# Computational Modelling of Imidazole Protection of Coor-dinated Gadolinium Tetraphenylporphyrine against Mo-lecular Oxygen Attack

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ClGdTPP·2Im

| | | | |
|---|---|---|---|
| Gd | -0.036220 | 0.389051 | 1.025796 |
| Cl | -1.061924 | 2.177828 | 2.809043 |
| N | 0.037390 | 2.294610 | -0.438463 |
| N | 2.061827 | 0.213075 | -0.211045 |
| N | -2.072404 | 0.269137 | -0.259936 |
| N | -0.053356 | -1.818403 | -0.021306 |
| C | -1.045868 | 3.103754 | -0.573837 |
| C | -0.611967 | 4.461337 | -0.840183 |
| C | 0.745623 | 4.442748 | -0.855130 |
| C | 1.147006 | 3.073469 | -0.592124 |
| C | 2.476856 | 2.624216 | -0.542730 |
| C | 2.888481 | 1.280027 | -0.400799 |
| C | 4.260091 | 0.825397 | -0.468760 |
| C | 4.231285 | -0.531818 | -0.341783 |
| C | 2.841893 | -0.906635 | -0.188499 |
| C | 2.380131 | -2.229167 | -0.037865 |
| C | 1.034762 | -2.640919 | -0.013444 |
| C | 0.602102 | -4.022096 | -0.082802 |
| C | -0.756032 | -4.001129 | -0.160662 |
| C | -1.155797 | -2.609508 | -0.117779 |
| C | -2.491324 | -2.157597 | -0.181345 |
| C | -2.901174 | -0.814185 | -0.239168 |
| C | -4.280376 | -0.367715 | -0.297218 |
| C | -4.252049 | 0.989508 | -0.367738 |
| C | -2.855982 | 1.379577 | -0.364352 |
| C | -2.393021 | 2.702408 | -0.485310 |
| H | 1.421567 | 5.273115 | -1.045361 |
| H | 5.131035 | 1.460024 | -0.615149 |
| H | 5.074770 | -1.218173 | -0.364506 |
| H | 1.258138 | -4.889222 | -0.113950 |
| H | -1.428822 | -4.849240 | -0.264550 |
| H | -5.155294 | -1.013558 | -0.289286 |
| H | -5.096952 | 1.671385 | -0.429242 |
| C | 3.548298 | 3.657758 | -0.681492 |
| C | 4.281483 | 3.779520 | -1.867714 |
| C | 3.827954 | 4.527696 | 0.379063 |
| C | 5.276681 | 4.747744 | -1.989632 |
| H | 4.060785 | 3.108152 | -2.700956 |
| C | 4.822759 | 5.496441 | 0.257373 |
| H | 3.252496 | 4.440347 | 1.303956 |
| C | 5.550465 | 5.608101 | -0.926844 |
| H | 5.837974 | 4.833738 | -2.922767 |
| H | 5.029632 | 6.168669 | 1.093117 |
| H | 6.329001 | 6.368134 | -1.023045 |
| C | 3.414375 | -3.303987 | 0.068005 |
| C | 4.109605 | -3.757094 | -1.058710 |
| C | 3.697696 | -3.877732 | 1.313054 |
| C | 5.069848 | -4.760843 | -0.942269 |

| | | | |
|---|---|---|---|
| H | 3.887606 | -3.315803 | -2.033138 |
| C | 4.657578 | -4.881654 | 1.430722 |
| H | 3.153967 | -3.527550 | 2.194447 |
| C | 5.346685 | -5.325287 | 0.302571 |
| H | 5.602554 | -5.107008 | -1.830807 |
| H | 4.867927 | -5.320709 | 2.408670 |
| H | 6.098060 | -6.112814 | 0.392873 |
| C | -3.563004 | -3.199025 | -0.205409 |
| C | -3.840478 | -3.958214 | 0.937760 |
| C | -4.308460 | -3.433401 | -1.367091 |
| C | -4.842860 | -4.926391 | 0.921348 |
| H | -3.256372 | -3.779882 | 1.843494 |
| C | -5.310534 | -4.401998 | -1.384628 |
| H | -4.092969 | -2.847809 | -2.263822 |
| C | -5.581515 | -5.150738 | -0.239900 |
| H | -5.049160 | -5.509791 | 1.821802 |
| H | -5.880964 | -4.575054 | -2.299925 |
| H | -6.366684 | -5.909903 | -0.253707 |
| H | -1.269839 | 5.309851 | -1.012823 |
| C | -3.418404 | 3.789466 | -0.497556 |
| C | -4.179765 | 4.068032 | -1.637272 |
| C | -3.617740 | 4.547827 | 0.662523 |
| C | -5.127427 | 5.090828 | -1.619432 |
| H | -4.021079 | 3.478023 | -2.543244 |
| C | -4.566376 | 5.568745 | 0.678478 |
| H | -3.019495 | 4.319567 | 1.549022 |
| C | -5.322455 | 5.842800 | -0.461414 |
| H | -5.714082 | 5.303116 | -2.516183 |
| H | -4.715925 | 6.154006 | 1.588617 |
| H | -6.064307 | 6.644583 | -0.447815 |
| N | 1.681290 | -0.020614 | 2.976064 |
| C | 2.996153 | -0.075871 | 2.951260 |
| N | 3.496893 | -0.107122 | 4.204590 |
| C | 2.439075 | -0.062911 | 5.084032 |
| C | 1.319187 | -0.006229 | 4.301779 |
| H | 3.620577 | -0.090847 | 2.059674 |
| H | 4.478167 | -0.142700 | 4.444358 |
| H | 2.574092 | -0.063559 | 6.161087 |
| H | 0.276493 | 0.075681 | 4.596766 |
| N | -1.300805 | -1.175375 | 2.722952 |
| C | -2.427401 | -0.852680 | 3.316955 |
| N | -2.865507 | -1.870344 | 4.090234 |
| C | -1.961024 | -2.903250 | 3.983456 |
| C | -0.997296 | -2.451107 | 3.122877 |
| H | -2.925050 | 0.111768 | 3.223009 |
| H | -3.709649 | -1.865084 | 4.646347 |
| H | -2.081338 | -3.843193 | 4.513303 |
| H | -0.113942 | -2.968653 | 2.753667 |

ClGdTPP·Im

| | | | |
|---|---|---|---|
| Gd | -0.255661 | -0.059492 | 0.919065 |
| Cl | -1.050797 | 1.145402 | 3.111660 |
| N | -0.118604 | 1.999708 | -0.239232 |
| N | 1.904203 | -0.077449 | -0.106949 |
| N | -2.234886 | -0.060111 | -0.377319 |
| N | -0.207113 | -2.147529 | -0.312323 |
| C | -1.210422 | 2.807770 | -0.353843 |
| C | -0.777426 | 4.187805 | -0.453466 |
| C | 0.579592 | 4.181687 | -0.390523 |
| C | 0.987237 | 2.797863 | -0.244664 |
| C | 2.318461 | 2.353399 | -0.149910 |
| C | 2.733447 | 1.004635 | -0.107887 |
| C | 4.110073 | 0.556505 | -0.103139 |
| C | 4.081536 | -0.803464 | -0.127920 |
| C | 2.687452 | -1.196935 | -0.137822 |
| C | 2.232344 | -2.525688 | -0.234991 |
| C | 0.892344 | -2.951490 | -0.369465 |
| C | 0.472074 | -4.325008 | -0.550211 |
| C | -0.889891 | -4.317080 | -0.614681 |
| C | -1.305702 | -2.939763 | -0.465992 |
| C | -2.643823 | -2.488504 | -0.509549 |
| C | -3.060029 | -1.146124 | -0.482430 |
| C | -4.432491 | -0.694341 | -0.581256 |
| C | -4.405547 | 0.664850 | -0.544414 |
| C | -3.016209 | 1.056634 | -0.425506 |
| C | -2.553769 | 2.388203 | -0.395198 |
| H | 1.252964 | 5.033242 | -0.453200 |
| H | 4.984713 | 1.202537 | -0.102565 |
| H | 4.930107 | -1.482693 | -0.161106 |
| H | 1.132061 | -5.185051 | -0.635304 |
| H | -1.553873 | -5.164181 | -0.772462 |
| H | -5.303435 | -1.339411 | -0.670843 |
| H | -5.249355 | 1.348523 | -0.598774 |
| C | 3.383435 | 3.401991 | -0.113584 |
| C | 4.202036 | 3.632760 | -1.225386 |
| C | 3.570881 | 4.175503 | 1.038019 |
| C | 5.190108 | 4.614952 | -1.185397 |
| H | 4.054755 | 3.036094 | -2.128745 |
| C | 4.559079 | 5.157577 | 1.078205 |
| H | 2.931347 | 4.001208 | 1.906774 |
| C | 5.371456 | 5.379161 | -0.033153 |
| H | 5.819199 | 4.786927 | -2.061595 |
| H | 4.695057 | 5.752460 | 1.984054 |

| | | | |
|---|---|---|---|
| H | 6.145269 | 6.149325 | -0.002142 |
| C | 3.275904 | -3.593565 | -0.164164 |
| C | 3.639849 | -4.339096 | -1.290822 |
| C | 3.907240 | -3.860689 | 1.057464 |
| C | 4.609307 | -5.336534 | -1.196963 |
| H | 3.157554 | -4.127977 | -2.248074 |
| C | 4.876914 | -4.857178 | 1.151154 |
| H | 3.634243 | -3.269140 | 1.935816 |
| C | 5.228915 | -5.599568 | 0.024184 |
| H | 4.886061 | -5.908344 | -2.085458 |
| H | 5.363771 | -5.053215 | 2.109346 |
| H | 5.989868 | -6.379668 | 0.096340 |
| C | -3.705957 | -3.534229 | -0.630140 |
| C | -4.070559 | -4.306340 | 0.478703 |
| C | -4.347579 | -3.761262 | -1.853136 |
| C | -5.057009 | -5.284798 | 0.368332 |
| H | -3.577077 | -4.128863 | 1.437385 |
| C | -5.333596 | -4.740006 | -1.964624 |
| H | -4.064542 | -3.162237 | -2.721844 |
| C | -5.690627 | -5.504164 | -0.854191 |
| H | -5.335269 | -5.876088 | 1.243520 |
| H | -5.824618 | -4.907662 | -2.925745 |
| H | -6.464124 | -6.270250 | -0.941400 |
| H | -1.435224 | 5.044970 | -0.576481 |
| C | -3.590996 | 3.465744 | -0.403434 |
| C | -4.231481 | 3.845950 | -1.587424 |
| C | -3.927182 | 4.109021 | 0.793236 |
| C | -5.193480 | 4.854995 | -1.576180 |
| H | -3.967582 | 3.345405 | -2.522186 |
| C | -4.889930 | 5.116836 | 0.803252 |
| H | -3.426441 | 3.807145 | 1.716678 |
| C | -5.524432 | 5.492076 | -0.380717 |
| H | -5.685346 | 5.146289 | -2.506966 |
| H | -5.146455 | 5.610887 | 1.742953 |
| H | -6.278107 | 6.282627 | -0.371900 |
| N | 0.826514 | -1.698378 | 2.645889 |
| C | 0.653505 | -2.996378 | 2.764361 |
| N | 1.429937 | -3.493282 | 3.750691 |
| C | 2.145295 | -2.450069 | 4.291628 |
| C | 1.751674 | -1.340702 | 3.593403 |
| H | -0.003548 | -3.611447 | 2.150976 |
| H | 1.482726 | -4.464759 | 4.025744 |
| H | 2.843491 | -2.582856 | 5.112093 |
| H | 2.062199 | -0.306742 | 3.724415 |

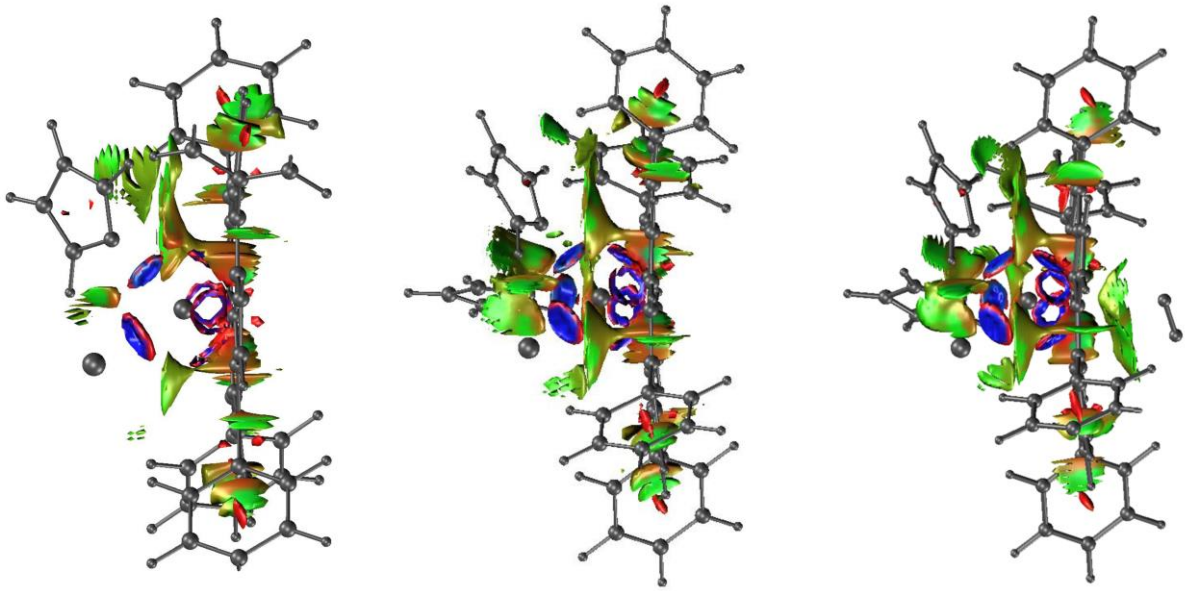

Figure S1. NCI representation (reduced electron density gradient isosurfaces = 0.6 a.u.) of bond types in co-ordinated complexes: non-covalent weak attractive coupling (dark blue), Van-der-Waals interac-tions (green) and repulsive interactions or steric effects (red).