

Supporting information for:

The Spin-Orbit Effects on Platinabenzene:

A Ring current and electron delocalization

approach

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S1 Nucleus-Independent Chemical Shift at M06-L and 0PBE

Level of theories.

Here presented in Table S1 the data obtained for M06-L and in Table S2 the data obtained for OPBE with the Spin-Orbit Contribution. Table S3 the comparison between Non-Relativistic, Scalar Relativistic and Spin-Orbit level of theory for M06-L level of theory. The plotted information of the comparison level of theory are presented in Figure S1. The molecular plane are highlighted in bold.

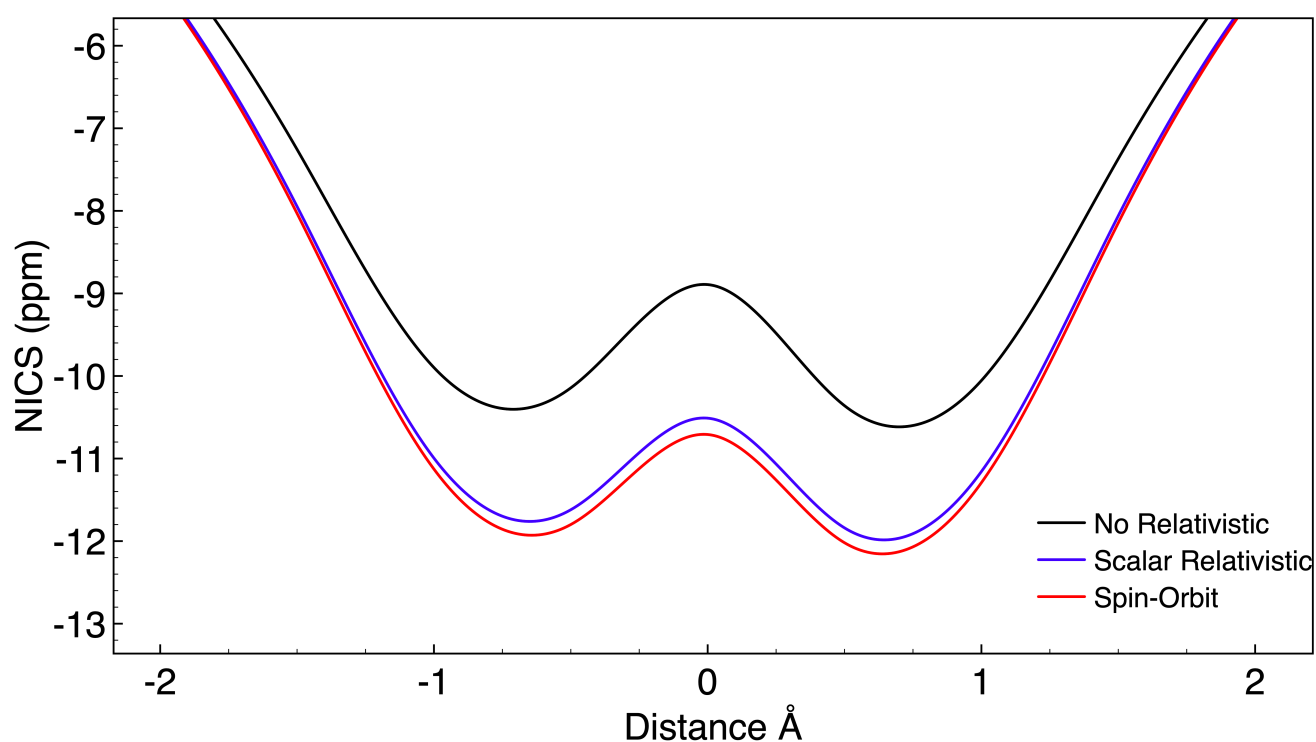


Figure S1: Comparison in the peak for different level of theory, No Relativistic, Scalar Relativistic and Spin-Orbit.

Table S1: NICS computed with M06-L Functional

| Position | Paramagnetic | Diamagnetic | Total Shielding |
|------------|---------------|---------------|-----------------|
| -6.0 | -0.732 | 0.211 | -0.521 |
| -5.5 | -0.927 | 0.279 | -0.648 |
| -5.0 | -1.19 | 0.375 | -0.815 |
| -4.5 | -1.552 | 0.512 | -1.041 |
| -4.0 | -2.059 | 0.708 | -1.352 |
| -3.5 | -2.784 | 0.989 | -1.796 |
| -3.0 | -3.847 | 1.386 | -2.461 |
| -2.5 | -5.434 | 1.916 | -3.518 |
| -2.0 | -7.777 | 2.506 | -5.271 |
| -1.5 | -10.782 | 2.751 | -8.032 |
| -1.0 | -12.643 | 1.514 | -11.128 |
| -0.5 | -9.655 | -2.145 | -11.799 |
| 0.0 | -5.993 | -4.716 | -10.709 |
| 0.5 | -10.02 | -2.001 | -12.02 |
| 1.0 | -12.88 | 1.588 | -11.292 |
| 1.5 | -10.899 | 2.753 | -8.146 |
| 2.0 | -7.855 | 2.492 | -5.363 |
| 2.5 | -5.498 | 1.905 | -3.592 |
| 3.0 | -3.898 | 1.38 | -2.518 |
| 3.5 | -2.825 | 0.987 | -1.838 |
| 4.0 | -2.091 | 0.708 | -1.383 |
| 4.5 | -1.577 | 0.512 | -1.065 |
| 5.0 | -1.21 | 0.376 | -0.834 |
| 5.5 | -0.943 | 0.28 | -0.663 |
| 6.0 | -0.745 | 0.211 | -0.533 |

Table S2: NICS computed with OPBE Functional

| Position | Paramagnetic | Diamagnetic | Spin-Ortbit | Total Shielding |
|------------|---------------|---------------|--------------|-----------------|
| -6.0 | -0.54 | 0.246 | -0.002 | -0.297 |
| -5.5 | -0.706 | 0.325 | -0.003 | -0.384 |
| -5.0 | -0.939 | 0.436 | -0.004 | -0.507 |
| -4.5 | -1.271 | 0.593 | -0.005 | -0.682 |
| -4.0 | -1.751 | 0.819 | -0.007 | -0.939 |
| -3.5 | -2.455 | 1.142 | -0.011 | -1.323 |
| -3.0 | -3.491 | 1.599 | -0.02 | -1.912 |
| -2.5 | -4.998 | 2.214 | -0.042 | -2.825 |
| -2.0 | -7.055 | 2.927 | -0.095 | -4.223 |
| -1.5 | -9.272 | 3.347 | -0.206 | -6.132 |
| -1.0 | -9.723 | 2.351 | -0.326 | -7.699 |
| -0.5 | -5.409 | -1.014 | -0.175 | -6.598 |
| 0.0 | -1.275 | -3.415 | 0.098 | -4.591 |
| 0.5 | -5.776 | -0.86 | -0.199 | -6.835 |
| 1.0 | -9.969 | 2.434 | -0.349 | -7.884 |
| 1.5 | -9.386 | 3.352 | -0.222 | -6.256 |
| 2.0 | -7.115 | 2.911 | -0.105 | -4.308 |
| 2.5 | -5.036 | 2.199 | -0.047 | -2.884 |
| 3.0 | -3.52 | 1.589 | -0.023 | -1.954 |
| 3.5 | -2.478 | 1.136 | -0.013 | -1.354 |
| 4.0 | -1.77 | 0.816 | -0.008 | -0.962 |
| 4.5 | -1.285 | 0.591 | -0.006 | -0.7 |
| 5.0 | -0.95 | 0.434 | -0.004 | -0.52 |
| 5.5 | -0.714 | 0.323 | -0.003 | -0.394 |
| 6.0 | -0.546 | 0.244 | -0.003 | -0.304 |

Table S3: NICS computed with M06-L Functional with different approximations. Non Relativistic, Scalar relativistic and Spin-Orbit

| Position | No Relativistic | Scalar Relativistic | Spin-Orbit |
|------------|-----------------|---------------------|----------------|
| -6,0 | -0,502 | -0,519 | -0,521 |
| -5.5 | -0.623 | -0.645 | -0.648 |
| -5.0 | -0.782 | -0.812 | -0.815 |
| -4.5 | -0.994 | -1.036 | -1.041 |
| -4.0 | -1.285 | -1.344 | -1.352 |
| -3.5 | -1.695 | -1.784 | -1.796 |
| -3.0 | -2.302 | -2.443 | -2.461 |
| -2.5 | -3.254 | -3.489 | -3.518 |
| -2.0 | -4.817 | -5.221 | -5.271 |
| -1.5 | -7.256 | -7.947 | -8.032 |
| -1.0 | -9.898 | -10.995 | -11.128 |
| -0.5 | -10.144 | -11.62 | -11.799 |
| 0.0 | -8.893 | -10.511 | -10.709 |
| 0.5 | -10.36 | -11.84 | -12.02 |
| 1.0 | -10.055 | -11.157 | -11.292 |
| 1.5 | -7.369 | -8.06 | -8.146 |
| 2.0 | -4.911 | -5.312 | -5.363 |
| 2.5 | -3.331 | -3.563 | -3.592 |
| 3.0 | -2.362 | -2.5 | -2.518 |
| 3.5 | -1.74 | -1.827 | -1.838 |
| 4.0 | -1.317 | -1.375 | -1.383 |
| 4.5 | -1.02 | -1.059 | -1.065 |
| 5.0 | -0.802 | -0.83 | -0.834 |
| 5.5 | -0.639 | -0.66 | -0.663 |
| 6,0 | -0,515 | -0,531 | -0,533 |

S2 4-Component Relativistic Current Density Plots and its components

Here presented the slices for the Magnetically Induced Current (MICD) Density at 4-Components Relativistic Level of Theory and decomposition of Current densities. From left to right. Total MICD, Diamagnetic MICD and Paramagnetic MICD.

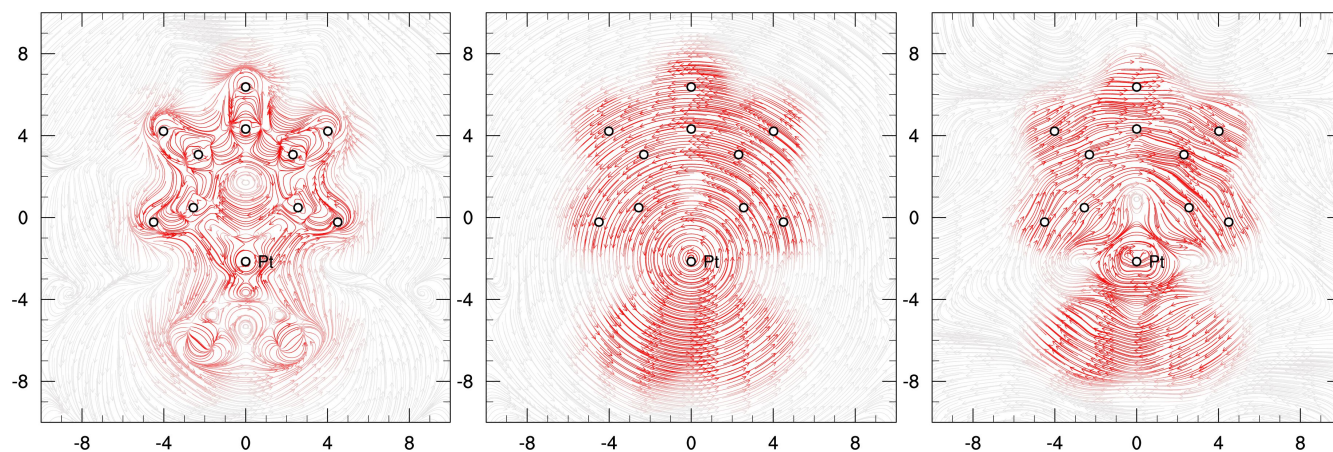


Figure S2: Plots for Magnetically Induced Current Density at $0a_0$ from molecular plane

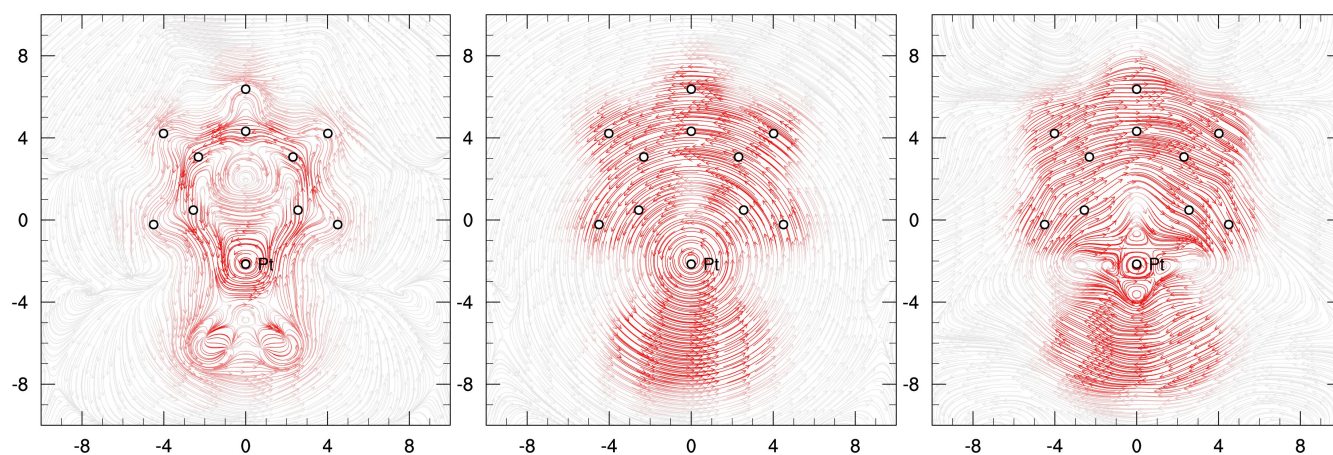


Figure S3: Plots for Magnetically Induced Current Density at $1a_0$ from molecular plane

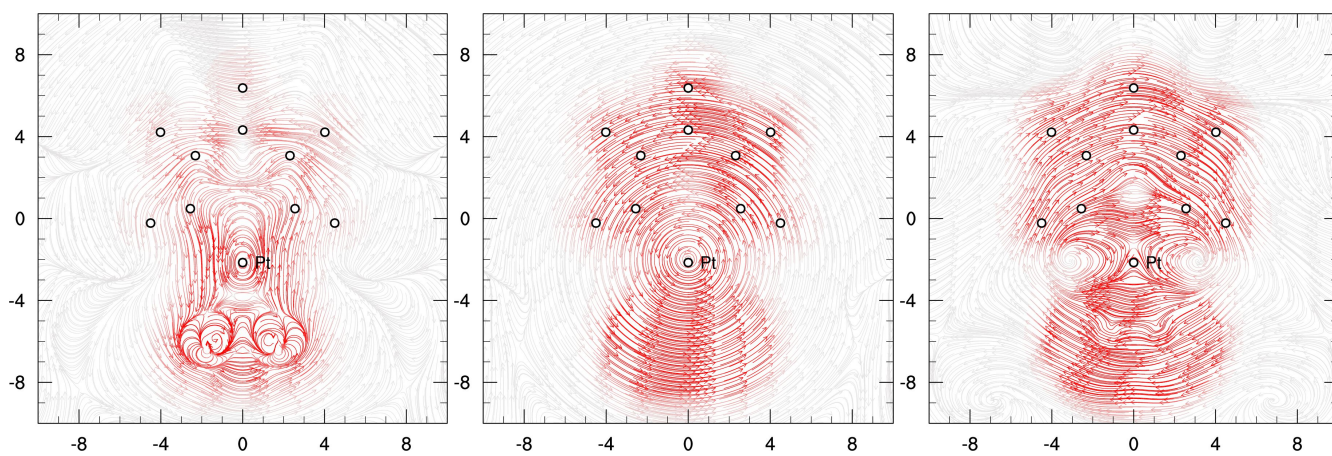


Figure S4: Plots for Magnetically Induced Current Density at $2a_0$ from molecular plane

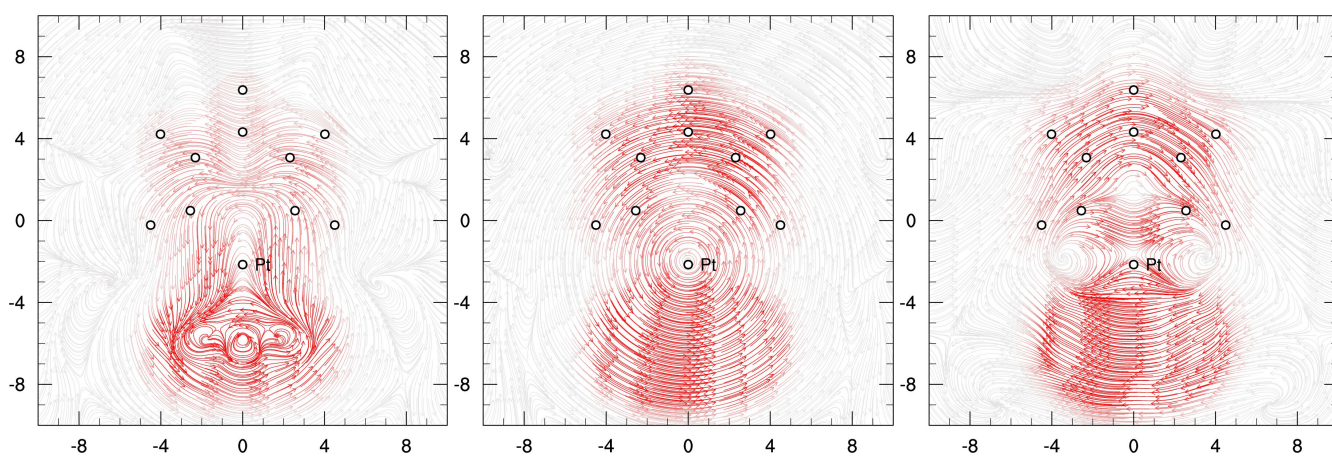


Figure S5: Plots for Magnetically Induced Current Density at $3a_0$ from molecular plane

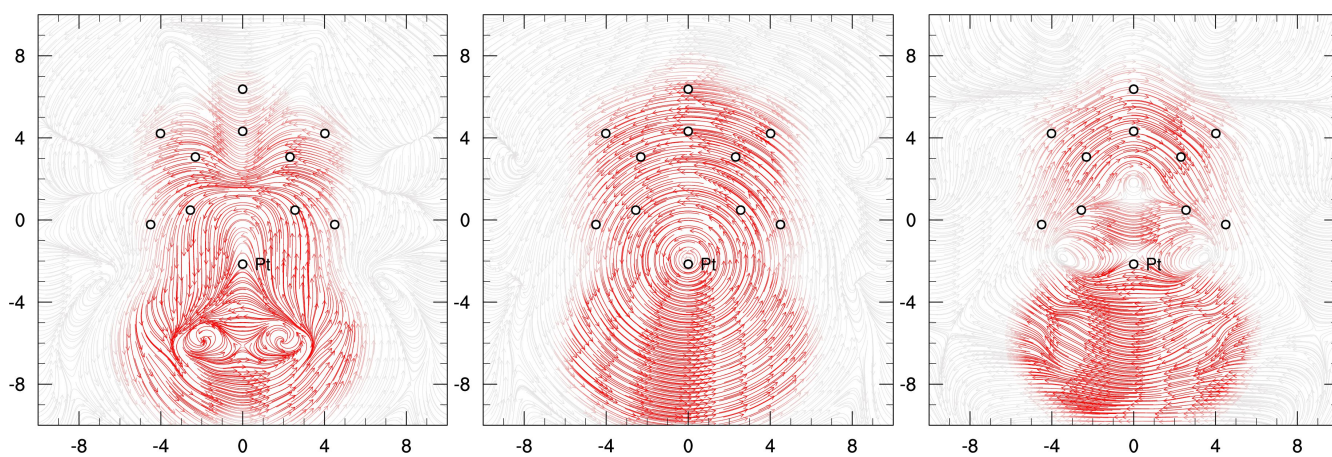


Figure S6: Plots for Magnetically Induced Current Density at $4a_0$ from molecular plane

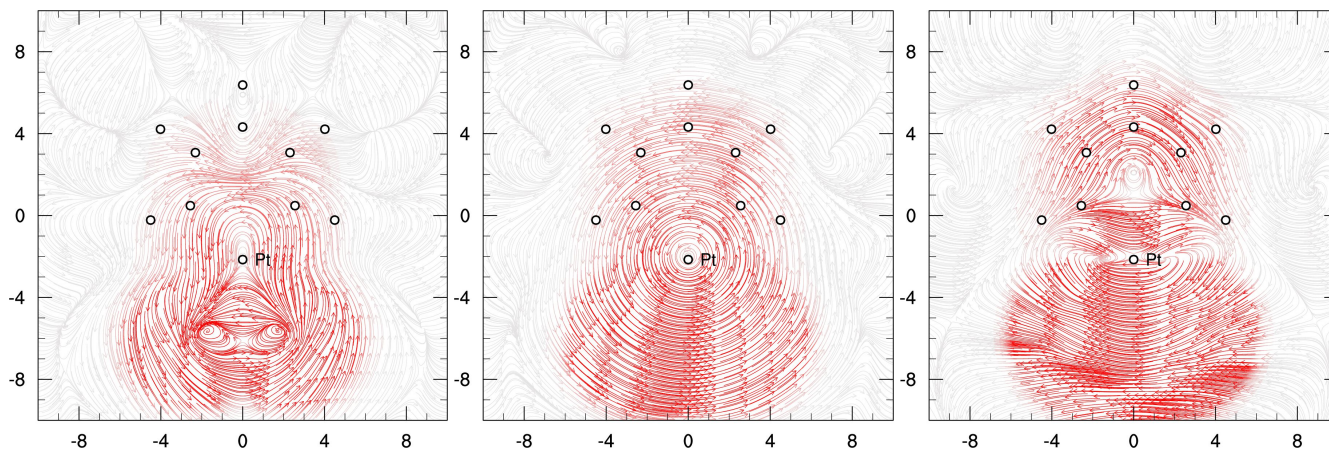


Figure S7: Plots for Magnetically Induced Current Density at $5a_0$ from molecular plane

S3 4-Component Relativistic Current Density Plots, Spin Free computation and, Spin-Orbit Effect

Here presented the slices for the Magnetically Induced Current (MICD) Density at 4-Components Relativistic Level of Theory and decomposition of Current densities. From left to right. Total MICD, Spin-Free MICD, and Spin-Orbit effect over the MICD.

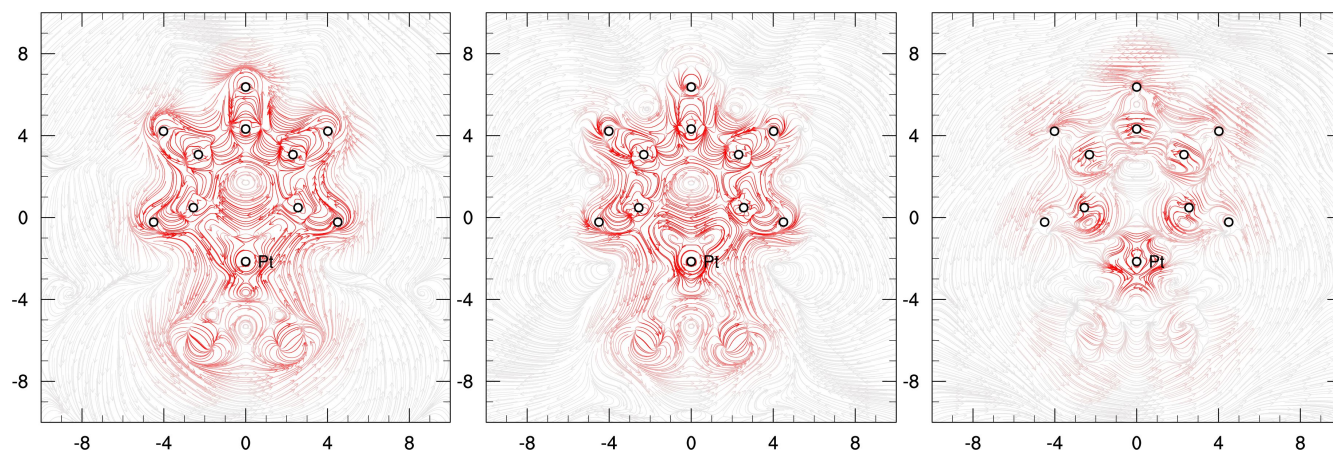


Figure S8: Plots for Magnetically Induced Current Density at $0a_0$ from molecular plane

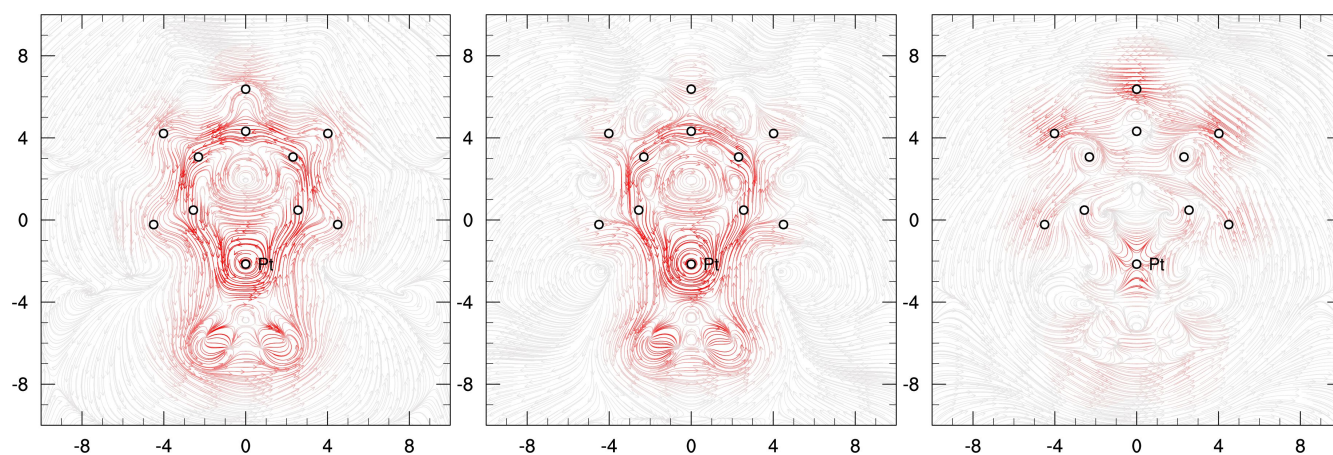


Figure S9: Plots for Magnetically Induced Current Density at $1a_0$ from molecular plane

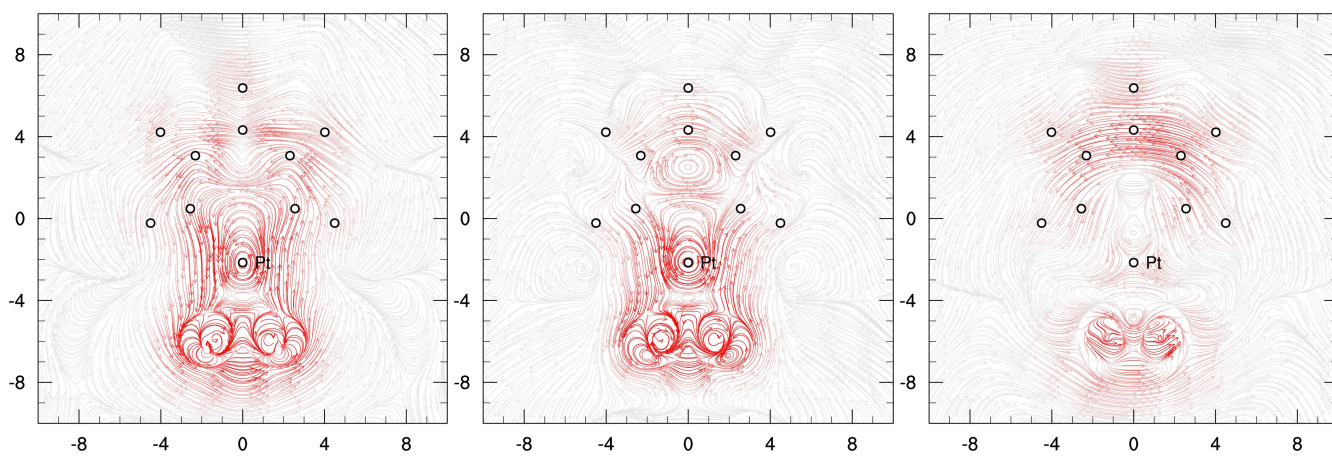


Figure S10: Plots for Magnetically Induced Current Density at $2a_0$ from molecular plane

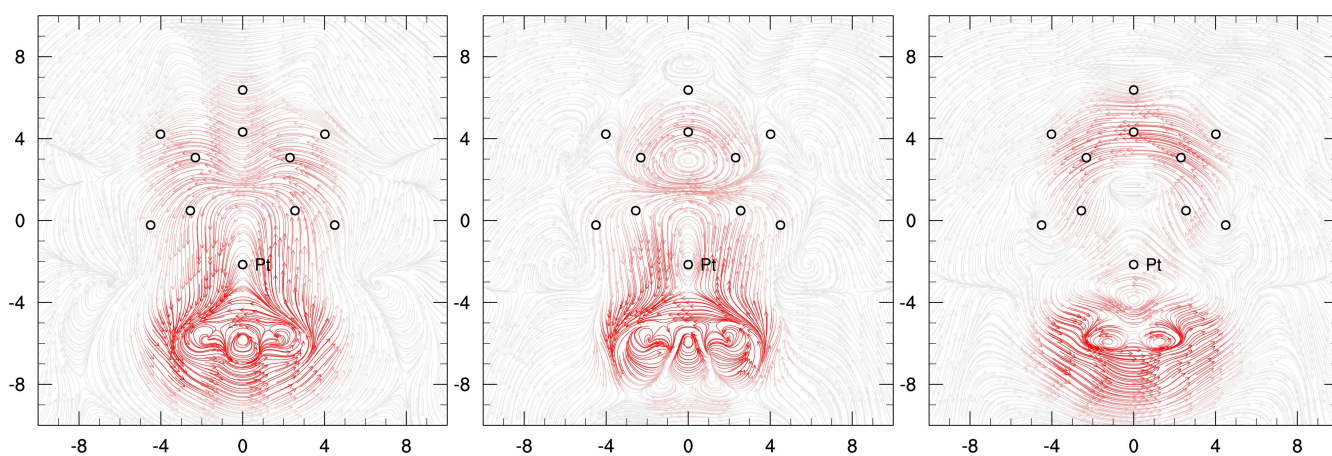


Figure S11: Plots for Magnetically Induced Current Density at $3a_0$ from molecular plane

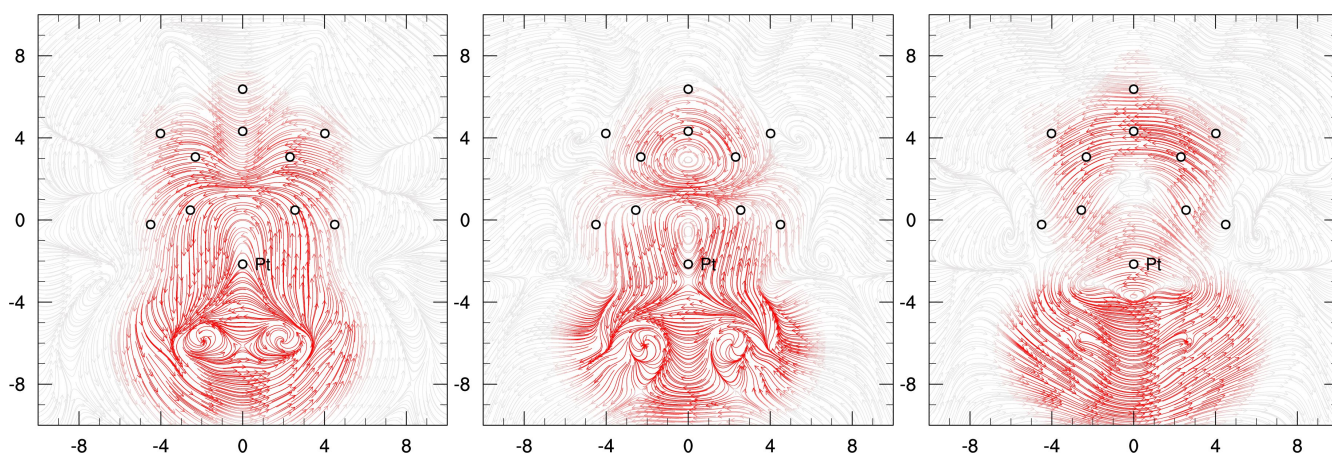


Figure S12: Plots for Magnetically Induced Current Density at $4a_0$ from molecular plane

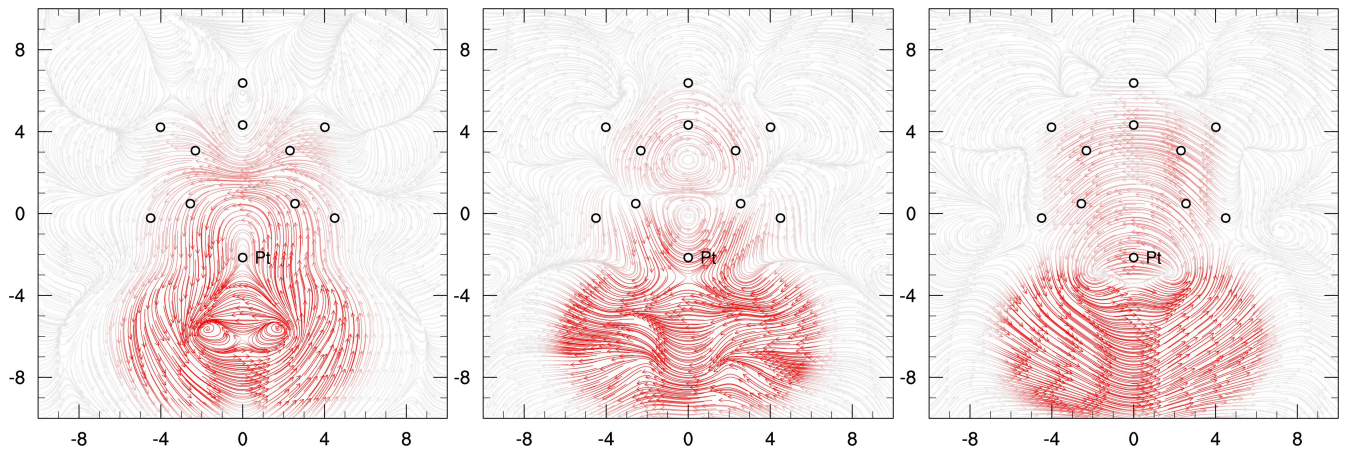


Figure S13: Plots for Magnetically Induced Current Density at $5a_0$ from molecular plane