## Electronic Supplementary Information for

# Metal complexes of tripodal ligands as ionophores for alkali metal ions

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# ESI 1: Summary of the results of DFT calculations
## (Cartesian coordinates and natural charges)

### Co•1 complex

| Atom | No. | X | Y | Z | Natural Charge |
|---|---|---|---|---|---|
| C | 1 | -0.017258 | 0.001903 | 3.360931 | -0.08318 |
| C | 2 | -0.024879 | 0.003818 | 4.896105 | -0.67109 |
| C | 3 | -0.97021 | -1.102814 | 2.832804 | -0.25946 |
| C | 4 | -0.493262 | 1.381079 | 2.832971 | -0.25948 |
| C | 5 | 1.419224 | -0.273955 | 2.844026 | -0.25954 |
| H | 6 | -0.468545 | -2.078413 | 2.895459 | 0.24443 |
| H | 7 | -1.866439 | -1.148461 | 3.46673 | 0.22815 |
| N | 8 | -1.353809 | -0.827308 | 1.451125 | -0.48492 |
| H | 9 | -1.589406 | 1.435048 | 2.889019 | 0.24438 |
| H | 10 | -0.088435 | 2.178041 | 3.471854 | 0.22815 |
| N | 11 | -0.053018 | 1.579187 | 1.454717 | -0.48497 |
| H | 12 | 2.014177 | 0.647819 | 2.906812 | 0.24441 |
| H | 13 | 1.901968 | -1.024838 | 3.484622 | 0.2282 |
| N | 14 | 1.381463 | -0.750449 | 1.464325 | -0.48488 |
| C | 15 | 2.211402 | -1.666286 | 1.071864 | 0.16223 |
| H | 16 | 2.987131 | -1.980019 | 1.779943 | 0.20445 |
| C | 17 | 2.191339 | -2.345676 | -0.18317 | -0.22192 |
| C | 18 | -2.56022 | -1.083297 | 1.050274 | 0.16207 |
| H | 19 | -3.225767 | -1.598436 | 1.752578 | 0.20443 |
| C | 20 | -3.129574 | -0.720949 | -0.207211 | -0.22212 |
| C | 21 | 0.33088 | 2.75299 | 1.059272 | 0.16212 |
| H | 22 | 0.21156 | 3.585464 | 1.762365 | 0.20445 |
| C | 23 | 0.940283 | 3.067512 | -0.192434 | -0.22206 |
| C | 24 | -2.470016 | 0.215272 | -1.076043 | 0.44293 |
| C | 25 | -4.420014 | -1.207365 | -0.535692 | -0.18233 |
| C | 26 | -5.06412 | -0.81932 | -1.691153 | -0.2906 |
| C | 27 | -3.173667 | 0.612711 | -2.25136 | -0.2932 |
| C | 28 | -4.422013 | 0.104174 | -2.5469 | -0.19637 |
| H | 29 | -4.8985 | -1.90635 | 0.148511 | 0.22599 |
| H | 30 | -6.046964 | -1.20854 | -1.937794 | 0.23387 |
| O | 31 | -1.31781 | 0.753155 | -0.830225 | -0.63981 |
| H | 32 | -2.680524 | 1.323439 | -2.907053 | 0.24574 |
| H | 33 | -4.92153 | 0.422305 | -3.459439 | 0.2344 |
| C | 34 | 1.430222 | 2.030254 | -1.058806 | 0.44292 |
| C | 35 | 1.166069 | 4.429089 | -0.51636 | -0.18235 |
| C | 36 | 1.835397 | 4.795624 | -1.664477 | -0.29058 |
| C | 37 | 2.137302 | 2.443766 | -2.226465 | -0.29321 |
| C | 38 | 2.323485 | 3.779854 | -2.517319 | -0.19637 |
| H | 39 | 0.79271 | 5.191307 | 0.165736 | 0.22602 |
| H | 40 | 1.991644 | 5.84201 | -1.907338 | 0.23388 |
| O | 41 | 1.319457 | 0.762751 | -0.816156 | -0.6399 |
| H | 42 | 2.513418 | 1.662889 | -2.879932 | 0.24576 |
| H | 43 | 2.857709 | 4.055562 | -3.423983 | 0.23441 |
| C | 44 | 1.055456 | -2.249764 | -1.058925 | 0.44281 |
| C | 45 | 3.262668 | -3.217458 | -0.502482 | -0.18233 |
| C | 46 | 3.258593 | -3.972341 | -1.656056 | -0.2906 |
| C | 47 | 1.073419 | -3.060623 | -2.232117 | -0.29313 |
| C | 48 | 2.142832 | -3.884379 | -2.518954 | -0.19637 |
| H | 49 | 4.103362 | -3.277291 | 0.186948 | 0.226 |
| H | 50 | 4.090968 | -4.626563 | -1.895761 | 0.23389 |
| O | 51 | 0.008758 | -1.524905 | -0.820632 | -0.63985 |
| H | 52 | 0.215084 | -2.993908 | -2.893234 | 0.24576 |
| H | 53 | 2.124859 | -4.478518 | -3.430069 | 0.23442 |
| Co | 54 | -0.002528 | -0.001323 | 0.311976 | 1.0775 |
| H | 55 | -1.002578 | 0.311301 | 5.285822 | 0.23895 |
| H | 56 | 0.195232 | -0.994104 | 5.293643 | 0.23897 |
| H | 57 | 0.726687 | 0.695982 | 5.29411 | 0.23895 |

## Co•2 complex

| Atom | No. | X | Y | Z | Natural Charge |
|---|---|---|---|---|---|
| C | 1 | -3.932899 | -0.018231 | 0.044045 | -0.08275 |
| C | 2 | -5.468305 | -0.024528 | 0.06161 | -0.67071 |
| C | 3 | -3.399695 | -1.437692 | 0.371734 | -0.25918 |
| C | 4 | -3.42811 | 0.404585 | -1.360144 | -0.2592 |
| C | 5 | -3.401403 | 0.984646 | 1.101585 | -0.25914 |
| H | 6 | -3.456102 | -1.606533 | 1.45631 | 0.2433 |
| H | 7 | -4.036628 | -2.189209 | -0.114995 | 0.2275 |
| N | 8 | -2.021788 | -1.584495 | -0.087335 | -0.48568 |
| H | 9 | -3.502288 | -0.451024 | -2.046076 | 0.24324 |
| H | 10 | -4.071245 | 1.203455 | -1.754544 | 0.22752 |
| N | 11 | -2.04656 | 0.870114 | -1.288127 | -0.48584 |
| H | 12 | -3.479213 | 2.007057 | 0.705774 | 0.24336 |
| H | 13 | -4.025771 | 0.929517 | 2.004108 | 0.22741 |
| N | 14 | -2.013902 | 0.683265 | 1.439708 | -0.48551 |
| C | 15 | -1.59801 | 0.825034 | 2.660631 | 0.16294 |
| H | 16 | -2.295023 | 1.271923 | 3.378859 | 0.20402 |
| C | 17 | -0.334128 | 0.420057 | 3.183636 | -0.22138 |
| C | 18 | -1.618813 | -2.715101 | -0.580502 | 0.16302 |
| H | 19 | -2.317408 | -3.558532 | -0.536565 | 0.20404 |
| C | 20 | -0.368041 | -2.970441 | -1.217372 | -0.22142 |
| C | 21 | -1.655201 | 1.859323 | -2.031156 | 0.16304 |
| H | 22 | -2.367696 | 2.243679 | -2.77003 | 0.20405 |
| C | 23 | -0.401457 | 2.536045 | -1.959389 | -0.22135 |
| C | 24 | 0.476673 | -1.885672 | -1.610936 | 0.42528 |
| C | 25 | -0.037266 | -4.312017 | -1.555927 | -0.2125 |
| C | 26 | 1.110364 | -4.595873 | -2.253811 | -0.27102 |
| C | 27 | 1.660179 | -2.222097 | -2.367424 | 0.27623 |
| C | 28 | 1.96088 | -3.538834 | -2.662487 | -0.3018 |
| H | 29 | -0.70805 | -5.109795 | -1.243972 | 0.22503 |
| H | 30 | 1.373681 | -5.619545 | -2.502219 | 0.2322 |
| O | 31 | 0.229581 | -0.638649 | -1.389195 | -0.62595 |
| O | 32 | 2.411267 | -1.144831 | -2.732355 | -0.50647 |
| H | 33 | 2.862415 | -3.778223 | -3.216346 | 0.23373 |
| C | 34 | 0.463108 | 2.336868 | -0.837705 | 0.42528 |
| C | 35 | -0.088969 | 3.498668 | -2.959081 | -0.21246 |
| C | 36 | 1.058678 | 4.247535 | -2.876296 | -0.27105 |
| C | 37 | 1.644308 | 3.165205 | -0.770158 | 0.27602 |
| C | 38 | 1.926733 | 4.077993 | -1.769352 | -0.30182 |
| H | 39 | -0.774267 | 3.624917 | -3.794661 | 0.22503 |
| H | 40 | 1.307852 | 4.973835 | -3.643979 | 0.2322 |
| O | 41 | 0.234144 | 1.521524 | 0.135949 | -0.62594 |
| O | 42 | 2.411357 | 2.950653 | 0.33601 | -0.50652 |
| H | 43 | 2.826751 | 4.681157 | -1.713977 | 0.23372 |
| C | 44 | 0.515018 | -0.448551 | 2.428955 | 0.42522 |
| C | 45 | 0.006952 | 0.800691 | 4.511248 | -0.21252 |
| C | 46 | 1.168967 | 0.355574 | 5.090988 | -0.27095 |
| C | 47 | 1.714331 | -0.91759 | 3.083168 | 0.2761 |
| C | 48 | 2.024285 | -0.512498 | 4.368106 | -0.30192 |
| H | 49 | -0.66783 | 1.458005 | 5.055655 | 0.22501 |
| H | 50 | 1.439503 | 0.65422 | 6.099246 | 0.23218 |
| O | 51 | 0.259485 | -0.881877 | 1.240493 | -0.62619 |
| O | 52 | 2.468977 | -1.760683 | 2.323529 | -0.50635 |
| H | 53 | 2.93646 | -0.860464 | 4.841307 | 0.23376 |
| Co | 54 | -0.887967 | -0.00503 | 0.00835 | 1.07564 |
| H | 55 | -5.870345 | -0.617644 | -0.768408 | 0.23831 |
| H | 56 | -5.850782 | -0.453107 | 0.995596 | 0.23831 |
| H | 57 | -5.86848 | 0.992355 | -0.028924 | 0.23832 |
| C | 58 | 3.599941 | -1.383544 | -3.456883 | -0.30844 |
| C | 59 | 3.593239 | 3.710896 | 0.476685 | -0.30845 |
| C | 60 | 3.673355 | -2.246606 | 2.878182 | -0.3085 |
| H | 61 | 4.369112 | -1.429682 | 3.117789 | 0.19632 |
| H | 62 | 3.494169 | -2.838042 | 3.787893 | 0.19428 |
| H | 63 | 4.119224 | -2.887063 | 2.114699 | 0.22609 |
| H | 64 | 4.308842 | -1.998512 | -2.883986 | 0.19626 |
| H | 65 | 3.399552 | -1.876985 | -4.419071 | 0.1943 |
| H | 66 | 4.042024 | -0.402408 | -3.640888 | 0.22612 |
| H | 67 | 4.295718 | 3.527605 | -0.349031 | 0.19618 |
| H | 68 | 3.380832 | 4.788672 | 0.528842 | 0.19437 |
| H | 69 | 4.048655 | 3.387898 | 1.41488 | 0.22609 |

## Al•2 complex

| Atom | No. | X | Y | Z | Natural Charge |
|---|---|---|---|---|---|
| C | 1 | -0.235916 | -0.400904 | 3.91433 | -0.08602 |
| C | 2 | -0.331241 | -0.554072 | 5.440313 | -0.66955 |
| C | 3 | -1.146742 | 0.77053 | 3.458245 | -0.25433 |
| C | 4 | 1.23457 | -0.102068 | 3.51886 | -0.25453 |
| C | 5 | -0.700851 | -1.718031 | 3.236023 | -0.25423 |
| H | 6 | -2.186854 | 0.420997 | 3.403286 | 0.24351 |
| H | 7 | -1.109153 | 1.575988 | 4.205202 | 0.22399 |
| N | 8 | -0.723852 | 1.281675 | 2.15229 | -0.64733 |
| H | 9 | 1.446136 | 0.962909 | 3.686888 | 0.24342 |
| H | 10 | 1.912292 | -0.677481 | 4.165238 | 0.22412 |
| N | 11 | 1.475931 | -0.442616 | 2.114496 | -0.64673 |
| H | 12 | 0.121365 | -2.44635 | 3.256503 | 0.24358 |
| H | 13 | -1.536018 | -2.148521 | 3.80634 | 0.22385 |
| N | 14 | -1.115262 | -1.47357 | 1.852497 | -0.6469 |
| C | 15 | -2.128122 | -2.144526 | 1.389366 | 0.17141 |
| H | 16 | -2.569839 | -2.917992 | 2.030657 | 0.19815 |
| C | 17 | -2.768897 | -1.949646 | 0.124175 | -0.21722 |
| C | 18 | -0.810587 | 2.561097 | 1.938259 | 0.17152 |
| H | 19 | -1.268305 | 3.183718 | 2.717701 | 0.19814 |
| C | 20 | -0.326382 | 3.264242 | 0.78941 | -0.21715 |
| C | 21 | 2.634396 | -0.938466 | 1.794904 | 0.17168 |
| H | 22 | 3.400541 | -1.004292 | 2.578073 | 0.19813 |
| C | 23 | 3.01193 | -1.455062 | 0.514337 | -0.21686 |
| C | 24 | 0.510054 | 2.606585 | -0.162037 | 0.42758 |
| C | 25 | -0.612441 | 4.651272 | 0.669867 | -0.21398 |
| C | 26 | -0.097786 | 5.382579 | -0.373611 | -0.26713 |
| C | 27 | 1.053171 | 3.408353 | -1.226625 | 0.27655 |
| C | 28 | 0.741129 | 4.754045 | -1.324425 | -0.29978 |
| H | 29 | -1.248955 | 5.121531 | 1.416458 | 0.22568 |
| H | 30 | -0.32113 | 6.44025 | -0.475968 | 0.23302 |
| O | 31 | 0.835518 | 1.354009 | -0.085584 | -0.80779 |
| O | 32 | 1.859489 | 2.72554 | -2.085426 | -0.50407 |
| H | 33 | 1.143785 | 5.346785 | -2.138892 | 0.23423 |
| C | 34 | 2.028922 | -1.665699 | -0.498708 | 0.42737 |
| C | 35 | 4.362816 | -1.845901 | 0.309175 | -0.214 |
| C | 36 | 4.74967 | -2.423956 | -0.87614 | -0.26699 |
| C | 37 | 2.46296 | -2.298985 | -1.715861 | 0.2766 |
| C | 38 | 3.790608 | -2.652002 | -1.891402 | -0.29979 |
| H | 39 | 5.084631 | -1.67496 | 1.105076 | 0.2257 |
| H | 40 | 5.782371 | -2.715084 | -1.042889 | 0.23302 |
| O | 41 | 0.776162 | -1.36351 | -0.355461 | -0.8084 |
| O | 42 | 1.472472 | -2.49324 | -2.629864 | -0.50404 |
| H | 43 | 4.111238 | -3.11497 | -2.818637 | 0.23423 |
| C | 44 | -2.455264 | -0.810986 | -0.676836 | 0.42745 |
| C | 45 | -3.793726 | -2.853542 | -0.266853 | -0.21404 |
| C | 46 | -4.494364 | -2.652237 | -1.431909 | -0.26707 |
| C | 47 | -3.22691 | -0.616193 | -1.875932 | 0.27653 |
| C | 48 | -4.20778 | -1.524443 | -2.237424 | -0.29986 |
| H | 49 | -4.009768 | -3.708358 | 0.370565 | 0.22574 |
| H | 50 | -5.271528 | -3.344723 | -1.740982 | 0.23305 |
| O | 51 | -1.557444 | 0.066844 | -0.355032 | -0.80776 |
| O | 52 | -2.893633 | 0.500826 | -2.579653 | -0.50406 |
| H | 53 | -4.77491 | -1.377162 | -3.150407 | 0.23429 |
| Al | 54 | -0.042527 | -0.080751 | 0.727303 | 2.05008 |
| H | 55 | 0.126223 | 0.300774 | 5.952814 | 0.23726 |
| H | 56 | -1.376256 | -0.619419 | 5.766235 | 0.23727 |
| H | 57 | 0.182691 | -1.461685 | 5.77903 | 0.23727 |
| C | 58 | 2.407538 | 3.431222 | -3.179831 | -0.30911 |
| C | 59 | 1.820311 | -3.085901 | -3.864187 | -0.30911 |
| C | 60 | -3.585457 | 0.753606 | -3.785194 | -0.3091 |
| H | 61 | -3.439037 | -0.055003 | -4.515552 | 0.19664 |
| H | 62 | -4.66376 | 0.888589 | -3.616688 | 0.19475 |
| H | 63 | -3.165493 | 1.679086 | -4.18429 | 0.22615 |
| H | 64 | 1.623915 | 3.836689 | -3.835774 | 0.19666 |
| H | 65 | 3.056486 | 4.255812 | -2.85071 | 0.19471 |
| H | 66 | 3.003332 | 2.705585 | -3.737152 | 0.22615 |
| H | 67 | 2.553529 | -2.479026 | -4.414473 | 0.1966 |
| H | 68 | 2.227039 | -4.098808 | -3.730324 | 0.19474 |
| H | 69 | 0.895229 | -3.143305 | -4.441324 | 0.22613 |

## $Na(Co•2)^{+}$ complex

| Atom | No. | X | Y | Z | Natural Charge |
|---|---|---|---|---|---|
| C | 1 | -4.097788 | -0.001449 | 0.004467 | -0.08828 |
| C | 2 | -5.633933 | -0.002396 | 0.00707 | -0.67506 |
| C | 3 | -3.573591 | -1.419623 | -0.330584 | -0.26309 |
| C | 4 | -3.575413 | 0.997685 | -1.057185 | -0.26307 |
| C | 5 | -3.571417 | 0.417411 | 1.399687 | -0.26306 |
| H | 6 | -3.623907 | -2.056183 | 0.562147 | 0.25277 |
| H | 7 | -4.208728 | -1.875274 | -1.100676 | 0.2388 |
| N | 8 | -2.189157 | -1.35861 | -0.808813 | -0.47062 |
| H | 9 | -3.626803 | 0.542863 | -2.054735 | 0.25284 |
| H | 10 | -4.210732 | 1.892257 | -1.065936 | 0.2388 |
| N | 11 | -2.190434 | 1.38109 | -0.767312 | -0.47054 |
| H | 12 | -3.622917 | 1.508616 | 1.505727 | 0.25285 |
| H | 13 | -4.204807 | -0.023567 | 2.179668 | 0.23873 |
| N | 14 | -2.185885 | -0.025135 | 1.58346 | -0.47049 |
| C | 15 | -1.838448 | -0.53697 | 2.721342 | 0.17143 |
| H | 16 | -2.58534 | -0.53205 | 3.521527 | 0.21908 |
| C | 17 | -0.564344 | -1.100396 | 3.0605 | -0.20537 |
| C | 18 | -1.843342 | -2.091071 | -1.819508 | 0.1715 |
| H | 19 | -2.590729 | -2.787894 | -2.212093 | 0.21913 |
| C | 20 | -0.570663 | -2.103574 | -2.479866 | -0.2054 |
| C | 21 | -1.84483 | 2.622712 | -0.896027 | 0.17148 |
| H | 22 | -2.593113 | 3.311632 | -1.300625 | 0.21913 |
| C | 23 | -0.571322 | 3.200541 | -0.579394 | -0.2054 |
| C | 24 | 0.391633 | -1.092112 | -2.218676 | 0.38784 |
| C | 25 | -0.292077 | -3.138474 | -3.407018 | -0.19213 |
| C | 26 | 0.937705 | -3.215581 | -4.024887 | -0.25398 |
| C | 27 | 1.683343 | -1.248912 | -2.811811 | 0.25122 |
| C | 28 | 1.938054 | -2.273024 | -3.708817 | -0.27046 |
| H | 29 | -1.058165 | -3.881579 | -3.612988 | 0.24145 |
| H | 30 | 1.153508 | -4.00632 | -4.735294 | 0.25111 |
| O | 31 | 0.171289 | -0.030305 | -1.483865 | -0.70098 |
| O | 32 | 2.621624 | -0.328104 | -2.380784 | -0.57378 |
| H | 33 | 2.915285 | -2.367972 | -4.16959 | 0.24744 |
| C | 34 | 0.393221 | 2.467839 | 0.162322 | 0.3878 |
| C | 35 | -0.294117 | 4.521216 | -1.01194 | -0.19207 |
| C | 36 | 0.936151 | 5.095037 | -0.772897 | -0.25401 |
| C | 37 | 1.684922 | 3.060613 | 0.320681 | 0.25116 |
| C | 38 | 1.938226 | 4.34983 | -0.117546 | -0.27029 |
| H | 39 | -1.06177 | 5.071112 | -1.550314 | 0.24141 |
| H | 40 | 1.150749 | 6.105868 | -1.102558 | 0.25111 |
| O | 41 | 0.174328 | 1.299783 | 0.713419 | -0.7013 |
| O | 42 | 2.624782 | 2.227586 | 0.901023 | -0.57385 |
| H | 43 | 2.915626 | 4.796323 | 0.028848 | 0.24742 |
| C | 44 | 0.398241 | -1.375811 | 2.053019 | 0.38772 |
| C | 45 | -0.284397 | -1.385833 | 4.420058 | -0.19211 |
| C | 46 | 0.947173 | -1.878358 | 4.795067 | -0.25397 |
| C | 47 | 1.691264 | -1.807793 | 2.484737 | 0.25112 |
| C | 48 | 1.947375 | -2.07248 | 3.81995 | -0.2704 |
| H | 49 | -1.05082 | -1.195121 | 5.166851 | 0.24143 |
| H | 50 | 1.164211 | -2.098052 | 5.83485 | 0.25112 |
| O | 51 | 0.176796 | -1.268953 | 0.766209 | -0.7014 |
| O | 52 | 2.629416 | -1.893961 | 1.47168 | -0.57371 |
| H | 53 | 2.925773 | -2.421806 | 4.131521 | 0.24744 |
| Co | 54 | -1.034554 | -0.000375 | 0.000437 | 1.08748 |
| H | 55 | -6.029652 | -0.162572 | -1.002288 | 0.24684 |
| H | 56 | -6.026704 | -0.79753 | 0.650936 | 0.24682 |
| H | 57 | -6.028623 | 0.951787 | 0.374242 | 0.24687 |
| C | 58 | 3.845393 | -0.240304 | -3.110815 | -0.31192 |
| C | 59 | 3.846296 | 2.817462 | 1.346205 | -0.31187 |
| C | 60 | 3.852345 | -2.572031 | 1.759257 | -0.31188 |
| H | 61 | 4.460534 | -2.016167 | 2.48376 | 0.20627 |
| H | 62 | 3.65587 | -3.579143 | 2.142802 | 0.21999 |
| H | 63 | 4.389695 | -2.642811 | 0.811886 | 0.22809 |
| H | 64 | 4.450742 | -1.147643 | -2.992299 | 0.2063 |
| H | 65 | 3.6506 | -0.066638 | -4.174778 | 0.22004 |
| H | 66 | 4.384687 | 0.613566 | -2.696843 | 0.22806 |
| H | 67 | 4.453027 | 3.171903 | 0.503568 | 0.20627 |
| H | 68 | 3.648238 | 3.649937 | 2.030217 | 0.22002 |
| H | 69 | 4.386055 | 2.031792 | 1.87787 | 0.22805 |
| Na | 70 | 2.040901 | 0.001892 | -0.002433 | 0.91603 |

## K(Co•2)$^{+}$ complex

| Atom | No. | X | Y | Z | Natural Charge |
|---|---|---|---|---|---|
| C | 1 | -4.073855 | -0.047733 | -0.016429 | -0.08713 |
| C | 2 | -5.609501 | -0.064815 | -0.021791 | -0.67513 |
| C | 3 | -3.527596 | -1.489272 | -0.175134 | -0.2627 |
| C | 4 | -3.550572 | 0.820254 | -1.189398 | -0.26261 |
| C | 5 | -3.556728 | 0.544107 | 1.319509 | -0.26264 |
| H | 6 | -3.564536 | -2.012981 | 0.788378 | 0.25204 |
| H | 7 | -4.155957 | -2.045467 | -0.881986 | 0.23864 |
| N | 8 | -2.147892 | -1.453869 | -0.667611 | -0.46947 |
| H | 9 | -3.577288 | 0.24362 | -2.122505 | 0.25206 |
| H | 10 | -4.199405 | 1.695499 | -1.318335 | 0.23853 |
| N | 11 | -2.17953 | 1.260917 | -0.918533 | -0.46951 |
| H | 12 | -3.608555 | 1.639723 | 1.28857 | 0.25212 |
| H | 13 | -4.193517 | 0.202767 | 2.145225 | 0.23856 |
| N | 14 | -2.174313 | 0.119512 | 1.558419 | -0.46935 |
| C | 15 | -1.831671 | -0.273193 | 2.743863 | 0.16992 |
| H | 16 | -2.572521 | -0.155741 | 3.541064 | 0.21832 |
| C | 17 | -0.592211 | -0.875134 | 3.134712 | -0.21118 |
| C | 18 | -1.790581 | -2.28041 | -1.598358 | 0.17006 |
| H | 19 | -2.516522 | -3.04608 | -1.889672 | 0.21831 |
| C | 20 | -0.552491 | -2.295952 | -2.317422 | -0.21114 |
| C | 21 | -1.851994 | 2.48817 | -1.16998 | 0.16998 |
| H | 22 | -2.594777 | 3.106261 | -1.684244 | 0.21827 |
| C | 23 | -0.628324 | 3.147963 | -0.827089 | -0.21106 |
| C | 24 | 0.362609 | -1.208782 | -2.222175 | 0.38951 |
| C | 25 | -0.298871 | -3.384619 | -3.190445 | -0.19299 |
| C | 26 | 0.853849 | -3.431913 | -3.94145 | -0.2584 |
| C | 27 | 1.567268 | -1.306323 | -2.99714 | 0.24445 |
| C | 28 | 1.793042 | -2.384976 | -3.836156 | -0.2732 |
| H | 29 | -1.030131 | -4.186465 | -3.253726 | 0.23982 |
| H | 30 | 1.050431 | -4.263775 | -4.60927 | 0.24974 |
| O | 31 | 0.170357 | -0.135344 | -1.504411 | -0.6908 |
| O | 32 | 2.457248 | -0.266716 | -2.81492 | -0.56547 |
| H | 33 | 2.70385 | -2.436556 | -4.423016 | 0.24617 |
| C | 34 | 0.303272 | 2.542791 | 0.06402 | 0.38908 |
| C | 35 | -0.40854 | 4.455471 | -1.330445 | -0.19292 |
| C | 36 | 0.726525 | 5.158149 | -0.994405 | -0.25841 |
| C | 37 | 1.488748 | 3.293055 | 0.36954 | 0.24398 |
| C | 38 | 1.681215 | 4.565857 | -0.141834 | -0.27296 |
| H | 39 | -1.151732 | 4.894351 | -1.991283 | 0.2399 |
| H | 40 | 0.897392 | 6.15817 | -1.378314 | 0.24979 |
| O | 41 | 0.140914 | 1.378002 | 0.630641 | -0.69192 |
| O | 42 | 2.397251 | 2.63625 | 1.175455 | -0.56607 |
| H | 43 | 2.577575 | 5.122807 | 0.109152 | 0.24619 |
| C | 44 | 0.343702 | -1.321674 | 2.158568 | 0.38874 |
| C | 45 | -0.35873 | -1.092026 | 4.516787 | -0.19307 |
| C | 46 | 0.793112 | -1.710229 | 4.948443 | -0.25841 |
| C | 47 | 1.545789 | -1.936687 | 2.646135 | 0.24391 |
| C | 48 | 1.751451 | -2.129392 | 4.002303 | -0.2731 |
| H | 49 | -1.105043 | -0.75781 | 5.233063 | 0.2399 |
| H | 50 | 0.973891 | -1.876652 | 6.004977 | 0.24978 |
| O | 51 | 0.172862 | -1.231157 | 0.867488 | -0.69079 |
| O | 52 | 2.453114 | -2.287178 | 1.66619 | -0.5652 |
| H | 53 | 2.66045 | -2.607096 | 4.351733 | 0.24623 |
| Co | 54 | -1.019417 | -0.010638 | -0.005652 | 1.08466 |
| H | 55 | -5.998249 | -0.322754 | -1.013553 | 0.24639 |
| H | 56 | -5.998892 | -0.799851 | 0.691923 | 0.24638 |
| H | 57 | -6.015788 | 0.915523 | 0.252215 | 0.24635 |
| C | 58 | 3.490203 | -0.109105 | -3.785272 | -0.31332 |
| C | 59 | 3.407386 | 3.422599 | 1.80397 | -0.31329 |
| C | 60 | 3.484515 | -3.20442 | 2.024467 | -0.31328 |
| H | 61 | 4.21904 | -2.748258 | 2.701182 | 0.20263 |
| H | 62 | 3.064304 | -4.099643 | 2.496768 | 0.21818 |
| H | 63 | 3.978756 | -3.484806 | 1.092108 | 0.22752 |
| H | 64 | 4.235103 | -0.913154 | -3.721449 | 0.20274 |
| H | 65 | 3.074046 | -0.080595 | -4.798742 | 0.2183 |
| H | 66 | 3.970922 | 0.846129 | -3.564491 | 0.22724 |
| H | 67 | 4.146043 | 3.791091 | 1.080078 | 0.20286 |
| H | 68 | 2.966444 | 4.273113 | 2.336237 | 0.21833 |
| H | 69 | 3.902392 | 2.764249 | 2.520783 | 0.22733 |
| K | 70 | 2.427985 | 0.041941 | 0.017472 | 0.96263 |

## $Rb(Co•2)^{+}$ complex

| Atom | No. | X | Y | Z | Natural Charge |
|---|---|---|---|---|---|
| C | 1 | -4.233046 | -0.006826 | 0.004541 | -0.08674 |
| C | 2 | -5.768311 | -0.009705 | 0.005756 | -0.67494 |
| C | 3 | -3.69865 | -1.41673 | 0.366413 | -0.26236 |
| C | 4 | -3.703062 | 0.385749 | -1.39894 | -0.26225 |
| C | 5 | -3.702139 | 1.012282 | 1.046189 | -0.26231 |
| H | 6 | -3.729153 | -1.563008 | 1.453423 | 0.25165 |
| H | 7 | -4.336923 | -2.18241 | -0.091907 | 0.23826 |
| N | 8 | -2.323899 | -1.57038 | -0.117475 | -0.47013 |
| H | 9 | -3.733189 | -0.483035 | -2.068262 | 0.25165 |
| H | 10 | -4.344462 | 1.163517 | -1.831708 | 0.23824 |
| N | 11 | -2.329494 | 0.884942 | -1.293338 | -0.47011 |
| H | 12 | -3.737149 | 2.027294 | 0.631144 | 0.2517 |
| H | 13 | -4.340365 | 0.993558 | 1.938325 | 0.23825 |
| N | 14 | -2.325869 | 0.674888 | 1.42039 | -0.47006 |
| C | 15 | -1.984663 | 0.715394 | 2.668871 | 0.16903 |
| H | 16 | -2.717297 | 1.124289 | 3.371836 | 0.2178 |
| C | 17 | -0.765381 | 0.244542 | 3.252363 | -0.21337 |
| C | 18 | -1.982789 | -2.672053 | -0.706343 | 0.16899 |
| H | 19 | -2.714223 | -3.486339 | -0.69987 | 0.21779 |
| C | 20 | -0.765745 | -2.940903 | -1.409702 | -0.21343 |
| C | 21 | -1.992786 | 1.946908 | -1.953305 | 0.169 |
| H | 22 | -2.727284 | 2.347913 | -2.658915 | 0.21778 |
| C | 23 | -0.776922 | 2.692705 | -1.837473 | -0.21344 |
| C | 24 | 0.146126 | -1.890965 | -1.723135 | 0.39119 |
| C | 25 | -0.546428 | -4.261098 | -1.881117 | -0.19395 |
| C | 26 | 0.56294 | -4.565426 | -2.636052 | -0.26029 |
| C | 27 | 1.297817 | -2.248347 | -2.505606 | 0.24326 |
| C | 28 | 1.488436 | -3.547164 | -2.947187 | -0.27511 |
| H | 29 | -1.27331 | -5.031523 | -1.636193 | 0.23918 |
| H | 30 | 0.732774 | -5.574004 | -2.997503 | 0.24905 |
| O | 31 | -0.00768 | -0.643436 | -1.377032 | -0.68393 |
| O | 32 | 2.175158 | -1.212506 | -2.750793 | -0.56064 |
| H | 33 | 2.360993 | -3.795589 | -3.541943 | 0.24533 |
| C | 34 | 0.139548 | 2.438701 | -0.775632 | 0.39132 |
| C | 35 | -0.563574 | 3.763463 | -2.743571 | -0.19398 |
| C | 36 | 0.545407 | 4.570405 | -2.633193 | -0.26025 |
| C | 37 | 1.290583 | 3.296069 | -0.697462 | 0.24335 |
| C | 38 | 1.476193 | 4.329541 | -1.600763 | -0.27524 |
| H | 39 | -1.294298 | 3.937242 | -3.529528 | 0.23916 |
| H | 40 | 0.711033 | 5.389356 | -3.325021 | 0.24903 |
| O | 41 | -0.008819 | 1.513193 | 0.13071 | -0.68393 |
| O | 42 | 2.172518 | 2.989322 | 0.31777 | -0.56054 |
| H | 43 | 2.348237 | 4.969901 | -1.52136 | 0.24535 |
| C | 44 | 0.149745 | -0.546819 | 2.498443 | 0.39126 |
| C | 45 | -0.546874 | 0.495795 | 4.631577 | -0.19391 |
| C | 46 | 0.56552 | -0.000637 | 5.271521 | -0.26024 |
| C | 47 | 1.304708 | -1.039858 | 3.198005 | 0.24318 |
| C | 48 | 1.494771 | -0.773025 | 4.543678 | -0.27509 |
| H | 49 | -1.276648 | 1.088786 | 5.177176 | 0.23916 |
| H | 50 | 0.734734 | 0.190207 | 6.325876 | 0.24905 |
| O | 51 | -0.003228 | -0.870512 | 1.244614 | -0.68403 |
| O | 52 | 2.185591 | -1.765484 | 2.422919 | -0.56078 |
| H | 53 | 2.369287 | -1.160559 | 5.055402 | 0.24533 |
| Co | 54 | -1.17803 | -0.001699 | 0.001403 | 1.08411 |
| H | 55 | -6.162085 | -0.626483 | -0.810231 | 0.24607 |
| H | 56 | -6.161633 | -0.409601 | 0.94738 | 0.24607 |
| H | 57 | -6.165323 | 1.004233 | -0.119366 | 0.2461 |
| C | 58 | 3.117719 | -1.384873 | -3.805787 | -0.31394 |
| C | 59 | 3.117459 | 3.988374 | 0.691825 | -0.31397 |
| C | 60 | 3.131189 | -2.58915 | 3.100035 | -0.31391 |
| H | 61 | 3.900203 | -1.993937 | 3.610223 | 0.20094 |
| H | 62 | 2.634297 | -3.238381 | 3.830113 | 0.21779 |
| H | 63 | 3.603688 | -3.204139 | 2.331223 | 0.22672 |
| H | 64 | 3.891233 | -2.120234 | -3.547073 | 0.20094 |
| H | 65 | 2.619049 | -1.696476 | -4.730793 | 0.21777 |
| H | 66 | 3.585185 | -0.409674 | -3.957553 | 0.22676 |
| H | 67 | 3.887784 | 4.131285 | -0.077703 | 0.20095 |
| H | 68 | 2.620129 | 4.945556 | 0.886232 | 0.21775 |
| H | 69 | 3.5884 | 3.632246 | 1.610481 | 0.22675 |
| Rb | 70 | 2.489418 | 0.003192 | -0.003973 | 0.9698 |

## $Cs(Co•2)^{+}$ complex

| Atom | No. | X | Y | Z | Natural Charge |
|---|---|---|---|---|---|
| C | 1 | -4.406149 | -0.039539 | -0.015031 | -0.08633 |
| C | 2 | -5.941397 | -0.054517 | -0.019143 | -0.6748 |
| C | 3 | -3.884732 | 0.701274 | 1.243629 | -0.26221 |
| C | 4 | -3.860506 | -1.491068 | -0.006453 | -0.26223 |
| C | 5 | -3.878214 | 0.687837 | -1.279383 | -0.26214 |
| H | 6 | -3.925968 | 1.78614 | 1.085158 | 0.25125 |
| H | 7 | -4.524934 | 0.464374 | 2.102434 | 0.238 |
| N | 8 | -2.508099 | 0.2884 | 1.52975 | -0.47068 |
| H | 9 | -3.889821 | -1.89839 | 1.011862 | 0.25133 |
| H | 10 | -4.492923 | -2.126106 | -0.639103 | 0.23801 |
| N | 11 | -2.485653 | -1.509001 | -0.512289 | -0.47064 |
| H | 12 | -3.899823 | 0.008751 | -2.140785 | 0.25126 |
| H | 13 | -4.526319 | 1.542385 | -1.510449 | 0.238 |
| N | 14 | -2.510193 | 1.158667 | -1.046978 | -0.47062 |
| C | 15 | -2.180463 | 2.352712 | -1.424682 | 0.16828 |
| H | 16 | -2.911367 | 2.903437 | -2.025226 | 0.21735 |
| C | 17 | -0.985593 | 3.068724 | -1.098044 | -0.21518 |
| C | 18 | -2.16845 | 0.025544 | 2.751375 | 0.16827 |
| H | 19 | -2.899821 | 0.258912 | 3.531653 | 0.21735 |
| C | 20 | -0.961248 | -0.595276 | 3.203021 | -0.21518 |
| C | 21 | -2.133871 | -2.429391 | -1.352792 | 0.16839 |
| H | 22 | -2.853275 | -3.232841 | -1.540066 | 0.21733 |
| C | 23 | -0.925619 | -2.492947 | -2.116844 | -0.21501 |
| C | 24 | -0.058335 | -1.199258 | 2.278038 | 0.39323 |
| C | 25 | -0.758607 | -0.711283 | 4.603114 | -0.19528 |
| C | 26 | 0.31924 | -1.402324 | 5.105545 | -0.26183 |
| C | 27 | 1.049208 | -1.925062 | 2.841533 | 0.24284 |
| C | 28 | 1.223512 | -2.015541 | 4.212451 | -0.27817 |
| H | 29 | -1.476492 | -0.247556 | 5.27509 | 0.23854 |
| H | 30 | 0.476433 | -1.491605 | 6.17518 | 0.24826 |
| O | 31 | -0.184374 | -1.16617 | 0.982404 | -0.67872 |
| O | 32 | 1.899439 | -2.492154 | 1.917693 | -0.55535 |
| H | 33 | 2.064881 | -2.568887 | 4.615907 | 0.24449 |
| C | 34 | -0.040302 | -1.376362 | -2.179717 | 0.39333 |
| C | 35 | -0.703021 | -3.647407 | -2.912081 | -0.19519 |
| C | 36 | 0.379182 | -3.723787 | -3.757589 | -0.26176 |
| C | 37 | 1.074331 | -1.489205 | -3.083076 | 0.24283 |
| C | 38 | 1.268281 | -2.631322 | -3.842016 | -0.27822 |
| H | 39 | -1.408475 | -4.471907 | -2.845168 | 0.23853 |
| H | 40 | 0.551688 | -4.605171 | -4.366066 | 0.24822 |
| O | 41 | -0.189446 | -0.268978 | -1.511355 | -0.67836 |
| O | 42 | 1.911269 | -0.394898 | -3.110664 | -0.55565 |
| H | 43 | 2.113572 | -2.694732 | -4.518967 | 0.24444 |
| C | 44 | -0.088446 | 2.578281 | -0.103244 | 0.39371 |
| C | 45 | -0.790425 | 4.342124 | -1.693849 | -0.1951 |
| C | 46 | 0.276302 | 5.13268 | -1.334729 | -0.2619 |
| C | 47 | 1.008771 | 3.438229 | 0.254738 | 0.24288 |
| C | 48 | 1.176248 | 4.672964 | -0.349869 | -0.27806 |
| H | 49 | -1.504403 | 4.685698 | -2.438268 | 0.23855 |
| H | 50 | 0.428383 | 6.106014 | -1.788953 | 0.24824 |
| O | 51 | -0.211468 | 1.438344 | 0.513064 | -0.67824 |
| O | 52 | 1.85854 | 2.927899 | 1.211998 | -0.55566 |
| H | 53 | 2.009156 | 5.307374 | -0.06575 | 0.24445 |
| Co | 54 | -1.355011 | -0.010391 | -0.007748 | 1.08312 |
| H | 55 | -6.332419 | -0.681445 | 0.790447 | 0.24579 |
| H | 56 | -6.346053 | 0.95525 | 0.114567 | 0.24576 |
| H | 57 | -6.329629 | -0.448681 | -0.965315 | 0.24578 |
| C | 58 | 2.780471 | -3.512697 | 2.375167 | -0.31456 |
| C | 59 | 2.800098 | -0.27579 | -4.216474 | -0.31468 |
| C | 60 | 2.724425 | 3.843751 | 1.874517 | -0.31454 |
| H | 61 | 3.516363 | 4.214303 | 1.209325 | 0.19902 |
| H | 62 | 2.164375 | 4.697006 | 2.274778 | 0.21713 |
| H | 63 | 3.178154 | 3.290427 | 2.699594 | 0.22629 |
| H | 64 | 3.57327 | -3.111788 | 3.021546 | 0.19893 |
| H | 65 | 2.233639 | -4.291168 | 2.920213 | 0.21702 |
| H | 66 | 3.231995 | -3.947465 | 1.480834 | 0.22648 |
| H | 67 | 3.60244 | -1.025491 | -4.180508 | 0.1989 |
| H | 68 | 2.262492 | -0.371837 | -5.167091 | 0.21717 |
| H | 69 | 3.237966 | 0.722409 | -4.14832 | 0.22643 |
| Cs | 70 | 2.549902 | 0.023142 | 0.010192 | 0.98111 |

## Na(Al•2)$^{+}$ complex

| Atom | No. | X | Y | Z | Natural Charge |
|---|---|---|---|---|---|
| C | 1 | -4.180409 | -0.01448 | -0.007031 | -0.09279 |
| C | 2 | -5.718593 | -0.021084 | -0.009407 | -0.67345 |
| C | 3 | -3.669401 | -1.476418 | -0.002163 | -0.2584 |
| C | 4 | -3.676599 | 0.716274 | -1.276315 | -0.25835 |
| C | 5 | -3.680295 | 0.723736 | 1.25906 | -0.25846 |
| H | 6 | -3.735475 | -1.884109 | 1.01522 | 0.25138 |
| H | 7 | -4.312379 | -2.091696 | -0.644224 | 0.23726 |
| N | 8 | -2.27649 | -1.564955 | -0.471286 | -0.65145 |
| H | 9 | -3.739431 | 0.039329 | -2.138584 | 0.25131 |
| H | 10 | -4.325849 | 1.575747 | -1.48622 | 0.23717 |
| N | 11 | -2.286531 | 1.176091 | -1.119808 | -0.65093 |
| H | 12 | -3.750751 | 1.808275 | 1.102635 | 0.25133 |
| H | 13 | -4.327076 | 0.472415 | 2.109146 | 0.23722 |
| N | 14 | -2.287391 | 0.368652 | 1.578192 | -0.65074 |
| C | 15 | -1.964148 | 0.301433 | 2.836045 | 0.18463 |
| H | 16 | -2.73554 | 0.541532 | 3.576088 | 0.21451 |
| C | 17 | -0.676674 | -0.039922 | 3.371736 | -0.20495 |
| C | 18 | -1.946253 | -2.617427 | -1.16027 | 0.18477 |
| H | 19 | -2.712804 | -3.383035 | -1.323578 | 0.21455 |
| C | 20 | -0.656997 | -2.902443 | -1.723785 | -0.20501 |
| C | 21 | -1.965188 | 2.302947 | -1.684064 | 0.18455 |
| H | 22 | -2.736094 | 2.82326 | -2.263193 | 0.21446 |
| C | 23 | -0.680205 | 2.942218 | -1.648764 | -0.20516 |
| C | 24 | 0.369464 | -1.922186 | -1.716474 | 0.39962 |
| C | 25 | -0.417524 | -4.183907 | -2.28013 | -0.19231 |
| C | 26 | 0.827769 | -4.510164 | -2.773312 | -0.25297 |
| C | 27 | 1.664314 | -2.311109 | -2.169387 | 0.25433 |
| C | 28 | 1.879783 | -3.572835 | -2.700303 | -0.26877 |
| H | 29 | -1.225562 | -4.910755 | -2.300058 | 0.24153 |
| H | 30 | 1.015547 | -5.489399 | -3.200521 | 0.25125 |
| O | 31 | 0.179939 | -0.687399 | -1.316498 | -0.86453 |
| O | 32 | 2.643226 | -1.349123 | -1.994778 | -0.5729 |
| H | 33 | 2.862284 | -3.857709 | -3.06041 | 0.24738 |
| C | 34 | 0.3506 | 2.450628 | -0.805895 | 0.40017 |
| C | 35 | -0.449136 | 4.068137 | -2.478246 | -0.1925 |
| C | 36 | 0.79215 | 4.666684 | -2.514388 | -0.25302 |
| C | 37 | 1.641612 | 3.045705 | -0.917157 | 0.25458 |
| C | 38 | 1.848873 | 4.139693 | -1.742042 | -0.26919 |
| H | 39 | -1.260472 | 4.444575 | -3.096002 | 0.24146 |
| H | 40 | 0.973477 | 5.529116 | -3.14685 | 0.25118 |
| O | 41 | 0.169284 | 1.484543 | 0.062105 | -0.8643 |
| O | 42 | 2.625277 | 2.41757 | -0.17409 | -0.57256 |
| H | 43 | 2.828255 | 4.600473 | -1.809585 | 0.24733 |
| C | 44 | 0.354912 | -0.52317 | 2.52511 | 0.39973 |
| C | 45 | -0.444479 | 0.120797 | 4.760774 | -0.19237 |
| C | 46 | 0.79824 | -0.141356 | 5.296886 | -0.25296 |
| C | 47 | 1.646998 | -0.718492 | 3.095521 | 0.25434 |
| C | 48 | 1.855299 | -0.546101 | 4.454632 | -0.26885 |
| H | 49 | -1.256318 | 0.466595 | 5.395562 | 0.24152 |
| H | 50 | 0.980157 | -0.020478 | 6.359422 | 0.25123 |
| O | 51 | 0.173203 | -0.796265 | 1.25515 | -0.86477 |
| O | 52 | 2.631262 | -1.048083 | 2.18062 | -0.57299 |
| H | 53 | 2.835885 | -0.713581 | 4.886399 | 0.24736 |
| Al | 54 | -1.002026 | -0.004323 | -0.002308 | 2.03725 |
| H | 55 | -6.109537 | -0.416908 | -0.953652 | 0.24569 |
| H | 56 | -6.111597 | -0.642876 | 0.803023 | 0.24569 |
| H | 57 | -6.117399 | 0.991405 | 0.120626 | 0.2457 |
| C | 58 | 3.893458 | -1.559224 | -2.651984 | -0.31177 |
| C | 59 | 3.876572 | 3.09203 | -0.040336 | -0.31178 |
| C | 60 | 3.880248 | -1.507192 | 2.698556 | -0.31179 |
| H | 61 | 4.412807 | -0.708277 | 3.228984 | 0.20796 |
| H | 62 | 3.732584 | -2.358946 | 3.37156 | 0.21975 |
| H | 63 | 4.468895 | -1.825455 | 1.836111 | 0.2257 |
| H | 64 | 4.43118 | -2.415775 | -2.227307 | 0.20793 |
| H | 65 | 3.746391 | -1.714659 | -3.726428 | 0.21977 |
| H | 66 | 4.476707 | -0.650056 | -2.494479 | 0.22571 |
| H | 67 | 4.403782 | 3.153593 | -1.000284 | 0.20795 |
| H | 68 | 3.733382 | 4.099907 | 0.364521 | 0.21968 |
| H | 69 | 4.46768 | 2.500801 | 0.66156 | 0.22555 |
| Na | 70 | 2.034037 | 0.002761 | 0.005277 | 0.91957 |

## $K(Al•2)^{+}$ complex

| Atom | No. | X | Y | Z | Natural Charge |
|---|---|---|---|---|---|
| C | 1 | -4.146371 | 0.001025 | 0.007231 | -0.09124 |
| C | 2 | -5.6841 | 0.001692 | 0.012686 | -0.67351 |
| C | 3 | -3.635292 | -1.461287 | 0.062843 | -0.25717 |
| C | 4 | -3.637411 | 0.683438 | -1.288445 | -0.2571 |
| C | 5 | -3.63129 | 0.780953 | 1.24408 | -0.25713 |
| H | 6 | -3.670831 | -1.827125 | 1.096887 | 0.25078 |
| H | 7 | -4.293999 | -2.102217 | -0.536546 | 0.23533 |
| N | 8 | -2.25749 | -1.555642 | -0.444369 | -0.64904 |
| H | 9 | -3.677202 | -0.029004 | -2.122131 | 0.25077 |
| H | 10 | -4.294609 | 1.524805 | -1.541452 | 0.23536 |
| N | 11 | -2.258176 | 1.16738 | -1.119712 | -0.64934 |
| H | 12 | -3.668516 | 1.859071 | 1.042151 | 0.25065 |
| H | 13 | -4.28642 | 0.583117 | 2.101759 | 0.23537 |
| N | 14 | -2.251627 | 0.390036 | 1.575194 | -0.64938 |
| C | 15 | -1.953665 | 0.26497 | 2.833242 | 0.18114 |
| H | 16 | -2.723391 | 0.522085 | 3.569535 | 0.21249 |
| C | 17 | -0.710435 | -0.198769 | 3.380941 | -0.20665 |
| C | 18 | -1.963796 | -2.583327 | -1.182113 | 0.18126 |
| H | 19 | -2.735761 | -3.347667 | -1.325563 | 0.21248 |
| C | 20 | -0.722288 | -2.82951 | -1.859268 | -0.20674 |
| C | 21 | -1.962838 | 2.319804 | -1.640722 | 0.18122 |
| H | 22 | -2.735042 | 2.829175 | -2.228067 | 0.21254 |
| C | 23 | -0.719879 | 3.02701 | -1.515802 | -0.20675 |
| C | 24 | 0.290906 | -1.832894 | -1.915936 | 0.39814 |
| C | 25 | -0.552542 | -4.071746 | -2.520324 | -0.19363 |
| C | 26 | 0.608861 | -4.347676 | -3.2083 | -0.25522 |
| C | 27 | 1.494127 | -2.160218 | -2.616248 | 0.24991 |
| C | 28 | 1.638223 | -3.38562 | -3.24882 | -0.27103 |
| H | 29 | -1.353106 | -4.805769 | -2.474224 | 0.24015 |
| H | 30 | 0.7428 | -5.296623 | -3.716598 | 0.25005 |
| O | 31 | 0.16468 | -0.644318 | -1.379277 | -0.85923 |
| O | 32 | 2.471743 | -1.185549 | -2.583153 | -0.56697 |
| H | 33 | 2.552808 | -3.618284 | -3.783475 | 0.24597 |
| C | 34 | 0.296108 | 2.573834 | -0.629 | 0.39807 |
| C | 35 | -0.552868 | 4.225307 | -2.254364 | -0.19366 |
| C | 36 | 0.608513 | 4.95877 | -2.148956 | -0.25515 |
| C | 37 | 1.500553 | 3.342396 | -0.564776 | 0.24999 |
| C | 38 | 1.641973 | 4.507248 | -1.30359 | -0.27123 |
| H | 39 | -1.355715 | 4.556144 | -2.908441 | 0.2401 |
| H | 40 | 0.740427 | 5.876397 | -2.712374 | 0.25 |
| O | 41 | 0.170547 | 1.513767 | 0.13085 | -0.85906 |
| O | 42 | 2.482427 | 2.822907 | 0.255382 | -0.56669 |
| H | 43 | 2.556995 | 5.086308 | -1.23956 | 0.24602 |
| C | 44 | 0.301803 | -0.74325 | 2.542604 | 0.39839 |
| C | 45 | -0.538568 | -0.155116 | 4.78713 | -0.19363 |
| C | 46 | 0.624703 | -0.61264 | 5.366285 | -0.25525 |
| C | 47 | 1.507749 | -1.184323 | 3.172248 | 0.24983 |
| C | 48 | 1.654012 | -1.12304 | 4.549864 | -0.27121 |
| H | 49 | -1.338639 | 0.248733 | 5.402454 | 0.2401 |
| H | 50 | 0.760925 | -0.580946 | 6.442045 | 0.25 |
| O | 51 | 0.170658 | -0.870754 | 1.245251 | -0.85914 |
| O | 52 | 2.485207 | -1.639582 | 2.309424 | -0.56672 |
| H | 53 | 2.569931 | -1.467991 | 5.016923 | 0.24596 |
| Al | 54 | -0.956134 | 0.000219 | 0.000515 | 2.03515 |
| H | 55 | -6.08316 | -0.421635 | -0.916182 | 0.2451 |
| H | 56 | -6.076839 | -0.591788 | 0.846326 | 0.24513 |
| H | 57 | -6.077734 | 1.019736 | 0.112438 | 0.24504 |
| C | 58 | 3.523356 | -1.281032 | -3.542845 | -0.31292 |
| C | 59 | 3.539843 | 3.699012 | 0.642517 | -0.31306 |
| C | 60 | 3.544905 | -2.411938 | 2.871879 | -0.31297 |
| H | 61 | 4.207742 | -1.798152 | 3.494902 | 0.20466 |
| H | 62 | 3.149384 | -3.241513 | 3.46864 | 0.21873 |
| H | 63 | 4.111325 | -2.811915 | 2.028176 | 0.22431 |
| H | 64 | 4.193071 | -2.123834 | -3.329455 | 0.20463 |
| H | 65 | 3.119272 | -1.384852 | -4.55613 | 0.21874 |
| H | 66 | 4.085663 | -0.347537 | -3.472082 | 0.22429 |
| H | 67 | 4.200826 | 3.935073 | -0.201188 | 0.20469 |
| H | 68 | 3.141928 | 4.628895 | 1.06399 | 0.21871 |
| H | 69 | 4.109138 | 3.169333 | 1.409326 | 0.22434 |
| K | 70 | 2.439693 | -0.001371 | -0.006813 | 0.9752 |

## $Rb(Al•2)^{+}$ complex

| Atom | No. | X | Y | Z | Natural Charge |
|---|---|---|---|---|---|
| C | 1 | -4.306601 | -0.023542 | 0.009804 | -0.0902 |
| C | 2 | -5.843502 | -0.031684 | 0.013472 | -0.67343 |
| C | 3 | -3.797505 | 0.621006 | -1.307041 | -0.25682 |
| C | 4 | -3.792749 | 0.796417 | 1.222746 | -0.25685 |
| C | 5 | -3.782955 | -1.480473 | 0.110285 | -0.25691 |
| H | 6 | -3.823544 | -0.121284 | -2.114951 | 0.25028 |
| H | 7 | -4.462634 | 1.445153 | -1.595003 | 0.23467 |
| N | 8 | -2.426546 | 1.125646 | -1.143315 | -0.64872 |
| H | 9 | -3.826594 | 1.867649 | 0.98683 | 0.25035 |
| H | 10 | -4.449816 | 0.628074 | 2.085564 | 0.23466 |
| N | 11 | -2.415981 | 0.410289 | 1.565678 | -0.64841 |
| H | 12 | -3.805181 | -1.810555 | 1.156677 | 0.25038 |
| H | 13 | -4.441024 | -2.148474 | -0.460231 | 0.23467 |
| N | 14 | -2.410271 | -1.5767 | -0.407081 | -0.64832 |
| C | 15 | -2.118087 | -2.608518 | -1.138639 | 0.1799 |
| H | 16 | -2.883333 | -3.38357 | -1.259606 | 0.2117 |
| C | 17 | -0.893757 | -2.839134 | -1.851652 | -0.20778 |
| C | 18 | -2.146772 | 2.277382 | -1.672944 | 0.17996 |
| H | 19 | -2.92016 | 2.763726 | -2.278145 | 0.21171 |
| C | 20 | -0.927515 | 3.019828 | -1.524214 | -0.20784 |
| C | 21 | -2.124344 | 0.294111 | 2.825415 | 0.1798 |
| H | 22 | -2.893312 | 0.56817 | 3.556532 | 0.21168 |
| C | 23 | -0.895924 | -0.19616 | 3.383072 | -0.20783 |
| C | 24 | 0.075042 | 2.608363 | -0.601143 | 0.39857 |
| C | 25 | -0.788673 | 4.225566 | -2.256514 | -0.19494 |
| C | 26 | 0.32832 | 5.01623 | -2.102325 | -0.256 |
| C | 27 | 1.226588 | 3.449 | -0.470333 | 0.24952 |
| C | 28 | 1.33936 | 4.621086 | -1.203413 | -0.27416 |
| H | 29 | -1.580501 | 4.517754 | -2.9417 | 0.23949 |
| H | 30 | 0.43857 | 5.939875 | -2.66056 | 0.24932 |
| O | 31 | -0.019286 | 1.529473 | 0.135646 | -0.85435 |
| O | 32 | 2.186178 | 2.994065 | 0.410463 | -0.56004 |
| H | 33 | 2.214077 | 5.252346 | -1.090774 | 0.24522 |
| C | 34 | 0.103933 | -0.782622 | 2.556515 | 0.39879 |
| C | 35 | -0.743672 | -0.161944 | 4.792049 | -0.19499 |
| C | 36 | 0.383374 | -0.680639 | 5.389931 | -0.25614 |
| C | 37 | 1.265487 | -1.307001 | 3.209399 | 0.24928 |
| C | 38 | 1.391207 | -1.255023 | 4.589525 | -0.27415 |
| H | 39 | -1.533098 | 0.28002 | 5.394845 | 0.23948 |
| H | 40 | 0.503851 | -0.656241 | 6.467776 | 0.24933 |
| O | 41 | -0.001466 | -0.882034 | 1.254973 | -0.85415 |
| O | 42 | 2.220451 | -1.837361 | 2.366887 | -0.56037 |
| H | 43 | 2.274238 | -1.66099 | 5.070679 | 0.24516 |
| C | 44 | 0.098164 | -1.823338 | -1.956529 | 0.39855 |
| C | 45 | -0.738412 | -4.077039 | -2.524564 | -0.19497 |
| C | 46 | 0.384215 | -4.329089 | -3.281515 | -0.25607 |
| C | 47 | 1.254215 | -2.119042 | -2.747767 | 0.24927 |
| C | 48 | 1.383759 | -3.34153 | -3.390004 | -0.27431 |
| H | 49 | -1.522084 | -4.825156 | -2.434815 | 0.2395 |
| H | 50 | 0.507482 | -5.275287 | -3.79765 | 0.24933 |
| O | 51 | -0.009827 | -0.646135 | -1.393054 | -0.85432 |
| O | 52 | 2.201725 | -1.117379 | -2.796829 | -0.56005 |
| H | 53 | 2.263219 | -3.551539 | -3.989009 | 0.24522 |
| Al | 54 | -1.113027 | -0.005577 | 0.001134 | 2.03645 |
| H | 55 | -6.243288 | 0.986089 | 0.088698 | 0.24482 |
| H | 56 | -6.237862 | -0.479117 | -0.906118 | 0.2448 |
| H | 57 | -6.233087 | -0.608265 | 0.860304 | 0.24482 |
| C | 58 | 3.171989 | 3.928939 | 0.841065 | -0.31436 |
| C | 59 | 3.218163 | -2.670828 | 2.951093 | -0.31439 |
| C | 60 | 3.189274 | -1.204369 | -3.820716 | -0.31436 |
| H | 61 | 3.894911 | -2.025495 | -3.638004 | 0.20259 |
| H | 62 | 2.725247 | -1.339036 | -4.804594 | 0.21817 |
| H | 63 | 3.730015 | -0.255452 | -3.804615 | 0.22415 |
| H | 64 | 3.866472 | 4.191733 | 0.032254 | 0.2027 |
| H | 65 | 2.705717 | 4.842448 | 1.227843 | 0.21815 |
| H | 66 | 3.725841 | 3.439408 | 1.645242 | 0.22402 |
| H | 67 | 3.917543 | -2.096583 | 3.573049 | 0.2027 |
| H | 68 | 2.763896 | -3.463744 | 3.55642 | 0.2182 |
| H | 69 | 3.764169 | -3.121592 | 2.119337 | 0.22404 |
| Rb | 70 | 2.495466 | 0.01242 | -0.005638 | 0.98385 |

## $Cs(Al•2)^{+}$ complex

| Atom | No. | X | Y | Z | Natural Charge |
|---|---|---|---|---|---|
| C | 1 | 4.484213 | -0.01279 | -0.014209 | -0.08944 |
| C | 2 | 6.021027 | -0.015994 | -0.020877 | -0.67337 |
| C | 3 | 3.962599 | 0.407539 | -1.414492 | -0.25655 |
| C | 4 | 3.965428 | -1.435629 | 0.325634 | -0.25656 |
| C | 5 | 3.973457 | 0.992286 | 1.052717 | -0.25653 |
| H | 6 | 3.986736 | 1.500623 | -1.506962 | 0.25008 |
| H | 7 | 4.620163 | -0.004006 | -2.190937 | 0.23403 |
| N | 8 | 2.589649 | -0.07528 | -1.620504 | -0.64726 |
| H | 9 | 3.983116 | -2.06223 | -0.574989 | 0.24998 |
| H | 10 | 4.62806 | -1.902607 | 1.065632 | 0.23402 |
| N | 11 | 2.596349 | -1.371534 | 0.856578 | -0.64662 |
| H | 12 | 3.99698 | 0.523851 | 2.044706 | 0.24994 |
| H | 13 | 4.637324 | 1.865698 | 1.084292 | 0.23402 |
| N | 14 | 2.6029 | 1.42201 | 0.741365 | -0.64692 |
| C | 15 | 2.324229 | 2.681006 | 0.887264 | 0.17846 |
| H | 16 | 3.094357 | 3.329418 | 1.320558 | 0.21075 |
| C | 17 | 1.116005 | 3.347428 | 0.491107 | -0.20828 |
| C | 18 | 2.30168 | -0.579875 | -2.780896 | 0.17856 |
| H | 19 | 3.066421 | -0.532322 | -3.564544 | 0.21081 |
| C | 20 | 1.08887 | -1.253113 | -3.151053 | -0.20826 |
| C | 21 | 2.3151 | -2.124105 | 1.875583 | 0.17852 |
| H | 22 | 3.08157 | -2.827477 | 2.220578 | 0.2108 |
| C | 23 | 1.107754 | -2.105911 | 2.652239 | -0.20813 |
| C | 24 | 0.106679 | -1.590156 | -2.176196 | 0.39882 |
| C | 25 | 0.952128 | -1.676101 | -4.497262 | -0.19587 |
| C | 26 | -0.138303 | -2.41737 | -4.894594 | -0.25722 |
| C | 27 | -1.008269 | -2.372747 | -2.620623 | 0.24876 |
| C | 28 | -1.118793 | -2.768185 | -3.945499 | -0.2751 |
| H | 29 | 1.727185 | -1.409941 | -5.211672 | 0.2389 |
| H | 30 | -0.24678 | -2.742092 | -5.924014 | 0.24866 |
| O | 31 | 0.191922 | -1.249241 | -0.914607 | -0.85238 |
| O | 32 | -1.937646 | -2.677239 | -1.649256 | -0.55695 |
| H | 33 | -1.968954 | -3.361238 | -4.264867 | 0.24447 |
| C | 34 | 0.127373 | -1.089885 | 2.464494 | 0.39854 |
| C | 35 | 0.974887 | -3.061445 | 3.690963 | -0.19584 |
| C | 36 | -0.110528 | -3.033313 | 4.538204 | -0.25722 |
| C | 37 | -0.982141 | -1.082116 | 3.370847 | 0.2487 |
| C | 38 | -1.089557 | -2.03341 | 4.374669 | -0.27499 |
| H | 39 | 1.749086 | -3.815049 | 3.81189 | 0.23894 |
| H | 40 | -0.216094 | -3.763533 | 5.333545 | 0.24868 |
| O | 41 | 0.21026 | -0.165401 | 1.5404 | -0.85262 |
| O | 42 | -1.911052 | -0.086716 | 3.15537 | -0.55714 |
| H | 43 | -1.935931 | -2.01285 | 5.052851 | 0.24451 |
| C | 44 | 0.128874 | 2.679833 | -0.289281 | 0.39862 |
| C | 45 | 0.98931 | 4.725235 | 0.800073 | -0.19591 |
| C | 46 | -0.095793 | 5.448737 | 0.35778 | -0.25724 |
| C | 47 | -0.980077 | 3.465032 | -0.743454 | 0.24883 |
| C | 48 | -1.080844 | 4.810463 | -0.421642 | -0.27512 |
| H | 49 | 1.768253 | 5.204074 | 1.388166 | 0.23886 |
| H | 50 | -0.196583 | 6.503017 | 0.59283 | 0.24863 |
| O | 51 | 0.204275 | 1.416547 | -0.626947 | -0.8522 |
| O | 52 | -1.914889 | 2.783918 | -1.492952 | -0.55681 |
| H | 53 | -1.92694 | 5.390196 | -0.774791 | 0.24446 |
| Al | 54 | 1.282254 | -0.004219 | -0.003961 | 2.03911 |
| H | 55 | 6.411141 | -0.816119 | -0.660454 | 0.24447 |
| H | 56 | 6.416057 | 0.935257 | -0.395769 | 0.24452 |
| H | 57 | 6.419615 | -0.169536 | 0.988555 | 0.24451 |
| C | 58 | -2.826639 | -3.759249 | -1.910957 | -0.3144 |
| C | 59 | -2.787947 | 0.232896 | 4.231727 | -0.31432 |
| C | 60 | -2.795078 | 3.558864 | -2.301795 | -0.31434 |
| H | 61 | -3.536011 | 4.100609 | -1.698548 | 0.20086 |
| H | 62 | -2.238075 | 4.275888 | -2.91622 | 0.21741 |
| H | 63 | -3.312624 | 2.851246 | -2.953484 | 0.22375 |
| H | 64 | -3.570155 | -3.502773 | -2.677559 | 0.20093 |
| H | 65 | -2.277319 | -4.653488 | -2.227944 | 0.21747 |
| H | 66 | -3.340037 | -3.966712 | -0.969341 | 0.22374 |
| H | 67 | -3.532245 | -0.556399 | 4.402982 | 0.20087 |
| H | 68 | -2.228159 | 0.406163 | 5.15828 | 0.21751 |
| H | 69 | -3.301717 | 1.152782 | 3.943455 | 0.22368 |
| Cs | 70 | -2.546804 | 0.0069 | 0.008807 | 0.99646 |

## ESI 2: Characterization of 1, 2, and their complexes

Characterization of the compounds were carried out using a JEOL JNM-LA400 or JNM-ECS400 FT-NMR spectrometer, a JEOL JMS-AX500 (FAB) or Thermo Fisher Exactive (ESI) mass spectrometer, and a Perkin-Elmer 2400 elemental analyzer at Chemical Analysis Center, Chiba University.

**1:** $\delta_H$ (400 MHz; $CDCl_3$; $Me_4Si$): 1.17 (3 H, s, $CH_3$), 3.65 (6 H, s, $CH_2$), 6.90 (3 H, t, $^3J$ 7.5, Ar-H), 6.98 (3 H, d, $^3J$ 8.5, Ar-H), 7.27 (3 H, dd, $^3J$ 7.7, $^4J$ 1.5, Ar-H), 7.34 (3 H, td, $^3J$ 7.8, $^4J$ 1.6, Ar-H), 8.39 (3 H, s, N=CH) and 13.37 (3 H, s, OH). Anal. Found: C, 72.61; H, 6.17; N, 9.80. Calc. for $C_{26}H_{27}N_3O_3$: C, 72.71; H, 6.34; N 9.78%.

**2:** $\delta_H$ (400 MHz; $CDCl_3$; $Me_4Si$): 1.16 (3 H, s, $CCH_3$), 3.66 (6 H, s, $CH_2$), 3.93 (9 H, s, $OCH_3$), 6.83 (3 H, t, $^3J$ 7.9, Ar-H), 6.89 (3 H, dd, $^3J$ 8.0, $^4J$ 1.7, Ar-H), 6.95 (3 H, dd, $^3J$ 7.7, $^4J$ 1.4, Ar-H), 8.39 (3 H, s, N=CH) and 13.96 (3 H, s, OH). Anal. Found: C, 66.92; H, 6.40; N, 8.03. Calc. for $C_{29}H_{33}N_3O_6$: C, 67.04; H, 6.40; N, 8.09%.

**Co•1 complex:** $\delta_H$ (400 MHz; $CDCl_3$; $Me_4Si$): 1.21 (3 H, s, $CH_3$), 3.09 (3 H, d, $^2J$ 12.5, $CH_2$), 3.85 (3 H, d, $^2J$ 12.3, $CH_2$), 6.44 (3 H, t, $^3J$ 7.4, Ar-H), 7.04 (6 H, d, $^3J$ 8.0, Ar-H), 7.11 (3 H, t, $^3J$ 7.6, Ar-H) and 7.43 (3 H, s, N=CH). MS (FAB+): *m*/*z* 486 $[M+H]^+$ and 508 $[M+Na]^+$. Anal. Found: C, 62.09; H, 5.13; N, 8.15. Calc. for $C_{26}H_{24}N_3O_3Co•H_2O$: C, 62.03; H, 5.21; N, 8.35%.

**Co•2 complex:** $\delta_H$ (400 MHz; $CDCl_3$; $Me_4Si$): 1.19 (3 H, s, $CCH_3$), 3.16 (3 H, d, $^2J$ 12.5, $CH_2$), 3.49 (9 H, s, $OCH_3$), 3.85 (3 H, d, $^2J$ 13.6, $CH_2$), 6.34 (3 H, t, $^3J$ 7.5, Ar-H), 6.74 (6 H, d, $^3J$ 7.9, Ar-H) and 7.43 (3 H, s, N=CH). MS (ESI+): *m*/*z* 576 $[M+H]^+$ and 598 $[M+Na]^+$. Anal. Found: C, 60.15; H, 5.01; N, 7.25. Calc. for $C_{29}H_{30}N_3O_6Co$: C, 60.52; H, 5.25; N, 7.30%.

**Al•2 complex:** $\delta_H$ (400 MHz; $CDCl_3$; $Me_4Si$): 1.16 (3 H, s, $CCH_3$), 3.32 (3 H, d, $^2J$ 13.4, $CH_2$), 3.60 (9 H, s, $OCH_3$), 4.09 (3 H, d, $^2J$ 13.6, $CH_2$), 6.48 (3 H, t, $^3J$ 7.8, Ar-H), 6.80 (3 H, dd, $^3J$ 7.9, $^4J$ 1.6, Ar-H), 6.90 (3 H, dd, $^3J$ 7.7, $^4J$ 1.6, Ar-H) and 8.06 (3 H, s, N=CH). MS (ESI+): *m*/*z* 544 $[M+H]^+$ and 566 $[M+Na]^+$. Anal. Found: C, 63.77; H, 5.51; N, 7.64. Calc. for $C_{29}H_{30}N_3O_6Al$: C, 64.08; H, 5.56; N, 7.73%.