Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


**Electronic Supplementary Information**

# Two electron reducing reaction of $CO_2$ to oxalate anion: theoretical study of delocalized (presolvated) electrons in $Al(CH_3)_n(NH_3)_m$ , n = 0 – 2 and m = 1 – 6, clusters

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# I. Cartesian coordinates

All the optimized structures were obtained at the CAM-B3LYP/6-311++G(2d,2p) EmpiricalDispersion=GD3BJ level of theory. No imaginary vibrational frequency has been found for the structures reported below.

## Al atom:

Charge = 0 Multiplicity = 2 HF = -242.3669814 S2 = 0.755372

## $NH_3$:

Charge = 0 Multiplicity = 1 HF = -56.5555218
Sum of electronic and zero-point Energies= -56.520969

| | | | | |
|---|---|---|---|---|
| 7 | 0 | 0.000000 | 0.000000 | 0.109457 |
| 1 | 0 | 0.000000 | 0.942961 | -0.255400 |
| 1 | 0 | 0.816629 | -0.471481 | -0.255400 |
| 1 | 0 | -0.816629 | -0.471481 | -0.255400 |

## Al($NH_3$):

Charge = 0 Multiplicity = 2 HF = -298.9401998 S2 = 0.757162
Sum of electronic and zero-point Energies= -298.906235

| | | | | |
|---|---|---|---|---|
| 7 | 0 | 0.000000 | 0.000000 | -1.270157 |
| 13 | 0 | 0.000000 | 0.000000 | 1.060371 |
| 1 | 0 | 0.000000 | 0.947011 | -1.631241 |
| 1 | 0 | 0.820136 | -0.473506 | -1.631241 |
| 1 | 0 | -0.820136 | -0.473506 | -1.631241 |

## Al(NH3)6:

### Al(0)-6 isomer:

Charge = 0 Multiplicity = 2 HF = -581.7433965 S2 = 0.835298
Sum of electronic and zero-point Energies= -581.518169

| | | | | |
|---|---|---|---|---|
| 13 | 0 | -0.000004 | -0.000002 | -0.000010 |
| 7 | 0 | -1.231888 | -0.686646 | -1.478147 |
| 7 | 0 | 1.239491 | -1.618927 | -0.147122 |
| 7 | 0 | 1.231948 | 0.942114 | -1.330070 |
| 7 | 0 | -1.239446 | 1.619011 | 0.146983 |
| 7 | 0 | -1.232017 | -0.941927 | 1.330125 |
| 7 | 0 | 1.231911 | 0.686375 | 1.478230 |
| 1 | 0 | -2.224212 | -0.554927 | -1.202905 |
| 1 | 0 | -1.131571 | -0.202805 | -2.376784 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | -1.136195 | -1.687609 | -1.679756 |
| 1 | 0 | 2.230367 | -1.310562 | -0.115498 |
| 1 | 0 | 1.142181 | -2.301210 | 0.612319 |
| 1 | 0 | 1.146828 | -2.148007 | -1.020744 |
| 1 | 0 | 2.224280 | 0.765862 | -1.081361 |
| 1 | 0 | 1.133796 | 0.624895 | -2.300357 |
| 1 | 0 | 1.133932 | 1.962761 | -1.351146 |
| 1 | 0 | -1.146484 | 2.148474 | 1.020342 |
| 1 | 0 | -1.142404 | 2.300963 | -0.612786 |
| 1 | 0 | -2.230338 | 1.310653 | 0.115794 |
| 1 | 0 | 2.224231 | 0.555567 | 1.202532 |
| 1 | 0 | 1.135577 | 1.687073 | 1.680841 |
| 1 | 0 | 1.132269 | 0.201607 | 2.376449 |
| 1 | 0 | -1.134217 | -0.624051 | 2.300236 |
| 1 | 0 | -2.224342 | -0.766132 | 1.081070 |
| 1 | 0 | -1.133646 | -1.962523 | 1.351879 |

Al(0)-51 isomer:

Charge = 0 Multiplicity = 2 HF = -581.7812666 S2 = 0.751688

Sum of electronic and zero-point Energies= -581.555265

| | | | | |
|---|---|---|---|---|
| 7 | 0 | -2.053916 | -1.475079 | -1.415801 |
| 13 | 0 | 0.567836 | 0.680897 | 0.677536 |
| 7 | 0 | -0.953837 | 1.705139 | -0.370840 |
| 7 | 0 | 2.535074 | -2.439828 | 0.607193 |
| 7 | 0 | 0.802109 | -0.521217 | -0.995270 |
| 7 | 0 | 1.868121 | 2.090963 | -0.183080 |
| 7 | 0 | -2.861783 | -0.257510 | 1.445944 |
| 1 | 0 | -2.495546 | -1.061863 | -2.227844 |
| 1 | 0 | -2.232758 | -2.470623 | -1.453186 |
| 1 | 0 | -2.513282 | -1.105113 | -0.584971 |
| 1 | 0 | -1.087489 | 2.637843 | 0.020204 |
| 1 | 0 | -0.767104 | 1.851720 | -1.368859 |
| 1 | 0 | -1.839363 | 1.207134 | -0.276972 |
| 1 | 0 | 3.540720 | -2.343752 | 0.667452 |
| 1 | 0 | 2.131502 | -1.931704 | 1.388876 |
| 1 | 0 | 2.316147 | -3.419931 | 0.731385 |
| 1 | 0 | 2.853823 | 1.832736 | -0.096037 |
| 1 | 0 | 1.700794 | 2.284734 | -1.183396 |
| 1 | 0 | 1.768070 | 2.995135 | 0.286627 |
| 1 | 0 | 1.458730 | -1.269570 | -0.749659 |
| 1 | 0 | -0.108253 | -0.953354 | -1.213895 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | 1.127391 | -0.060977 | -1.841579 |
| 1 | 0 | -3.281148 | -1.094532 | 1.833087 |
| 1 | 0 | -1.918339 | -0.192757 | 1.827050 |
| 1 | 0 | -3.386138 | 0.525943 | 1.816727 |

Al(0)-42 isomer:

Charge = 0 Multiplicity = 2 HF = -581.7835125 S2 = 0.751208

Sum of electronic and zero-point Energies= -581.557510

| | | | | |
|---|---|---|---|---|
| 7 | 0 | -0.935306 | -1.117065 | 1.473682 |
| 13 | 0 | 0.573258 | -1.285570 | -0.007993 |
| 7 | 0 | -0.651317 | -0.077376 | -1.216702 |
| 7 | 0 | 1.395925 | 0.495455 | 0.778451 |
| 7 | 0 | -0.757112 | 2.753574 | 0.261306 |
| 7 | 0 | -3.575211 | -0.493861 | -0.720891 |
| 1 | 0 | -1.377141 | -0.197079 | 1.629257 |
| 1 | 0 | -1.649067 | -0.339724 | -1.151368 |
| 1 | 0 | 0.832918 | 1.331122 | 0.604181 |
| 1 | 0 | -0.583050 | -1.410342 | 2.385575 |
| 1 | 0 | -1.703571 | -1.755881 | 1.261611 |
| 1 | 0 | -0.377015 | -0.161587 | -2.189052 |
| 1 | 0 | -0.605627 | 0.909829 | -0.957353 |
| 1 | 0 | 1.535199 | 0.432955 | 1.782262 |
| 1 | 0 | 2.322200 | 0.604406 | 0.349233 |
| 1 | 0 | -3.985565 | -1.393108 | -0.487269 |
| 1 | 0 | -1.436199 | 2.391010 | 0.935742 |
| 1 | 0 | -3.666013 | 0.090621 | 0.110200 |
| 1 | 0 | -0.264431 | 3.505360 | 0.737246 |
| 1 | 0 | -4.165343 | -0.076789 | -1.434816 |
| 1 | 0 | -1.305193 | 3.196381 | -0.472534 |
| 7 | 0 | 3.995481 | -0.063720 | -0.650921 |
| 1 | 0 | 3.558878 | -0.970925 | -0.791260 |
| 1 | 0 | 4.263981 | 0.290117 | -1.560252 |
| 1 | 0 | 4.845461 | -0.213012 | -0.121969 |

Al(0)-33 isomer:

Charge = 0 Multiplicity = 2 HF = -581.7850183 S2 = 0.750337

Sum of electronic and zero-point Energies= -581.558084

| | | | | |
|---|---|---|---|---|
| 13 | 0 | 0.005580 | -0.017301 | 2.067625 |
| 7 | 0 | 0.088823 | -1.693208 | 0.741424 |
| 7 | 0 | 1.419450 | 0.912250 | 0.760358 |

| | | | | |
|---|---|---|---|---|
| 7 | 0 | -1.502821 | 0.761287 | 0.767201 |
| 1 | 0 | -0.728123 | -1.748718 | 0.127642 |
| 1 | 0 | 1.879266 | 0.241936 | 0.138743 |
| 1 | 0 | -1.149942 | 1.501004 | 0.154405 |
| 7 | 0 | -2.123944 | -1.360388 | -1.476052 |
| 7 | 0 | 2.246913 | -1.134550 | -1.484809 |
| 7 | 0 | -0.134359 | 2.532258 | -1.449474 |
| 1 | 0 | 0.134379 | -2.549646 | 1.281414 |
| 1 | 0 | 0.904096 | -1.664474 | 0.123617 |
| 1 | 0 | 2.135445 | 1.372743 | 1.310320 |
| 1 | 0 | 0.988784 | 1.612268 | 0.150784 |
| 1 | 0 | -1.894975 | 0.046406 | 0.148916 |
| 1 | 0 | -2.259046 | 1.146675 | 1.321057 |
| 1 | 0 | -2.159899 | -2.347913 | -1.719331 |
| 1 | 0 | 2.385858 | -2.113541 | -1.725510 |
| 1 | 0 | -0.093400 | 1.766555 | -2.128043 |
| 1 | 0 | -3.041827 | -0.984335 | -1.703629 |
| 1 | 0 | 1.555989 | -0.780600 | -2.152470 |
| 1 | 0 | -0.975913 | 3.057092 | -1.677589 |
| 1 | 0 | -1.476681 | -0.934109 | -2.145215 |
| 1 | 0 | 3.119229 | -0.664467 | -1.716717 |
| 1 | 0 | 0.645789 | 3.144496 | -1.678055 |

Al(0)-24 isomer:

Charge = 0 Multiplicity = 2 HF = -581.789818 S2 = 0.763702

Sum of electronic and zero-point Energies= -581.563856

| | | | | |
|---|---|---|---|---|
| 7 | 0 | -0.400925 | 0.269319 | -1.404806 |
| 13 | 0 | -0.000317 | 1.922825 | -0.000017 |
| 7 | 0 | 0.400523 | 0.270142 | 1.405722 |
| 7 | 0 | -1.653991 | -1.947721 | 0.826574 |
| 7 | 0 | 1.654954 | -1.948097 | -0.825801 |
| 1 | 0 | -0.242938 | -0.525013 | 1.322423 |
| 1 | 0 | 0.242630 | -0.525653 | -1.320780 |
| 1 | 0 | 0.328517 | 0.639744 | 2.345828 |
| 1 | 0 | -0.329158 | 0.637903 | -2.345324 |
| 1 | 0 | 1.351236 | -0.060770 | 1.271496 |
| 1 | 0 | -1.351582 | -0.061579 | -1.270067 |
| 1 | 0 | -2.115795 | -2.493882 | 1.542192 |
| 1 | 0 | 2.116762 | -2.491513 | -1.543533 |
| 1 | 0 | -2.343438 | -1.311092 | 0.425464 |
| 1 | 0 | 2.343636 | -1.310234 | -0.425222 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | -1.370726 | -2.588568 | 0.095955 |
| 1 | 0 | 1.375809 | -2.591332 | -0.095682 |
| 7 | 0 | 3.425017 | 0.457769 | 0.236642 |
| 7 | 0 | -3.425394 | 0.456751 | -0.238040 |
| 1 | 0 | 4.138200 | 0.420392 | -0.482949 |
| 1 | 0 | 2.785062 | 1.215872 | -0.027046 |
| 1 | 0 | 3.892600 | 0.754587 | 1.085920 |
| 1 | 0 | -3.892933 | 0.752915 | -1.087572 |
| 1 | 0 | -4.138820 | 0.418906 | 0.481289 |
| 1 | 0 | -2.786231 | 1.215440 | 0.025794 |

Al(0)-15 isomer:

Charge = 0 Multiplicity = 2 HF = -581.7814964 S2 = 0.759758

Sum of electronic and zero-point Energies= -581.558259

| | | | | |
|---|---|---|---|---|
| 7 | 0 | 0.131525 | 0.620533 | 0.442032 |
| 13 | 0 | 0.003601 | -0.219804 | -1.449700 |
| 7 | 0 | -1.545146 | -1.456012 | 1.939762 |
| 7 | 0 | -3.515710 | -1.422800 | -0.511362 |
| 1 | 0 | -0.353983 | -0.025398 | 1.081723 |
| 1 | 0 | -0.374876 | 1.508340 | 0.471791 |
| 1 | 0 | 1.089838 | 0.760811 | 0.789413 |
| 1 | 0 | -1.968768 | -1.241275 | 2.833075 |
| 1 | 0 | -2.292111 | -1.535713 | 1.247315 |
| 1 | 0 | -1.107659 | -2.364349 | 2.027681 |
| 1 | 0 | -2.870889 | -0.877129 | -1.082854 |
| 1 | 0 | -3.686796 | -2.289316 | -1.006637 |
| 1 | 0 | -4.392996 | -0.918171 | -0.482184 |
| 7 | 0 | 3.045710 | 0.889310 | 1.306317 |
| 1 | 0 | 3.493228 | 1.785696 | 1.164275 |
| 1 | 0 | 3.279708 | 0.585632 | 2.242753 |
| 1 | 0 | 3.459733 | 0.225717 | 0.648214 |
| 7 | 0 | 3.823772 | -1.169779 | -0.906529 |
| 1 | 0 | 4.425918 | -0.918859 | -1.681019 |
| 1 | 0 | 4.018196 | -2.137230 | -0.679382 |
| 1 | 0 | 2.863084 | -1.129737 | -1.249749 |
| 7 | 0 | -1.841315 | 2.888281 | -0.267499 |
| 1 | 0 | -1.620040 | 3.777352 | -0.697071 |
| 1 | 0 | -1.975278 | 2.210944 | -1.014526 |
| 1 | 0 | -2.724966 | 2.993409 | 0.214235 |

$Al(NH_3)_6^+$: global minimum

Charge = 1 Multiplicity = 1 HF = -581.6761191

Sum of electronic and zero-point Energies= -581.447467

| | | | | |
|---|---|---|---|---|
| 13 | 0 | -0.003964 | 0.002832 | 1.904902 |
| 7 | 0 | -1.621704 | -0.540334 | 0.539502 |
| 7 | 0 | 1.276619 | -1.150169 | 0.558933 |
| 7 | 0 | 0.356381 | 1.661325 | 0.530066 |
| 1 | 0 | -1.913610 | 0.235103 | -0.056783 |
| 1 | 0 | 0.754137 | -1.791024 | -0.040206 |
| 1 | 0 | 1.177028 | 1.518449 | -0.060874 |
| 7 | 0 | -2.358825 | 2.090837 | -1.223209 |
| 7 | 0 | -0.631868 | -3.070810 | -1.251218 |
| 7 | 0 | 2.986307 | 1.002599 | -1.236115 |
| 1 | 0 | -2.417685 | -0.806061 | 1.108836 |
| 1 | 0 | -1.390569 | -1.334582 | -0.058389 |
| 1 | 0 | 1.894076 | -1.706825 | 1.139509 |
| 1 | 0 | 1.859869 | -0.561316 | -0.035844 |
| 1 | 0 | -0.442197 | 1.861473 | -0.072877 |
| 1 | 0 | 0.526799 | 2.485393 | 1.095684 |
| 1 | 0 | -3.342057 | 1.891147 | -1.071769 |
| 1 | 0 | -1.507397 | -3.537910 | -1.041287 |
| 1 | 0 | 2.749308 | 0.918651 | -2.218852 |
| 1 | 0 | -2.257354 | 3.085789 | -1.050559 |
| 1 | 0 | -0.678766 | -2.805496 | -2.229004 |
| 1 | 0 | 3.293409 | 1.960081 | -1.099731 |
| 1 | 0 | -2.194813 | 1.955937 | -2.214578 |
| 1 | 0 | 0.080035 | -3.791495 | -1.188098 |
| 1 | 0 | 3.812946 | 0.431717 | -1.094618 |

$Al(CH_3)(NH_3)_6$:

Al(I)-5 isomer:

Charge = 0 Multiplicity = 1 HF = -565.134835

Sum of electronic and zero-point Energies= -564.908687

| | | | | |
|---|---|---|---|---|
| 13 | 0 | -0.013013 | 0.000086 | 0.125650 |
| 6 | 0 | -0.200761 | 0.001960 | 2.113478 |
| 7 | 0 | -1.507569 | -1.419136 | -0.215128 |
| 7 | 0 | -1.504948 | 1.421065 | -0.218908 |
| 7 | 0 | 1.423114 | 1.522491 | 0.152017 |
| 7 | 0 | 1.421790 | -1.523518 | 0.154073 |

| | | | | |
|---|---|---|---|---|
| 7 | 0 | 0.356631 | -0.002689 | -1.924949 |
| 1 | 0 | 0.775648 | 0.001766 | 2.612554 |
| 1 | 0 | -0.731175 | 0.876851 | 2.505391 |
| 1 | 0 | -0.732273 | -0.871663 | 2.506738 |
| 1 | 0 | -2.202965 | -1.373563 | 0.533828 |
| 1 | 0 | -2.011628 | -1.303686 | -1.098025 |
| 1 | 0 | -1.154291 | -2.380058 | -0.226768 |
| 1 | 0 | -1.149188 | 2.380868 | -0.241941 |
| 1 | 0 | -2.014306 | 1.298633 | -1.097838 |
| 1 | 0 | -2.196087 | 1.384471 | 0.534434 |
| 1 | 0 | 1.271372 | 2.251284 | -0.550344 |
| 1 | 0 | 1.431861 | 1.981437 | 1.064357 |
| 1 | 0 | 2.374104 | 1.177411 | -0.016990 |
| 1 | 0 | -0.023151 | -0.823518 | -2.416731 |
| 1 | 0 | -0.026691 | 0.814352 | -2.420186 |
| 1 | 0 | 1.366614 | -0.000977 | -2.136093 |
| 1 | 0 | 1.265374 | -2.256425 | -0.543034 |
| 1 | 0 | 2.372205 | -1.180560 | -0.022473 |
| 1 | 0 | 1.435189 | -1.976984 | 1.069068 |

Al(I)-23 isomer:

Charge = 0 Multiplicity = 1 HF = -565.1555745

Sum of electronic and zero-point Energies= -564.931275

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 2.094746 | -1.027384 | -1.284585 |
| 13 | 0 | 0.107787 | -0.561612 | -1.156470 |
| 7 | 0 | 0.497646 | 1.457207 | -0.548608 |
| 7 | 0 | 0.038942 | -0.948258 | 0.977074 |
| 7 | 0 | -2.978136 | -1.349940 | 0.745058 |
| 7 | 0 | 2.777496 | 0.682010 | 1.606670 |
| 1 | 0 | -0.921469 | -0.875428 | 1.311503 |
| 1 | 0 | 1.154572 | 1.505216 | 0.228249 |
| 1 | 0 | 0.339386 | -1.905379 | 1.125263 |
| 1 | 0 | 0.887050 | 1.973190 | -1.329082 |
| 1 | 0 | 0.654627 | -0.341502 | 1.514477 |
| 1 | 0 | -0.385028 | 1.902475 | -0.283931 |
| 1 | 0 | -2.545343 | -1.303696 | -0.180729 |
| 1 | 0 | 3.075957 | 0.098730 | 0.831347 |
| 1 | 0 | -3.896359 | -0.929499 | 0.669028 |
| 1 | 0 | 3.018672 | 0.196490 | 2.461863 |
| 1 | 0 | -3.125566 | -2.330826 | 0.952438 |
| 1 | 0 | 3.338477 | 1.524701 | 1.584959 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | 2.299069 | -1.635723 | -2.167259 |
| 1 | 0 | 2.741955 | -0.145232 | -1.372096 |
| 1 | 0 | 2.458551 | -1.612397 | -0.429509 |
| 7 | 0 | -2.444390 | 1.892671 | -0.144355 |
| 1 | 0 | -3.121328 | 2.595794 | -0.410347 |
| 1 | 0 | -2.388356 | 1.201112 | -0.889810 |
| 1 | 0 | -2.795481 | 1.411404 | 0.674387 |

$Al(CH_3)_2(NH_3)_6$:

Al(II)-4 isomer:

Charge = 0 Multiplicity = 2 HF = -548.5034949 S2 = 0.750254

Sum of electronic and zero-point Energies= -548.279162

| | | | | |
|---|---|---|---|---|
| 7 | 0 | 0.156961 | -1.355683 | 1.498646 |
| 13 | 0 | 0.000158 | -0.000146 | -0.212735 |
| 6 | 0 | -0.064134 | 1.610039 | -1.432563 |
| 6 | 0 | 0.066066 | -1.611284 | -1.431173 |
| 7 | 0 | -2.119025 | -0.146689 | -0.075104 |
| 7 | 0 | -0.158994 | 1.356796 | 1.497452 |
| 7 | 0 | 2.119138 | 0.146855 | -0.072553 |
| 1 | 0 | 0.910172 | -1.129095 | 2.153215 |
| 1 | 0 | -0.684813 | -1.396330 | 2.079854 |
| 1 | 0 | 0.327584 | -2.302257 | 1.163865 |
| 1 | 0 | -0.228360 | -1.352504 | -2.452987 |
| 1 | 0 | 1.059507 | -2.066469 | -1.516762 |
| 1 | 0 | -0.597923 | -2.426889 | -1.121558 |
| 1 | 0 | -2.411411 | -0.343998 | -1.028405 |
| 1 | 0 | -2.481813 | -0.891001 | 0.514490 |
| 1 | 0 | -2.578937 | 0.711651 | 0.213084 |
| 1 | 0 | -0.329298 | 2.303054 | 1.161617 |
| 1 | 0 | -0.913021 | 1.130682 | 2.151248 |
| 1 | 0 | 0.682035 | 1.398029 | 2.079686 |
| 1 | 0 | -1.057672 | 2.064563 | -1.520514 |
| 1 | 0 | 0.598791 | 2.426297 | -1.122401 |
| 1 | 0 | 0.232417 | 1.350516 | -2.453578 |
| 1 | 0 | 2.412626 | 0.342135 | -1.025933 |
| 1 | 0 | 2.480877 | 0.892659 | 0.515792 |
| 1 | 0 | 2.579040 | -0.710637 | 0.218162 |

Al(II)-13 isomer:

Charge = 0 Multiplicity = 2 HF = -548.5021799 S2 = 0.75088

Sum of electronic and zero-point Energies= -548.281224

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 1.993591 | -0.282112 | 1.263748 |
| 13 | 0 | 0.059180 | 0.142816 | 1.061273 |
| 7 | 0 | -0.324794 | -0.327841 | -0.848544 |
| 6 | 0 | -0.407561 | 2.070914 | 1.178335 |
| 7 | 0 | 0.120324 | -3.290525 | -0.251752 |
| 7 | 0 | -3.284806 | 0.328654 | -0.540004 |
| 7 | 0 | 1.894968 | 1.414611 | -2.007692 |
| 1 | 0 | -0.170318 | -1.329625 | -0.985624 |
| 1 | 0 | -1.301795 | -0.117052 | -1.065944 |
| 1 | 0 | 0.294029 | 0.199418 | -1.472608 |
| 1 | 0 | 2.272757 | -1.217784 | 0.773714 |
| 1 | 0 | 2.622249 | 0.508584 | 0.840167 |
| 1 | 0 | 2.283051 | -0.376029 | 2.311282 |
| 1 | 0 | 0.180447 | 2.660987 | 0.466887 |
| 1 | 0 | -1.458993 | 2.282127 | 0.976160 |
| 1 | 0 | -0.192134 | 2.470032 | 2.171171 |
| 1 | 0 | -0.435986 | -4.101596 | -0.488860 |
| 1 | 0 | 1.083606 | -3.591505 | -0.175701 |
| 1 | 0 | -0.168965 | -2.976496 | 0.669935 |
| 1 | 0 | -4.125686 | -0.135717 | -0.856999 |
| 1 | 0 | -3.117524 | 0.045042 | 0.419997 |
| 1 | 0 | -3.468329 | 1.323849 | -0.529283 |
| 1 | 0 | 2.616718 | 1.004523 | -1.427481 |
| 1 | 0 | 2.285669 | 1.567145 | -2.927945 |
| 1 | 0 | 1.675843 | 2.320390 | -1.611971 |

Al(II)-22 isomer:

Charge = 0 Multiplicity = 2 HF = -548.5140942 S2 = 0.750264

Sum of electronic and zero-point Energies= -548.292164

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 1.775121 | -1.853751 | -0.115310 |
| 13 | 0 | 1.078149 | -0.028490 | -0.048922 |
| 7 | 0 | 0.344171 | 0.296439 | 1.774856 |
| 6 | 0 | 2.142731 | 1.523039 | -0.580073 |
| 7 | 0 | -0.601753 | 0.020683 | -1.065749 |
| 7 | 0 | -2.258876 | -2.236309 | -0.104913 |
| 7 | 0 | -2.255177 | 2.252685 | -0.057391 |
| 1 | 0 | 1.059805 | -2.587463 | 0.260860 |
| 1 | 0 | 2.685449 | -1.966236 | 0.477043 |
| 1 | 0 | 2.030781 | -2.149658 | -1.136136 |
| 1 | 0 | 0.128150 | 1.282735 | 1.964466 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | -0.539905 | -0.205032 | 1.974728 |
| 1 | 0 | 0.993321 | 0.004762 | 2.512784 |
| 1 | 0 | -1.169232 | 0.857223 | -0.832284 |
| 1 | 0 | -0.435415 | 0.034548 | -2.067978 |
| 1 | 0 | -1.192129 | -0.805604 | -0.855777 |
| 1 | 0 | 1.580686 | 2.457307 | -0.519640 |
| 1 | 0 | 3.028470 | 1.645669 | 0.046476 |
| 1 | 0 | 2.501611 | 1.431665 | -1.608624 |
| 1 | 0 | -2.433189 | -1.882659 | 0.834013 |
| 1 | 0 | -3.163188 | -2.429852 | -0.521061 |
| 1 | 0 | -1.777949 | -3.122946 | 0.000659 |
| 1 | 0 | -2.571404 | 1.819455 | 0.808666 |
| 1 | 0 | -1.762854 | 3.099036 | 0.211318 |
| 1 | 0 | -3.084615 | 2.537205 | -0.568860 |

## II. Extension and application:

$Al(CH_3)_2(NH_3)_2$:

Charge = 0 Multiplicity = 2 HF = -435.372514\S2=0.750267

Sum of electronic and zero-point Energies= -435.225482

| | | | | |
|---|---|---|---|---|
| 13 | 0 | 0.000000 | 0.000000 | 0.212071 |
| 7 | 0 | 0.000000 | 1.465574 | -1.142355 |
| 7 | 0 | 0.000000 | -1.465574 | -1.142355 |
| 1 | 0 | 0.000000 | 2.407822 | -0.739206 |
| 1 | 0 | 0.000000 | -2.407822 | -0.739206 |
| 1 | 0 | 0.815718 | -1.400029 | -1.764248 |
| 1 | 0 | 0.815718 | 1.400029 | -1.764248 |
| 1 | 0 | -0.815718 | -1.400029 | -1.764248 |
| 1 | 0 | -0.815718 | 1.400029 | -1.764248 |
| 6 | 0 | 1.712440 | 0.000000 | 1.141164 |
| 6 | 0 | -1.712440 | 0.000000 | 1.141164 |
| 1 | 0 | 2.567612 | 0.000000 | 0.463828 |
| 1 | 0 | -2.567612 | 0.000000 | 0.463828 |
| 1 | 0 | 1.814885 | 0.875344 | 1.787454 |
| 1 | 0 | -1.814885 | 0.875344 | 1.787454 |
| 1 | 0 | 1.814885 | -0.875344 | 1.787454 |
| 1 | 0 | -1.814885 | -0.875344 | 1.787454 |

$Al_2(CH_3)_2(CH_2)_2(NH_3)_4$:

Singlet state:

Charge = 0 Multiplicity = 1 HF = -869.5472555

Sum of electronic and zero-point Energies= -869.269736

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -3.958371 | -0.847947 | -0.173278 |
| 13 | 0 | -2.117207 | -0.199881 | -0.064109 |
| 7 | 0 | -2.017415 | 1.502445 | -1.087725 |
| 6 | 0 | -0.642836 | -1.444100 | -0.432189 |
| 6 | 0 | 0.642712 | -1.444777 | 0.430513 |
| 13 | 0 | 2.117012 | -0.199874 | 0.064454 |
| 7 | 0 | 2.016230 | 1.503308 | 1.086484 |
| 6 | 0 | 3.958129 | -0.847661 | 0.176324 |
| 1 | 0 | 4.703508 | -0.085133 | -0.057365 |
| 7 | 0 | 1.876644 | 0.650326 | -1.728844 |
| 7 | 0 | -1.875003 | 0.651418 | 1.728379 |
| 1 | 0 | 1.596905 | -0.003003 | -2.463565 |
| 1 | 0 | 1.953993 | 1.379528 | 2.102933 |
| 1 | 0 | 1.156993 | 2.024897 | 0.811408 |
| 1 | 0 | 1.129061 | 1.362030 | -1.661202 |
| 1 | 0 | 2.803001 | 2.137147 | 0.909195 |
| 1 | 0 | 2.709499 | 1.141991 | -2.058947 |
| 1 | 0 | 1.121153 | -2.430079 | 0.363060 |
| 1 | 0 | 4.129682 | -1.683088 | -0.507244 |
| 1 | 0 | 0.391398 | -1.352655 | 1.493898 |
| 1 | 0 | 4.188853 | -1.217516 | 1.178633 |
| 1 | 0 | -0.391396 | -1.349634 | -1.495342 |
| 1 | 0 | -1.120955 | -2.429681 | -0.366820 |
| 1 | 0 | -4.703510 | -0.085372 | 0.061046 |
| 1 | 0 | -4.190490 | -1.218418 | -1.175033 |
| 1 | 0 | -4.128872 | -1.682991 | 0.511027 |
| 1 | 0 | -2.803840 | 2.136624 | -0.910280 |
| 1 | 0 | -1.157812 | 2.024087 | -0.813937 |
| 1 | 0 | -1.956195 | 1.377616 | -2.104092 |
| 1 | 0 | -2.707991 | 1.141943 | 2.059862 |
| 1 | 0 | -1.592916 | -0.001224 | 2.462824 |
| 1 | 0 | -1.128545 | 1.364170 | 1.659182 |

Triplet state:

Charge = 0 Multiplicity = 3 HF = -869.5344543 S2 = 2.000533

Sum of electronic and zero-point Energies= -869.257641

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 3.799283 | -1.479591 | -0.478939 |
| 13 | 0 | 2.397312 | -0.189244 | -0.066329 |
| 7 | 0 | 2.761878 | 0.615709 | 1.722554 |
| 6 | 0 | 0.486340 | -0.604570 | -0.196540 |
| 6 | 0 | -0.486358 | 0.604669 | -0.196455 |
| 13 | 0 | -2.397318 | 0.189279 | -0.066259 |
| 7 | 0 | -2.761843 | -0.615983 | 1.722493 |
| 6 | 0 | -3.799373 | 1.479572 | -0.478757 |
| 1 | 0 | -4.803708 | 1.077771 | -0.338198 |
| 7 | 0 | -2.747874 | -1.503952 | -1.063498 |
| 7 | 0 | 2.747941 | 1.504136 | -1.063280 |
| 1 | 0 | -2.676324 | -1.416237 | -2.081721 |
| 1 | 0 | -2.702018 | 0.048029 | 2.501207 |
| 1 | 0 | -2.122426 | -1.391767 | 1.935267 |
| 1 | 0 | -2.104128 | -2.249638 | -0.775711 |
| 1 | 0 | -3.701753 | -1.035237 | 1.753540 |
| 1 | 0 | -3.686656 | -1.867100 | -0.854838 |
| 1 | 0 | -0.327230 | 1.207285 | -1.097454 |
| 1 | 0 | -3.733484 | 1.823979 | -1.513845 |
| 1 | 0 | -0.241656 | 1.294429 | 0.621657 |
| 1 | 0 | -3.719325 | 2.369832 | 0.149905 |
| 1 | 0 | 0.241675 | -1.294418 | 0.621511 |
| 1 | 0 | 0.327179 | -1.207094 | -1.097594 |
| 1 | 0 | 4.803649 | -1.077871 | -0.338374 |
| 1 | 0 | 3.719175 | -2.369862 | 0.149703 |
| 1 | 0 | 3.733365 | -1.823973 | -1.514033 |
| 1 | 0 | 3.701814 | 1.034896 | 1.753676 |
| 1 | 0 | 2.122513 | 1.391498 | 1.935465 |
| 1 | 0 | 2.702009 | -0.048436 | 2.501152 |
| 1 | 0 | 3.686735 | 1.867212 | -0.854545 |
| 1 | 0 | 2.676392 | 1.416621 | -2.081520 |
| 1 | 0 | 2.104219 | 2.249790 | -0.775350 |

$Al_2(CH_3)_2(CH_2)_2(NH_3)_4 + 2CO_2$:

Singlet state:

Charge = 0 Multiplicity = 1 HF = -1246.9077178

Sum of electronic and zero-point Energies= -1246.595118

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 3.975934 | -2.028688 | 0.220697 |
| 13 | 0 | 2.272077 | -1.059389 | 0.138316 |
| 6 | 0 | 0.566675 | -1.961560 | 0.536061 |

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.566662 | -1.961847 | -0.535230 |
| 13 | 0 | -2.272069 | -1.059388 | -0.138145 |
| 6 | 0 | -3.975899 | -2.028724 | -0.220589 |
| 7 | 0 | 2.213592 | -0.220796 | -1.656154 |
| 7 | 0 | 2.449437 | 0.539829 | 1.264527 |
| 7 | 0 | -2.214134 | -0.219800 | 1.655869 |
| 7 | 0 | -2.449076 | 0.539431 | -1.265031 |
| 1 | 0 | -4.840671 | -1.397614 | -0.001375 |
| 1 | 0 | -2.209877 | -0.919084 | 2.391082 |
| 1 | 0 | -1.491769 | 0.857100 | -1.564925 |
| 1 | 0 | -2.778859 | 1.362144 | -0.757334 |
| 1 | 0 | -1.374678 | 0.398371 | 1.791047 |
| 1 | 0 | -3.033424 | 0.404157 | -2.081623 |
| 1 | 0 | -3.016403 | 0.380198 | 1.821601 |
| 1 | 0 | -0.838796 | -2.995251 | -0.769401 |
| 1 | 0 | -4.005818 | -2.862492 | 0.484719 |
| 1 | 0 | -0.216619 | -1.558774 | -1.491831 |
| 1 | 0 | -4.146291 | -2.462062 | -1.209029 |
| 1 | 0 | 0.216624 | -1.557924 | 1.492394 |
| 1 | 0 | 0.838748 | -2.994832 | 0.770817 |
| 1 | 0 | 4.840599 | -1.397724 | 0.000863 |
| 1 | 0 | 4.146679 | -2.461460 | 1.209267 |
| 1 | 0 | 4.005648 | -2.862817 | -0.484126 |
| 1 | 0 | 2.779094 | 1.362390 | 0.756503 |
| 1 | 0 | 1.492210 | 0.857541 | 1.564618 |
| 1 | 0 | 3.034015 | 0.404772 | 2.080987 |
| 1 | 0 | 3.016784 | 0.377505 | -1.823382 |
| 1 | 0 | 2.207206 | -0.920748 | -2.390707 |
| 1 | 0 | 1.374869 | 0.398482 | -1.790944 |
| 6 | 0 | -0.492794 | 2.081012 | 0.593653 |
| 6 | 0 | 0.492849 | 2.081166 | -0.593723 |
| 8 | 0 | 1.631593 | 2.535265 | -0.462060 |
| 8 | 0 | -1.631721 | 2.534703 | 0.461963 |
| 8 | 0 | -0.074322 | 1.438389 | 1.615133 |
| 8 | 0 | 0.074608 | 1.438321 | -1.615179 |

Triplet state:

Charge = 0 Multiplicity = 3 HF = -1246.8172495 S2 = 2.007293

Sum of electronic and zero-point Energies= -1246.508594

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 3.800263 | 1.698380 | -1.305847 |
| 13 | 0 | 2.152965 | 0.992652 | -0.514292 |

| | | | | |
|---|---|---|---|---|
| 7 | 0 | 1.999518 | -0.871034 | -1.121767 |
| 6 | 0 | 0.484494 | 2.024681 | -0.601505 |
| 6 | 0 | -0.493326 | 2.028407 | 0.605875 |
| 13 | 0 | -2.155937 | 0.984821 | 0.523775 |
| 7 | 0 | -1.991939 | -0.882679 | 1.115473 |
| 7 | 0 | 2.511359 | 0.641607 | 1.401887 |
| 6 | 0 | -3.806216 | 1.673939 | 1.323605 |
| 7 | 0 | -2.518744 | 0.646474 | -1.394074 |
| 8 | 0 | -0.593409 | -1.200401 | -2.103142 |
| 8 | 0 | 0.599312 | -1.222273 | 2.094974 |
| 1 | 0 | -4.661653 | 1.011151 | 1.171661 |
| 1 | 0 | -2.629020 | 1.498619 | -1.932842 |
| 1 | 0 | -1.061669 | -1.095955 | 1.515222 |
| 1 | 0 | -2.151546 | -1.535815 | 0.334510 |
| 1 | 0 | -1.726181 | 0.101234 | -1.791355 |
| 1 | 0 | -2.678283 | -1.106328 | 1.828672 |
| 1 | 0 | -3.339705 | 0.067621 | -1.547238 |
| 1 | 0 | -0.854385 | 3.049288 | 0.775962 |
| 1 | 0 | -4.085135 | 2.647788 | 0.915747 |
| 1 | 0 | 0.017690 | 1.778821 | 1.541432 |
| 1 | 0 | -3.705513 | 1.813440 | 2.402431 |
| 1 | 0 | -0.024940 | 1.756961 | -1.533084 |
| 1 | 0 | 0.835352 | 3.046754 | -0.786243 |
| 1 | 0 | 4.662260 | 1.043763 | -1.155945 |
| 1 | 0 | 3.700049 | 1.843089 | -2.384258 |
| 1 | 0 | 4.067983 | 2.672992 | -0.892024 |
| 1 | 0 | 2.159796 | -1.531300 | -0.345909 |
| 1 | 0 | 1.070179 | -1.082512 | -1.524227 |
| 1 | 0 | 2.687399 | -1.085863 | -1.835527 |
| 1 | 0 | 3.337049 | 0.069164 | 1.553952 |
| 1 | 0 | 2.612196 | 1.490766 | 1.947197 |
| 1 | 0 | 1.721843 | 0.086723 | 1.792727 |
| 6 | 0 | -1.295922 | -2.210735 | -1.887173 |
| 8 | 0 | -2.377100 | -2.340257 | -1.330475 |
| 6 | 0 | 1.304656 | -2.228656 | 1.869604 |
| 8 | 0 | 2.386174 | -2.350098 | 1.312127 |

# III. Full Gaussian package citations

**Ref. 37**: Gaussian 09, Revision D.01,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

**Ref. 38**: Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.