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Supplementary Information - GIGA: A Versatile Genetic Algorithm for Free and Supported Clusters and Nanoparticles in the Presence of Ligands

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1 GA Analysis Tool

In the following, the GA analysis tool is described. The purpose of the analysis algorithm is to provide a fast, handy and thorough analysis of all structural motifs found during the GO independent of the specific quantum chemical software used for local minimisations. Therefore, the analysis software consists of three subprograms, written in object oriented Python: **Extraction**, **Analysis1** and **Analysis2**. With Extraction, all information of the cluster structures generated during the GO are extracted, **Analysis1** is used for automatic grouping of different cluster structures according to structural and energy criteria, **Analysis2** is used for automatic visualisation and checking of the results of **Analysis1** as well as for automatic documentation of the results.

Extraction

The purpose of the **Extraction** class is: i) extraction of the quantum chemical output calculation in an uniform format with and fix units ([r] = Å, [E] = eV) independent of the quantum chemical backend used; ii) to save space on the hard disk, since typical quantum chemical output files of a local optimisation are in the range between 1 MB and 80 MB and the files generated with the **Extraction** program are smaller than 1 kB. The **Extraction** class iterates through all generated quantum chemical outputs (all cluster structures) and extracts information such as the final coordinates, the energy in eV, the CPU time taken, the number of the cluster structure (*strucNr*). With this information, for each cluster three small ASCII files are generated: *clusterName_strucNr.energy*, *clusterName_strucNr.xyz*, *clusterName_strucNr_aligned.xyz*. All the extracted information is saved for each cluster structure in the *clusterName_strucNr.energy* files and are used in the **Analysis1** program. The two geometry files only differ in the orientation of the cluster. The files *clusterName_strucNr.xyz* contain the cluster in the same orientation as in the corresponding quantum chemical output. In clusterName_strucNr_aligned.xyz the cluster is aligned in a distinct, specified way: first the cluster is transformed so its center of mass (CoM) is at the origin. Than the cluster is rotated so that the most distant atom (with respect to the CoM) lies on the x-axis; second a rotation around the x-axis is performed so that the z component of the second most distant atom (with respect to the CoM) vanishes. The generated geometry files are used for cluster structure visualisation in the **Analysis2** program.

Analysis1

In **Analysis1**, the assignment of the individual cluster structure into different geometry motifs takes place. First the data from all .energy files are imported into an array and arranged in order of ascending energy. Then an iterative process is performed. Starting with the GM, all cluster structures in the array are compared to the GM structure according to a structural *diff* (relative value) criterion and an energetic criterion *Ediff* (in eV). Regarding the structural criterion, all atomic distances (taking into account the element types) within two clusters are compared and if the relative deviation exceeds *diff* then the two structures are considered to be different. The energetic criterion *Ediff* is the maximum allowable energy difference (in eV) between two cluster structures for them to be assigned to the same geometry group. According to *Ediff* and *diff* all generated cluster structures are grouped into several geometry groups. The first group (*GroupNr 1*) exhibits the GM geometry. Additionally the moment of inertia eigenvalues are calculated for each cluster structure, since they can be used as additional structural comparison criteria. Four different output ASCII files are generated by **Analysis1**: *AllClusters*, *AllClusters_Ordered*, *ErrorList* and *results*. *ErrorList* contains all structures, which are not converged. All groups with the lowest and highest energy structure within each group are listed in results. The geometry group, total Energy and the *strucNr* of all generated cluster structures ordered according to the *strucNr* are specified in *AllClusters_Ordered*. The *strucNr* of all clusters, the assigned geometry group and moment of inertia eigenvalues are written in *AllClusters*. This file is ordered according to the assigned groups (*GroupNr*) and all cluster geometries within each group are listed in ascending energy order.

Analysis2

Analysis2 provides a selection menu with different automatic vi-

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sualisation analysis modes to check and, if necessary, correct the clustering results of **Analysis1**. A screenshot of the selection menu is shown in Fig. 1. During this process, the user should note the *strucNr* of each cluster representing a new geometry. At the end of the analysis process, all extracted *strucNr* are passed as input to the program and an Excel output file is generated.

Fig. 2 and Fig. 3 illustrate several geometry groups found with the analysis tool for the example of $[Cd_3Se_3(H_2S)_3]^+$ obtained with optimisation mode **a** (optimisation from scratch at the PBE level of theory using Quantum Espresso as the quantum chemical software package).

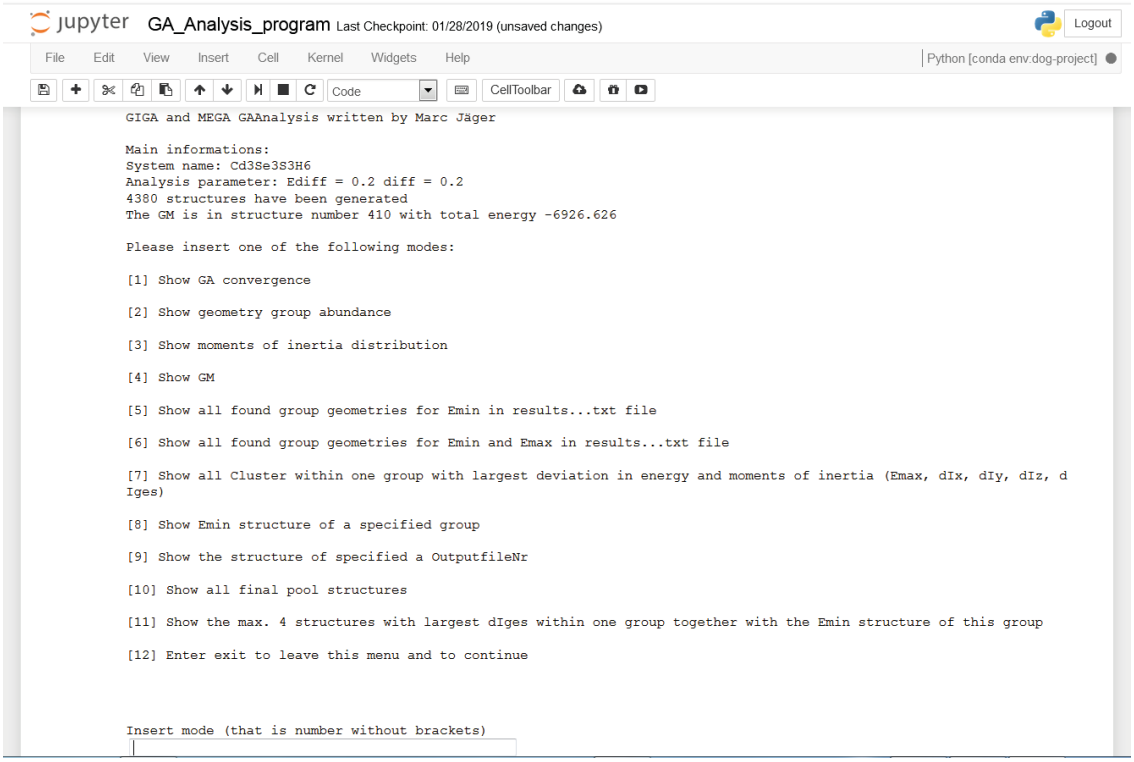

Fig. 1 Selection menu of **Analysis2** for automatic visualisation oft the results of **Analysis1**.

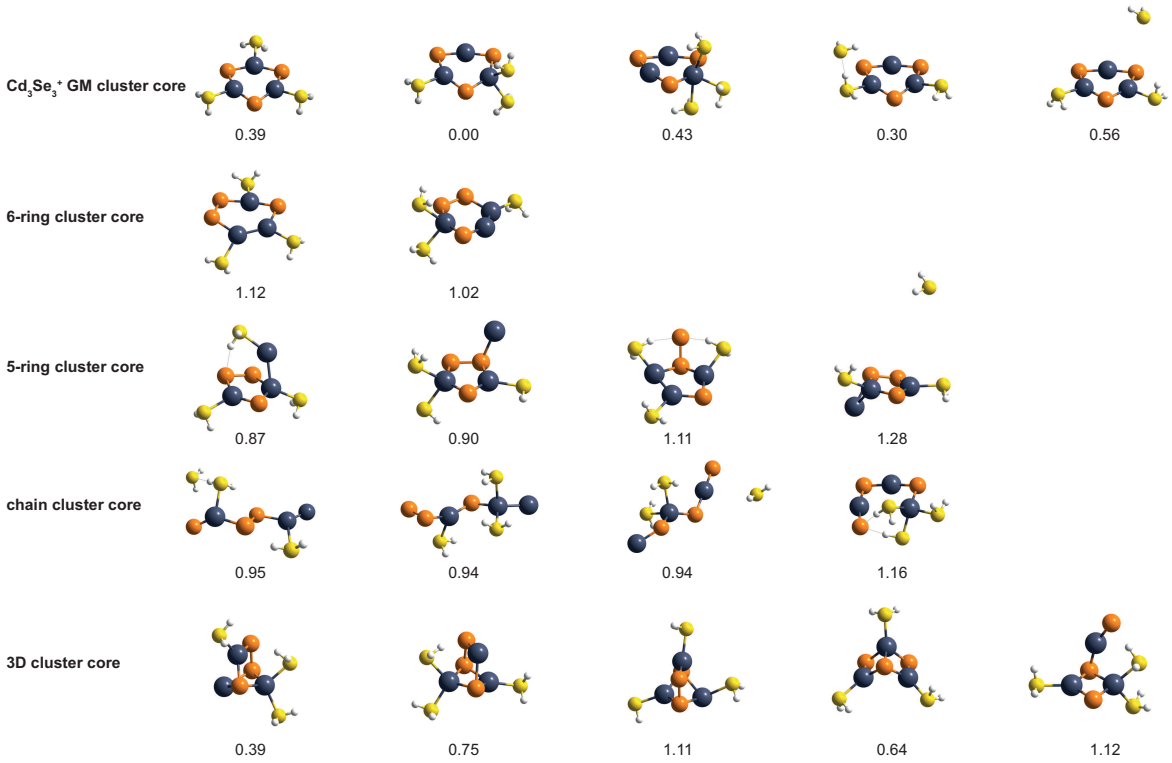

Fig. 2 $[Cd_3Se_3(H_2S)_3]^+$ structural motifs with intact ligands. Relative energies are in eV.

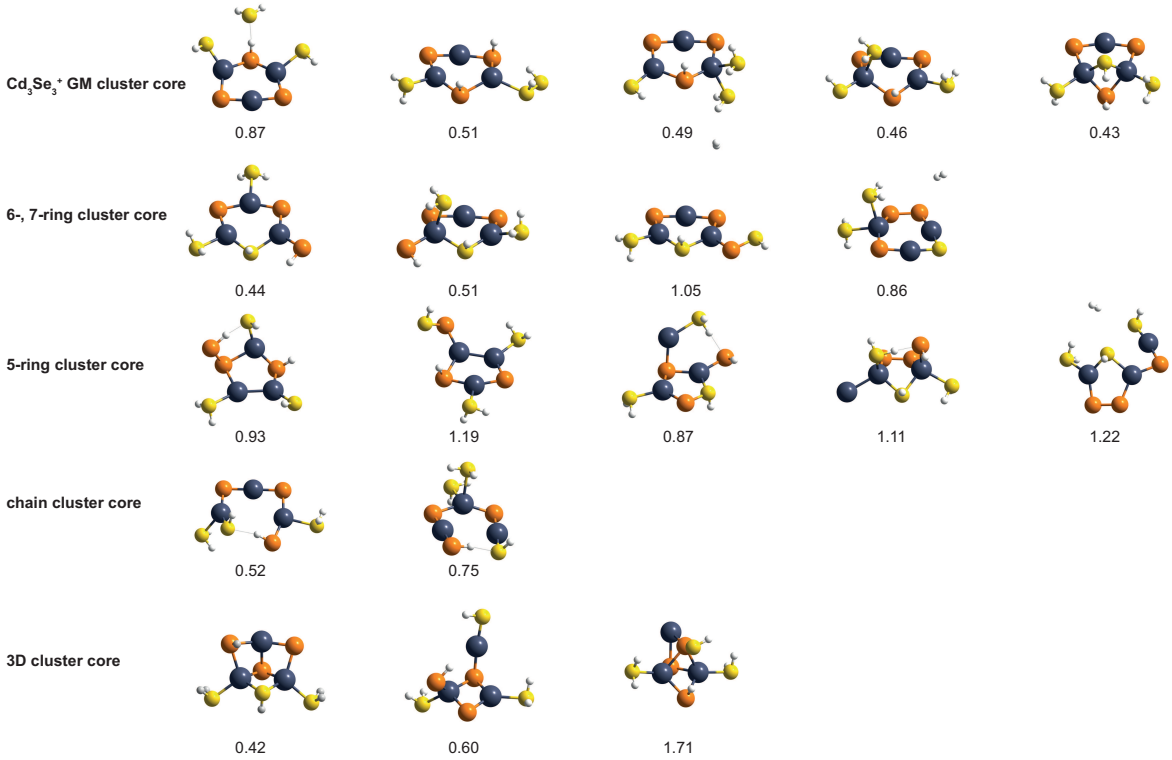

Fig. 3 $[Cd_3Se_3(H_2S)_3]^+$ structural motifs where ligand dissociation occurs. Relative energies are in eV.

2 Coordinates

All coordinates are given in Å.

bare $Cd_3Se_3^+$ GM
Cd -1.615317880000 -0.942005430000 0.385045470000
Cd 0.076601170000 1.287039780000 -1.426184050000
Cd 1.535914140000 -0.373574290000 1.072359350000
Se 2.390389030000 1.384933200000 -0.559370730000
Se -2.273131930000 0.542177620000 -1.575073410000
Se -0.113300530000 -1.886819150000 2.090367790000
$[Cd_3Se_3(H_2S)_3]^+$ Iso-I
Cd 1.304584100000 1.410252650000 -0.785410130000
Cd -0.640241600000 -1.496428240000 -1.265483080000
Se 0.875542380000 -0.124522780000 -2.668089100000
Cd -0.695349230000 0.108632590000 1.984557590000
Se 0.732441520000 2.132040310000 1.611937290000
Se -1.869661360000 -1.818691260000 0.952239160000
S -1.232517750000 0.049207910000 4.688082590000
H -2.502288240000 -0.393526230000 4.616892620000
H -1.605119550000 1.332954310000 4.850832970000
S -1.314746910000 -3.763602510000 -2.703363590000
H -1.245495810000 -3.200665360000 -3.924557780000
H -2.655758890000 -3.658040900000 -2.644835570000
S 3.333939300000 3.154434620000 -1.483339990000
H 3.149039110000 3.065315970000 -2.814200150000
H 2.658186980000 4.315292830000 -1.389055590000
$[Cd_3Se_3(H_2S)_3]^+$ Iso-II
Cd 0.732641310000 -0.884430280000 -1.764306270000
Cd -1.617500190000 -0.795899200000 1.018501000000
Cd 0.881523540000 1.690986080000 0.803653610000
Se -0.972154790000 1.177748820000 2.358457350000
Se 2.197797230000 1.076870290000 -1.308057490000
Se -1.137862440000 -2.333895530000 -0.977444990000
S 1.536641730000 -1.909803890000 -4.197248580000
H 2.868131880000 -1.835531750000 -4.010457240000
H 1.486141640000 -3.219453530000 -3.888270860000
S -3.923179820000 -1.879617700000 2.098423880000
H -3.704163160000 -1.465066630000 3.360723800000
H -3.476066100000 -3.125043190000 2.347272780000
S 2.187837270000 3.951839030000 1.721912800000
H 1.121557240000 4.501040810000 2.334007170000
H 2.059187700000 4.729255720000 0.630130330000
$[Cd_3Se_3(H_2S)_3]^+$ Iso-III
Cd -1.687033330000 1.001702430000 -0.962479550000
Cd 0.585188810000 -1.120327920000 1.462053030000
Se 2.795838430000 -0.794135710000 0.306710290000
Se -0.074407480000 1.805763730000 -2.656952830000
Cd 1.624851550000 0.560207140000 -1.345599510000
Se -1.962660000000 -0.479970290000 1.089281330000
S -4.157094690000 2.104355360000 -1.383416690000
H -4.018030590000 2.321628100000 -2.705466770000
H -4.866651580000 0.973917790000 -1.563410180000
S 0.387074630000 -3.824770840000 2.072274000000
H -0.623262380000 -4.163755520000 1.250002250000
H 1.332312880000 -4.176317210000 1.179327170000
S 0.946766630000 -0.469854710000 4.139105710000
H 0.301657760000 0.711294340000 4.163019750000
H 2.143478430000 0.105274770000 3.911049960000
$[Cd_3Se_3(H_2S)_3]^+$ Iso-IV
Cd -1.519737230000 0.702223200000 0.989402990000
Cd 0.190219020000 0.650553620000 -1.686936850000
Cd 1.067165670000 -1.398232090000 0.777745510000
Se 1.118376970000 1.287148700000 0.719169400000
Se -2.436554210000 1.331124450000 -1.354375650000
Se -0.856451390000 -1.168425040000 2.533352090000
S 3.157610300000 -2.777678840000 1.677444340000
H 3.066668250000 -2.363184570000 2.956455290000
H 2.510262120000 -3.932559490000 1.928365840000
S 0.684407140000 -1.874039210000 -1.721620740000
H -2.995901300000 -0.005872300000 -1.601464890000
H 1.974567200000 -1.719111600000 -2.075135710000
S 1.207180040000 1.887237770000 -3.813481870000
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Pt_6^+ GM structure A
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Pt 8.162366000000 9.227809000000 5.634964000000
Pt 10.234219000000 10.533209000000 5.615701000000
Pt 6.088850000000 7.924995000000 5.617413000000
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Pt 10.253932000000 10.500210000000 8.064520000000
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$[Pt_6/graphene]^+$ Structure B

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$[Pt_6(H_20)_2/graphene]^+$ Iso-I GM from scratch

Pt 9.591760000000 8.038258000000 7.336730000000
Pt 7.075475000000 7.835244000000 7.455812000000
Pt 11.831684000000 9.010458000000 8.062968000000
Pt 8.472416000000 5.776700000000 7.933167000000
Pt 8.292145000000 6.537162000000 5.521014000000
Pt 10.067904000000 10.449889000000 6.998715000000
O 8.359435000000 11.313807000000 6.279129000000
H 8.252149000000 12.188380000000 6.705122000000
H 12.671533000000 8.515376000000 6.876124000000
O 6.401596000000 9.807607000000 6.962930000000
H 7.217687000000 10.438184000000 6.690942000000
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$[Pt_6(H_20)_2/graphene]^+$ Iso-II

Pt 9.525978000000 8.177644000000 8.057671000000
Pt 10.028314000000 8.396857000000 5.631311000000
Pt 7.530781000000 6.715337000000 7.282077000000
Pt 9.641930000000 5.606910000000 8.030813000000
Pt 9.265435000000 5.901903000000 5.489948000000
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$[Pt_6(H_20)_2/graphene]^+$ Iso-III
Pt 7.752678000000 11.727653000000 8.107608000000
Pt 8.866219000000 9.626071000000 7.495204000000
Pt 11.091224000000 10.787179000000 7.263778000000
Pt 7.244093000000 9.604561000000 5.495659000000
Pt 6.273387000000 9.671251000000 7.828983000000
Pt 9.964370000000 12.890348000000 7.982269000000
O 11.982309000000 9.235700000000 6.280994000000
H 12.801445000000 9.026171000000 6.776772000000
H 10.803549000000 8.125254000000 6.763928000000
O 9.949500000000 7.747617000000 7.186715000000
H 10.296721000000 13.100766000000 9.472418000000
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$[Pt_6(H_2O)_2/graphene]^+$ Iso-IV
Pt 6.736917000000 11.461173000000 8.126200000000
Pt 7.913234000000 9.768441000000 6.811009000000
Pt 9.361343000000 11.418672000000 5.508624000000
Pt 5.783593000000 9.137373000000 5.515471000000
Pt 5.691931000000 9.119459000000 8.029318000000
Pt 9.296781000000 11.635350000000 8.014642000000
O 9.151147000000 7.967835000000 6.050302000000
H 9.882568000000 7.909699000000 6.696250000000
H 8.578891000000 7.196126000000 6.232857000000
O 5.494615000000 12.699090000000 9.392271000000
H 5.640971000000 12.507859000000 10.339508000000
H 5.626707000000 13.660281000000 9.281538000000
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$[Pt_6(H_20)_2/graphene]^+$ Iso-V

Pt 8.108456000000 9.224766000000 8.067659000000
Pt 8.131827000000 9.301033000000 5.641475000000
Pt 10.146043000000 10.805126000000 5.707503000000
Pt 6.313420000000 7.561571000000 5.608593000000
Pt 6.373310000000 7.506439000000 8.059845000000
Pt 9.950894000000 10.839643000000 8.187200000000
O 12.322037000000 11.993988000000 6.163930000000
H 12.629450000000 11.407952000000 6.885158000000
H 12.089688000000 12.832641000000 6.608856000000
O 5.273177000000 6.132126000000 9.392706000000
H 4.608503000000 6.511016000000 10.002360000000
H 5.795365000000 5.479864000000 9.899282000000
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C 14.909998000000 9.838051000000 3.349999000000
C 16.329997000000 9.838051000000 3.349999000000
C 1.420000000000 8.608290000000 3.349999000000
C 4.259999000000 8.608290000000 3.349999000000
C 5.679998000000 8.608290000000 3.349999000000
C 8.519997000000 8.608290000000 3.349999000000
C 9.940002000000 8.608290000000 3.349999000000
C 12.780001000000 8.608290000000 3.349999000000
C 14.200001000000 8.608290000000 3.349999000000
C 17.040000000000 8.608290000000 3.349999000000
C 2.130002000000 7.378535000000 3.349999000000
C 3.550001000000 7.378535000000 3.349999000000
C 6.390000000000 7.378535000000 3.349999000000
C 7.810000000000 7.378535000000 3.349999000000
C 10.649999000000 7.378535000000 3.349999000000
C 12.069999000000 7.378535000000 3.349999000000
C 14.909998000000 7.378535000000 3.349999000000
C 16.329997000000 7.378535000000 3.349999000000
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C 5.679998000000 6.148780000000 3.349999000000
C 8.519997000000 6.148780000000 3.349999000000
C 9.940002000000 6.148780000000 3.349999000000
C 12.780001000000 6.148780000000 3.349999000000
C 14.200001000000 6.148780000000 3.349999000000
C 17.040000000000 6.148780000000 3.349999000000
C 2.130002000000 4.919025000000 3.349999000000
C 3.550001000000 4.919025000000 3.349999000000
C 6.390000000000 4.919025000000 3.349999000000
C 7.810000000000 4.919025000000 3.349999000000
C 10.649999000000 4.919025000000 3.349999000000
C 12.069999000000 4.919025000000 3.349999000000
C 14.909998000000 4.919025000000 3.349999000000
C 16.329997000000 4.919025000000 3.349999000000
C 1.420000000000 3.689270000000 3.349999000000
C 4.259999000000 3.689270000000 3.349999000000
C 5.679998000000 3.689270000000 3.349999000000
C 8.519997000000 3.689270000000 3.349999000000
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C 12.780001000000 3.689270000000 3.349999000000
C 14.200001000000 3.689270000000 3.349999000000
C 17.040000000000 3.689270000000 3.349999000000
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C 3.550001000000 2.459510000000 3.349999000000
C 6.390000000000 2.459510000000 3.349999000000
C 7.810000000000 2.459510000000 3.349999000000
C 10.649999000000 2.459510000000 3.349999000000
C 12.069999000000 2.459510000000 3.349999000000
C 14.909998000000 2.459510000000 3.349999000000
C 16.329997000000 2.459510000000 3.349999000000
C 1.420000000000 1.229755000000 3.349999000000
C 4.259999000000 1.229755000000 3.349999000000
C 5.679998000000 1.229755000000 3.349999000000
C 8.519997000000 1.229755000000 3.349999000000
C 9.940002000000 1.229755000000 3.349999000000
C 12.780001000000 1.229755000000 3.349999000000
C 14.200001000000 1.229755000000 3.349999000000
C 17.040000000000 1.229755000000 3.349999000000
C 2.130002000000 0.000000000000 3.349999000000
C 3.550001000000 0.000000000000 3.349999000000
C 6.390000000000 0.000000000000 3.349999000000
C 7.810000000000 0.000000000000 3.349999000000
C 10.649999000000 0.000000000000 3.349999000000
C 12.069999000000 0.000000000000 3.349999000000
C 14.909998000000 0.000000000000 3.349999000000

C 16.329997000000 0.000000000000 3.349999000000
Pt_4V_2 Iso-I PBE0/def-tzvp
Pt -1.123813050000 -1.412168260000 0.332821980000
Pt -1.702593610000 0.301296860000 -1.515390590000
Pt 1.655406860000 1.591566650000 0.146800560000
V -0.766059920000 1.151908070000 0.663024920000
Pt 1.188657950000 -0.722921060000 1.201431920000
V 0.745865630000 -0.239317370000 -1.325253980000
Pt_4V_2 Iso-II PBE/def2-tzvp
V 0.045252010000 -0.505039540000 -0.114465430000
V -0.179472250000 1.995046520000 0.471624620000
Pt 0.235324720000 -2.579506640000 -0.537180110000
Pt -0.221914170000 1.148348290000 -1.758726890000
Pt 1.758677150000 0.682006340000 0.971508240000
Pt -1.734949350000 0.318514760000 1.180411790000