

| $[\text{Au}_6\text{Pd}(\text{PPh}_3)_7]^{2+}$ | | | | | 47 | 1 | 2.777512 | -3.387827 | -0.095424 |
|---|---------------|-------------------------|-----------|-----------|----|---|-----------|-----------|-----------|
| Center | Atomic Number | Coordinates (Angstroms) | | | 48 | 6 | -1.604094 | 0.178195 | 5.039638 |
| | | X | Y | Z | 49 | 6 | -2.182031 | 0.296554 | 6.316568 |
| 1 | 79 | 1.295603 | -1.219035 | 1.218229 | 50 | 1 | -3.263789 | 0.31463 | 6.432571 |
| 2 | 79 | -1.411058 | -0.041586 | 1.348301 | 51 | 6 | -1.360495 | 0.390197 | 7.447715 |
| 3 | 79 | -2.515118 | -1.506688 | -0.988859 | 52 | 1 | -1.80744 | 0.483409 | 8.43252 |
| 4 | 79 | 1.068948 | 1.557955 | 0.758854 | 53 | 6 | 0.037313 | 0.352472 | 7.311302 |
| 5 | 79 | 2.681071 | -0.099667 | -1.12898 | 54 | 1 | 0.668598 | 0.418948 | 8.191811 |
| 6 | 79 | -2.426682 | 1.262496 | -1.049395 | 55 | 6 | 0.615928 | 0.219882 | 6.041491 |
| 7 | 46 | -0.046365 | -0.222193 | -1.048599 | 56 | 1 | 1.697733 | 0.184615 | 5.927164 |
| 8 | 15 | 2.532613 | -2.725233 | 2.723849 | 57 | 6 | -0.205495 | 0.135391 | 4.908189 |
| 9 | 15 | -2.628058 | -0.002568 | 3.492783 | 58 | 1 | 0.239766 | 0.027349 | 3.915174 |
| 10 | 15 | -3.391568 | -3.811096 | -1.155708 | 59 | 6 | -3.629189 | -1.558905 | 3.727694 |
| 11 | 15 | 1.833468 | 3.744814 | 1.538976 | 60 | 6 | -4.801306 | -1.586541 | 4.502895 |
| 12 | 15 | 5.059405 | -0.219922 | -1.80244 | 61 | 1 | -5.185856 | -0.669857 | 4.946469 |
| 13 | 15 | -3.546342 | 3.427424 | -1.387078 | 62 | 6 | -5.485328 | -2.795827 | 4.684824 |
| 14 | 15 | 0.164625 | -0.464947 | -3.45047 | 63 | 1 | -6.389194 | -2.818997 | 5.285809 |
| 15 | 6 | 3.396686 | -1.674432 | 4.001434 | 64 | 6 | -5.004682 | -3.974764 | 4.092242 |
| 16 | 6 | 3.797237 | -2.200897 | 5.241509 | 65 | 1 | -5.543277 | -4.908266 | 4.227127 |
| 17 | 1 | 3.581021 | -3.237686 | 5.493413 | 66 | 6 | -3.84255 | -3.945692 | 3.30864 |
| 18 | 6 | 4.45857 | -1.380045 | 6.166584 | 67 | 1 | -3.478206 | -4.852945 | 2.832008 |
| 19 | 1 | 4.77016 | -1.787929 | 7.122997 | 68 | 6 | -3.155719 | -2.737987 | 3.126126 |
| 20 | 6 | 4.713431 | -0.033939 | 5.859532 | 69 | 1 | -2.257099 | -2.712515 | 2.505745 |
| 21 | 1 | 5.223636 | 0.598273 | 6.579551 | 70 | 6 | -3.865542 | 1.386771 | 3.472503 |
| 22 | 6 | 4.304091 | 0.496343 | 4.625849 | 71 | 6 | -3.762533 | 2.508687 | 4.308783 |
| 23 | 1 | 4.49132 | 1.539824 | 4.382802 | 72 | 1 | -2.981728 | 2.563613 | 5.066009 |
| 24 | 6 | 3.649077 | -0.32343 | 3.696466 | 73 | 6 | -4.668028 | 3.571628 | 4.165476 |
| 25 | 1 | 3.32769 | 0.095127 | 2.740365 | 74 | 1 | -4.589704 | 4.435881 | 4.818661 |
| 26 | 6 | 1.646317 | -4.040135 | 3.694495 | 75 | 6 | -5.662744 | 3.524615 | 3.180058 |
| 27 | 6 | 0.429507 | -3.682886 | 4.30382 | 76 | 1 | -6.35558 | 4.352873 | 3.06432 |
| 28 | 1 | 0.050395 | -2.663812 | 4.215338 | 77 | 6 | -5.760841 | 2.406514 | 2.335782 |
| 29 | 6 | -0.298204 | -4.638483 | 5.022363 | 78 | 1 | -6.526753 | 2.368732 | 1.564873 |
| 30 | 1 | -1.236235 | -4.358668 | 5.492826 | 79 | 6 | -4.865209 | 1.341572 | 2.479779 |
| 31 | 6 | 0.184214 | -5.952776 | 5.128733 | 80 | 1 | -4.937447 | 0.480215 | 1.81524 |
| 32 | 1 | -0.38148 | -6.695283 | 5.682552 | 81 | 6 | -4.930825 | -4.033246 | -0.134724 |
| 33 | 6 | 1.397807 | -6.307399 | 4.522246 | 82 | 6 | -5.543213 | -2.886336 | 0.398002 |
| 34 | 1 | 1.77342 | -7.322179 | 4.60939 | 83 | 1 | -5.09806 | -1.906316 | 0.219092 |
| 35 | 6 | 2.133874 | -5.351645 | 3.805551 | 84 | 6 | -6.712489 | -3.005014 | 1.160734 |
| 36 | 1 | 3.069326 | -5.634146 | 3.326846 | 85 | 1 | -7.181615 | -2.117335 | 1.575097 |
| 37 | 6 | 3.877807 | -3.583257 | 1.764133 | 86 | 6 | -7.268546 | -4.270435 | 1.394514 |
| 38 | 6 | 5.064792 | -4.029199 | 2.36981 | 87 | 1 | -8.176493 | -4.363963 | 1.982461 |
| 39 | 1 | 5.223276 | -3.891566 | 3.438298 | 88 | 6 | -6.652008 | -5.418797 | 0.871682 |
| 40 | 6 | 6.05863 | -4.640151 | 1.592107 | 89 | 1 | -7.084104 | -6.398178 | 1.051795 |
| 41 | 1 | 6.977218 | -4.979887 | 2.059994 | 90 | 6 | -5.484017 | -5.302302 | 0.106847 |
| 42 | 6 | 5.869723 | -4.803606 | 0.211369 | 91 | 1 | -5.014218 | -6.195298 | -0.300941 |
| 43 | 1 | 6.643801 | -5.267469 | -0.392677 | 92 | 6 | -2.137885 | -5.033765 | -0.515526 |
| 44 | 6 | 4.683688 | -4.364268 | -0.394312 | 93 | 6 | -2.192584 | -6.399179 | -0.845996 |
| 45 | 1 | 4.534984 | -4.488401 | -1.463791 | 94 | 1 | -2.946672 | -6.765417 | -1.540374 |
| 46 | 6 | 3.688191 | -3.75561 | 0.380655 | 95 | 6 | -1.252727 | -7.287221 | -0.305217 |
| | | | | | 96 | 1 | -1.29765 | -8.34101 | -0.561975 |
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| 98 | 1 | 0.466154 | -7.503857 | 0.991498 | 149 | 1 | 4.737207 | 2.669438 | -1.579258 |
| 99 | 6 | -0.193122 | -5.451295 | 0.88209 | 150 | 6 | 5.8668 | 3.586808 | -3.176579 |
| 100 | 1 | 0.579998 | -5.082958 | 1.553454 | 151 | 1 | 5.635427 | 4.59823 | -2.855785 |
| 101 | 6 | -1.128624 | -4.560192 | 0.3406 | 152 | 6 | 6.660676 | 3.371238 | -4.313997 |
| 102 | 1 | -1.065335 | -3.493659 | 0.571824 | 153 | 1 | 7.051711 | 4.216207 | -4.87256 |
| 103 | 6 | -3.808786 | -4.422932 | -2.862704 | 154 | 6 | 6.949379 | 2.063295 | -4.729566 |
| 104 | 6 | -2.74802 | -4.625876 | -3.766095 | 155 | 1 | 7.560934 | 1.893862 | -5.610262 |
| 105 | 1 | -1.713494 | -4.487979 | -3.443242 | 156 | 6 | 6.459884 | 0.96834 | -4.001831 |
| 106 | 6 | -3.015598 | -5.010856 | -5.084252 | 157 | 1 | 6.690299 | -0.044705 | -4.325256 |
| 107 | 1 | -2.190508 | -5.163405 | -5.774146 | 158 | 6 | 6.283262 | -0.272146 | -0.395508 |
| 108 | 6 | -4.341765 | -5.194235 | -5.508024 | 159 | 6 | 7.581777 | 0.250247 | -0.531403 |
| 109 | 1 | -4.550124 | -5.494051 | -6.530158 | 160 | 1 | 7.893631 | 0.708981 | -1.467852 |
| 110 | 6 | -5.397289 | -4.991573 | -4.608259 | 161 | 6 | 8.475418 | 0.190208 | 0.547971 |
| 111 | 1 | -6.423069 | -5.137071 | -4.932163 | 162 | 1 | 9.478984 | 0.588954 | 0.437761 |
| 112 | 6 | -5.135196 | -4.600942 | -3.286246 | 163 | 6 | 8.073338 | -0.381975 | 1.765468 |
| 113 | 1 | -5.96029 | -4.440752 | -2.595505 | 164 | 1 | 8.765456 | -0.421242 | 2.600838 |
| 114 | 6 | 3.619356 | 3.659137 | 2.058497 | 165 | 6 | 6.778105 | -0.901705 | 1.901287 |
| 115 | 6 | 4.453333 | 2.72753 | 1.415509 | 166 | 1 | 6.454287 | -1.337688 | 2.844061 |
| 116 | 1 | 4.031078 | 2.030079 | 0.686898 | 167 | 6 | 5.885876 | -0.850956 | 0.821279 |
| 117 | 6 | 5.821222 | 2.685201 | 1.714465 | 168 | 1 | 4.88245 | -1.266237 | 0.925696 |
| 118 | 1 | 6.461847 | 1.972893 | 1.200548 | 169 | 6 | 5.372296 | -1.754443 | -2.807617 |
| 119 | 6 | 6.355087 | 3.560648 | 2.671474 | 170 | 6 | 6.583713 | -2.460762 | -2.741548 |
| 120 | 1 | 7.415114 | 3.526141 | 2.904285 | 171 | 1 | 7.370413 | -2.14044 | -2.060807 |
| 121 | 6 | 5.519858 | 4.475671 | 3.331592 | 172 | 6 | 6.774771 | -3.591218 | -3.549877 |
| 122 | 1 | 5.931444 | 5.150033 | 4.076007 | 173 | 1 | 7.71417 | -4.133694 | -3.504684 |
| 123 | 6 | 4.15234 | 4.529779 | 3.023685 | 174 | 6 | 5.75982 | -4.014815 | -4.422263 |
| 124 | 1 | 3.508563 | 5.242228 | 3.535574 | 175 | 1 | 5.914827 | -4.886855 | -5.050003 |
| 125 | 6 | 0.932607 | 4.410494 | 3.020263 | 176 | 6 | 4.546397 | -3.311568 | -4.482244 |
| 126 | 6 | 0.826058 | 5.784511 | 3.28531 | 177 | 1 | 3.750777 | -3.637297 | -5.148176 |
| 127 | 1 | 1.228779 | 6.510347 | 2.580162 | 178 | 6 | 4.35162 | -2.184421 | -3.67332 |
| 128 | 6 | 0.185649 | 6.215294 | 4.456819 | 179 | 1 | 3.403053 | -1.646351 | -3.709993 |
| 129 | 1 | 0.111046 | 7.27725 | 4.671262 | 180 | 6 | -5.390597 | 3.250492 | -1.215632 |
| 130 | 6 | -0.344902 | 5.278681 | 5.358787 | 181 | 6 | -5.984546 | 2.046231 | -1.635432 |
| 131 | 1 | -0.828214 | 5.619503 | 6.269365 | 182 | 1 | -5.367962 | 1.24857 | -2.051438 |
| 132 | 6 | -0.241087 | 3.90452 | 5.088662 | 183 | 6 | -7.369806 | 1.871482 | -1.512697 |
| 133 | 1 | -0.638236 | 3.167136 | 5.784405 | 184 | 1 | -7.828171 | 0.943608 | -1.840321 |
| 134 | 6 | 0.395863 | 3.472863 | 3.918332 | 185 | 6 | -8.161889 | 2.895152 | -0.968885 |
| 135 | 1 | 0.475934 | 2.405821 | 3.705939 | 186 | 1 | -9.234864 | 2.759857 | -0.875225 |
| 136 | 6 | 1.779967 | 5.049238 | 0.212322 | 187 | 6 | -7.568324 | 4.095888 | -0.550144 |
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| 138 | 1 | -0.319723 | 4.658459 | -0.210354 | 189 | 6 | -6.182648 | 4.275486 | -0.672299 |
| 139 | 6 | 0.499351 | 6.166094 | -1.525291 | 190 | 1 | -5.723498 | 5.202368 | -0.333229 |
| 140 | 1 | -0.437248 | 6.303545 | -2.061259 | 191 | 6 | -3.234475 | 4.223627 | -3.037646 |
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| 200 | 6 | -1.906738 | 4.242321 | -3.50103 |
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| 212 | 1 | -3.212262 | 6.403561 | -1.509267 |
| 213 | 6 | 0.577195 | -2.221324 | -3.939095 |
| 214 | 6 | 0.543735 | -2.678125 | -5.269443 |
| 215 | 1 | 0.282524 | -1.994981 | -6.07582 |
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| 217 | 1 | 0.768674 | -4.377537 | -6.581154 |
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| 221 | 1 | 1.243753 | -5.183959 | -2.364662 |
| 222 | 6 | 0.838277 | -3.131752 | -2.898736 |
| 223 | 1 | 0.829256 | -2.773542 | -1.866555 |
| 224 | 6 | -1.401588 | -0.124051 | -4.424158 |
| 225 | 6 | -2.424446 | -1.088484 | -4.403293 |
| 226 | 1 | -2.253272 | -2.058655 | -3.936121 |
| 227 | 6 | -3.663073 | -0.817706 | -4.993123 |
| 228 | 1 | -4.437942 | -1.579533 | -4.976888 |
| 229 | 6 | -3.892231 | 0.426508 | -5.604856 |
| 230 | 1 | -4.853851 | 0.640436 | -6.061427 |
| 231 | 6 | -2.869287 | 1.38378 | -5.639772 |
| 232 | 1 | -3.033085 | 2.343525 | -6.122978 |
| 233 | 6 | -1.624165 | 1.109992 | -5.051495 |
| 234 | 1 | -0.83471 | 1.858637 | -5.093938 |
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| 236 | 6 | 2.169085 | 0.423222 | -5.361194 |
| 237 | 1 | 2.115062 | -0.55433 | -5.836805 |
| 238 | 6 | 3.032285 | 1.401368 | -5.881892 |
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| 245 | 1 | 0.905996 | 2.183367 | -2.718799 |