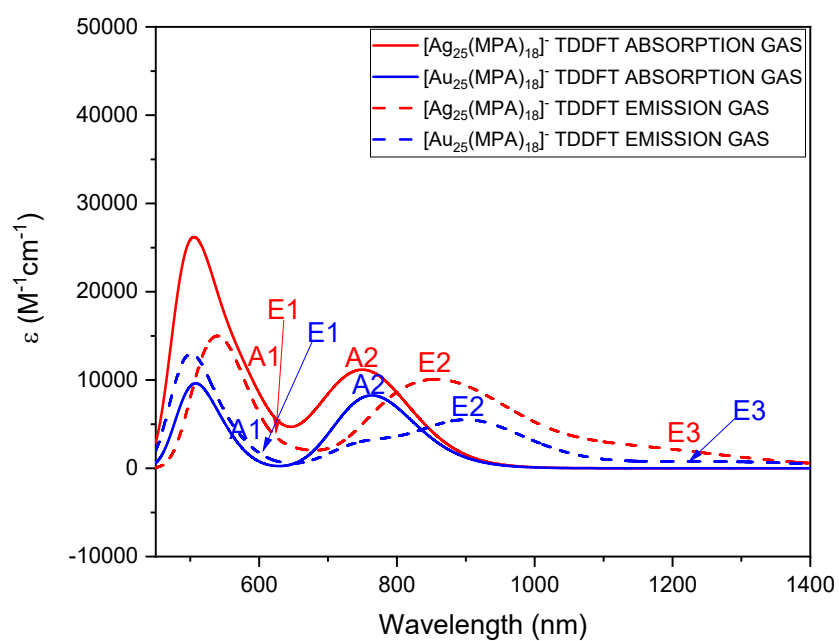


S12. Gaussian absorption and emission spectra obtained using the sTDDFT methodology and B3LYP functional, for the complexes $[M_{25}(MPA)_{18}]^-$ (M = Au, Ag) in gas phase.

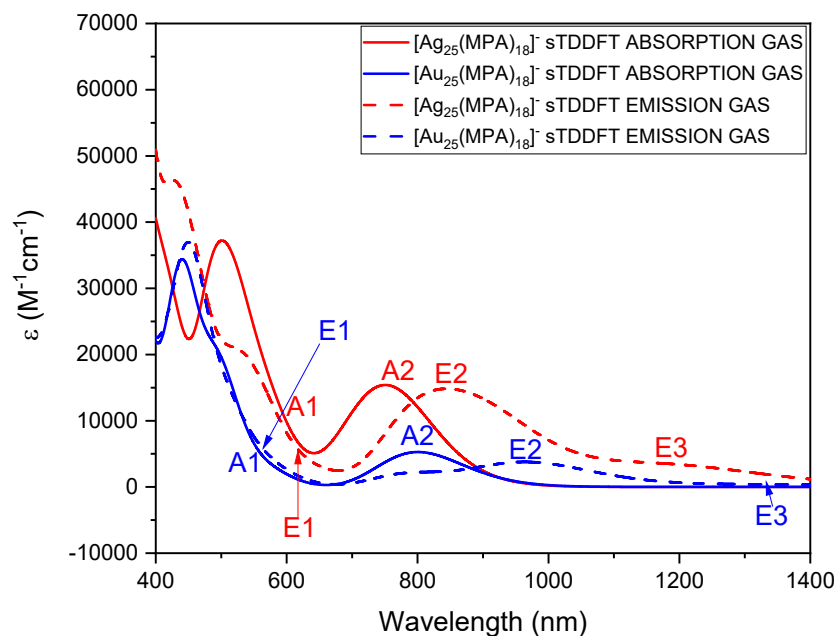




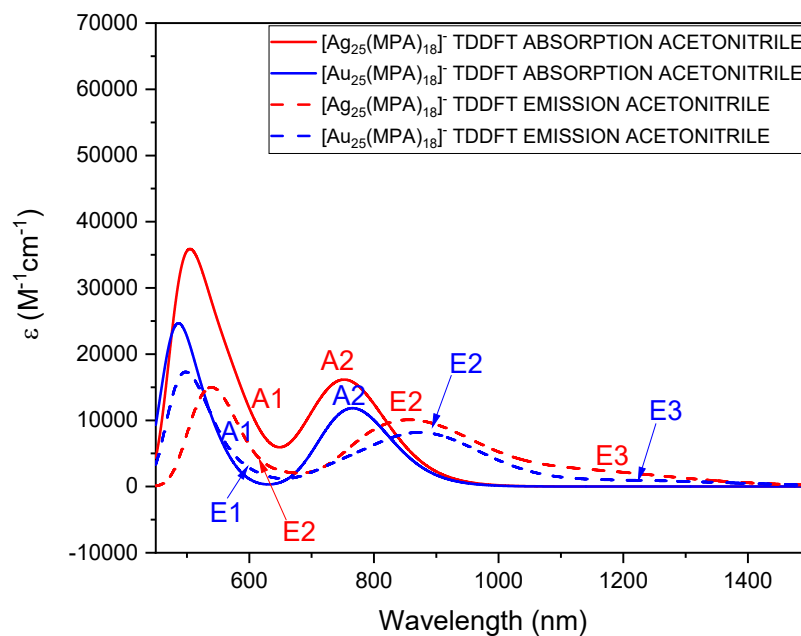
S13. Gaussian absorption and emission spectra obtained using the TDDFT methodology and TPSSh functional, for the complexes $[\text{M}_{25}(\text{MPA})_{18}]^-$ ($\text{M} = \text{Au}, \text{Ag}$) in gas phase.



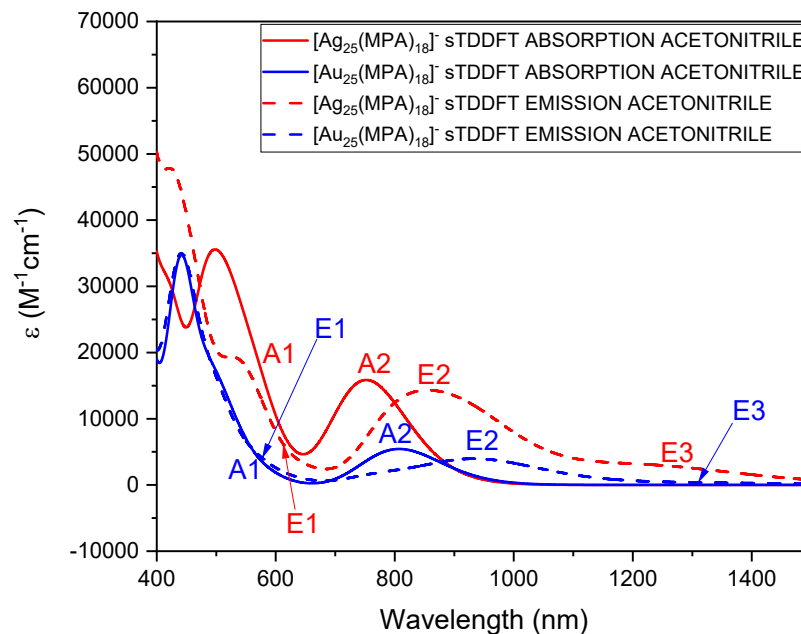
S14. Gaussian absorption and emission spectra obtained using the sTDDFT methodology and TPSSh functional, for the complexes $[M_{25}(MPA)_{18}]^-$ ($M = Au, Ag$) in gas phase.



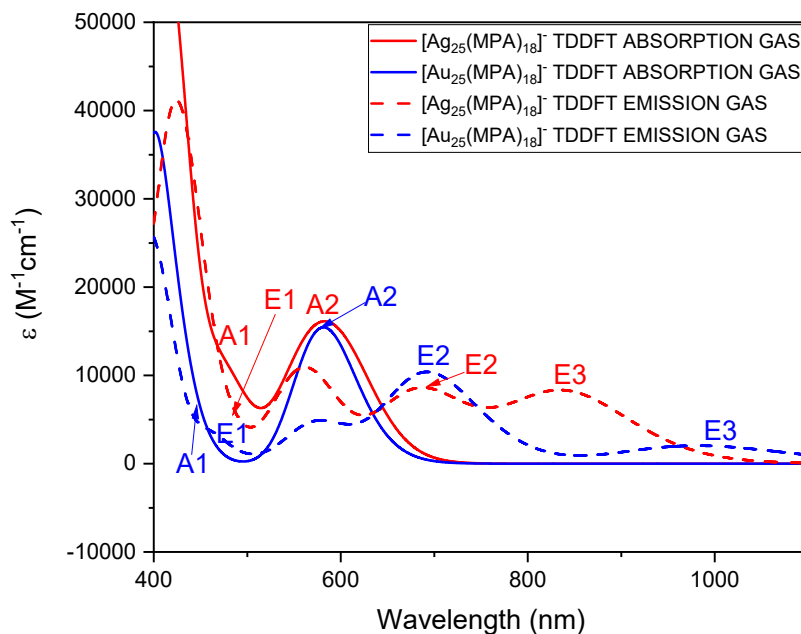
S15. Gaussian absorption and emission spectra obtained using the TDDFT methodology and TPSSh functional, for the complexes $[M_{25}(MPA)_{18}]^-$ ($M = Au, Ag$) in acetonitrile phase.



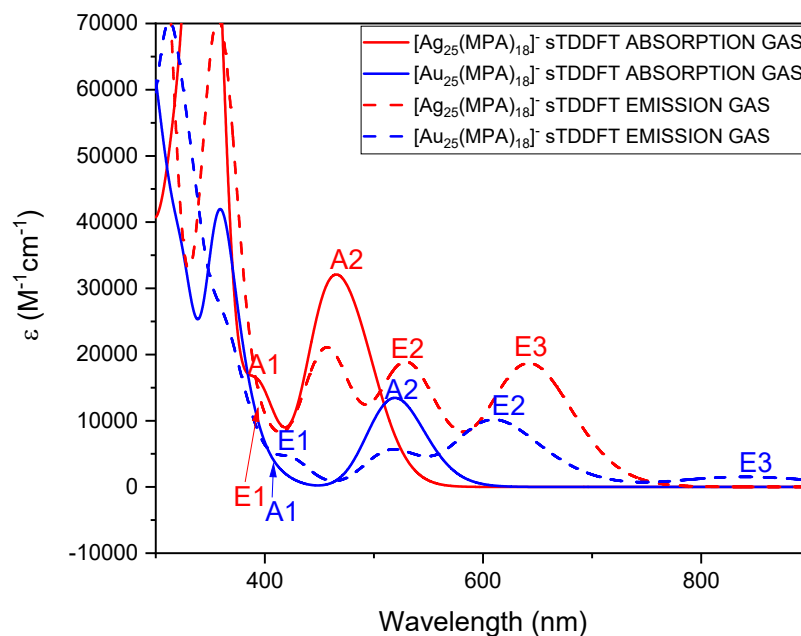
S16. Gaussian absorption and emission spectra obtained using the sTDDFT methodology and TPSSh functional, for the complexes $[M_{25}(MPA)_{18}]^-$ ($M = Au, Ag$) in acetonitrile phase.



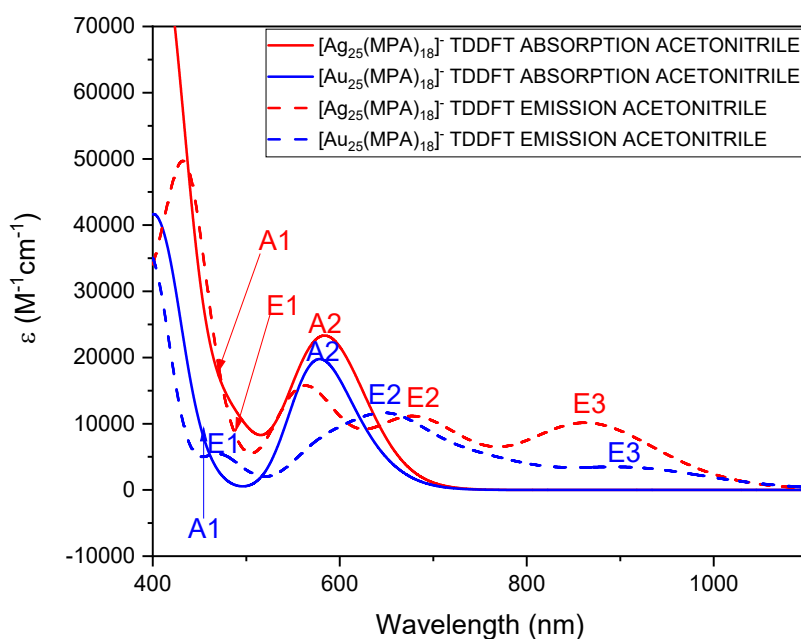
S17. Gaussian absorption and emission spectra obtained using the TDDFT methodology and PBEh-3c functional, for the complexes $[M_{25}(MPA)_{18}]^-$ ($M = Au, Ag$) in gas phase.



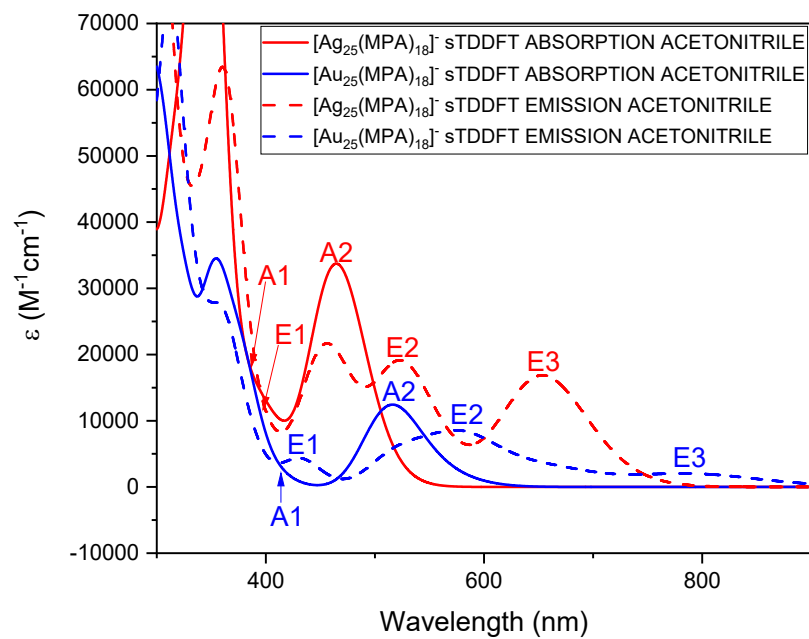
S18. Gaussian absorption and emission spectra obtained using the sTDDFT methodology and PBEh-3c functional, for the complexes $[M_{25}(MPA)_{18}]^-$ ($M = Au, Ag$) in gas phase.



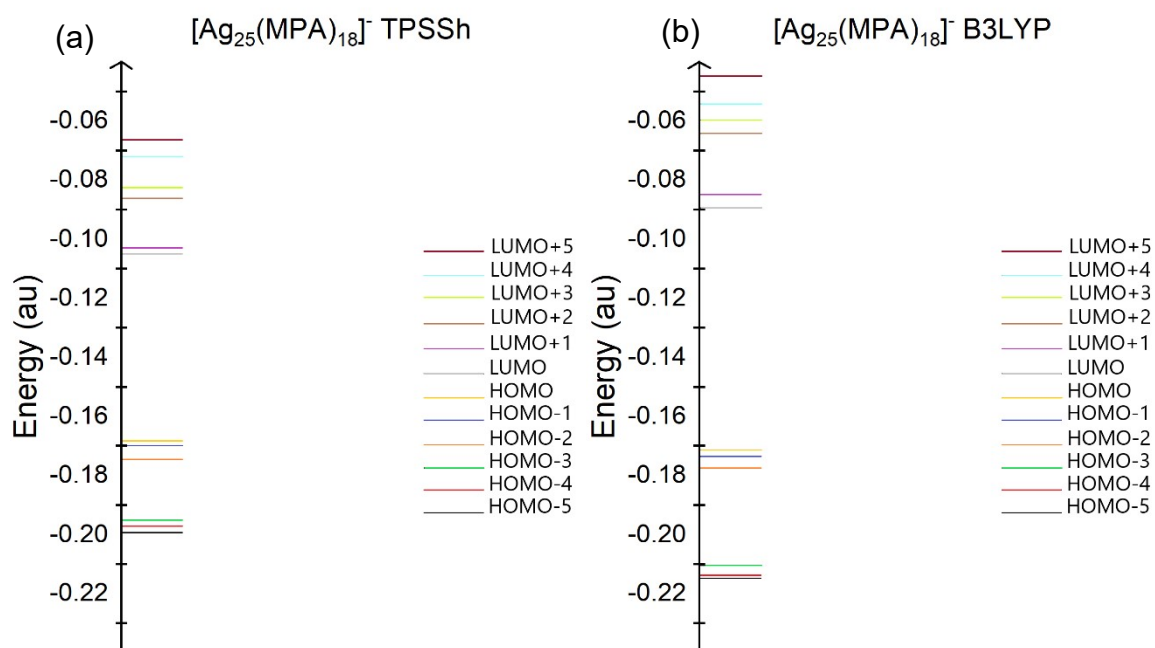
S19. Gaussian absorption and emission spectra obtained using the TDDFT methodology and PBEh-3c functional, for the complexes $[M_{25}(MPA)_{18}]^-$ ($M = Au, Ag$) in acetonitrile.



S20. Gaussian absorption and emission spectra obtained using the sTDDFT methodology and PBEh-3c functional, for the complexes $[M_{25}(MPA)_{18}]^-$ ($M = Au, Ag$) in acetonitrile.



S21. Molecular orbitals diagrams of the systems $[\text{Ag}_{25}(\text{MPA})_{18}]^-$ using the functional B3LYP (a) and TPSSh (b).



S22. Molecular orbitals diagrams of the systems $[\text{Au}_{25}(\text{MPA})_{18}]^-$ using the functional B3LYP (a) and TPSSh (b).

