Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Method/basis set dependence of NICS values among metallic nano-clusters and hydrocarbons

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Figure S-1A. NICS (0) values of $C_3H_3^+$ at different levels of theory. Numbers 1 to 13 on the horizontal axis denote different basis sets which are employed for optimization and computation of NICS values, (1) 6-31G, (2) 6-31G(d), (3) 6-31G(d,p), (4) 6-31+G(d), (5) 6-31+G(d,p), (6) 6-31++G(d,p), (7) 6-311++G(d,p), (8) 6-311++G(2df,2pd), (9) 6-311++G(3df,3pd), (10) cc-pVDZ, (11) cc-pVTZ, (12) aug-cc-pVDZ, (13) aug-cc-pVTZ, page S-33.

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At BP86/Aug-cc-pVTZ-PP level of theory Self Consistent Field calculations did not converge, page S-47.

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At M06/Aug-cc-pVTZ-PP, BP86/ cc-pVDZ-PP and B3LYP/cc-pVDZ-PP levels of theory Self Consistent Field calculations did not converge, page S-53.

Figure S-22A. NICS (0) values of Ag_4^{2-} at different levels of theory. Numbers 1 to 12 on the horizontal axis denote different basis sets which are employed for optimization and computation of NICS values, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) Lanl2TZ, (5) Lanl2TZ(f), (6) DZVP(DFT orbital), (7) cc-pVDZ-PP, (8) cc-pVTZ-PP, (9) Def2-TZVP, (10) Def2-TZVPP, (11) Def2-QZVP and (12) Def2-QZVPP, page S-54.

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Figure S-23B. NICS (1) values of Au_4^{2-} at different levels of theory. Numbers 1 to 11 on the horizontal axis denote different basis sets which are employed for optimization and computation of NICS values, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) Lanl2TZ, (5) Lanl2TZ(f), (6) cc-pVDZ-PP, (7) cc-pVTZ-PP, (8) Def2-TZVP, (9) Def2-TZVPP, (10) Def2-QZVP and (11) Def2-QZVPP, page S-55.

Figure S-24. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in CH_3^+. This plot includes all data, computed by HF, B3LYP, B3PW91 and BLYP methods and different basis sets. Sky blue circles and orange circles represent NICS values which are different from the other data, page S-56.

Figure S-25. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in CH_3^-. This plot includes all data, computed by HF, B3LYP, B3PW91 and BLYP methods and different basis sets, page S-56.

Figure S-26. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in $C_4H_4^{2+}$. This plot includes all data, computed by HF, B3LYP, B3PW91 and BLYP methods and different basis sets. Orange circles represent NICS values which are different from the other data, page S-57.

Figure S-27. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in C_4H_4. This plot includes all data, computed by HF, B3LYP, B3PW91 and BLYP methods and different basis sets, page S-57.

Figure S-28. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in $C_5H_5^+$. This plot includes all data, computed by HF, B3LYP, B3PW91 and BLYP methods and different basis sets, page S-58.

Figure S-29. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in $C_5H_5^-$. This plot includes all data, computed by HF, B3LYP, B3PW91 and BLYP methods and different basis sets. Sky blue circles and orange circles represent NICS values which are different from the other data, page S-58.

Figure S-30. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in C_6H_6. This plot includes all data, computed by HF, B3LYP, B3PW91 and BLYP methods and different basis sets. Orange circles represent NICS values which are different from the other data, page S-59.

Figure S-31. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in $C_7H_7^+$. This plot includes all data, computed by HF, B3LYP, B3PW91 and

BLYP methods and different basis sets. Orange circles represent NICS values which are different from the other data, page S-59.

Figure S-32. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in $C_8H_8^{2+}$. This plot includes all data, computed by HF, B3LYP, B3PW91 and BLYP methods and different basis sets. Orange circles represent NICS values which are different from the other data, page S-60.

Figure S-33. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in $C_8H_8^{2-}$. This plot includes all data, computed by HF, B3LYP, B3PW91 and BLYP methods and different basis sets. Orange circles represent NICS values which are different from the other data, page S-60.

Figure S-34. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in $C_9H_9^-$. This plot includes all data, computed by HF, B3LYP, B3PW91 and BLYP methods and different basis sets. Orange circles represent NICS values which are different from the other data, page S-61.

Figure S-35. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in Li_3^+. This plot includes all data, computed by B3LYP and BP86 and M06 methods and different basis sets. Sky blue circles and orange circles represent NICS values which are different from the other data, page S-61.

Figure S-36. $NICS(1)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in Cu_3^+. This plot includes all data, computed by B3LYP and BP86 and M06 methods and different basis sets. Sky blue circles and orange circles represent NICS values which are different from the other data, page S-62.

Figure S-37. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in Ag_3^+. This plot includes all data, computed by B3LYP and BP86 and M06 methods and different basis sets. Sky blue circles and orange circles represent NICS values which are different from the other data, page S-62.

Figure S-38. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in Au_3^+. This plot includes all data, computed by B3LYP and BP86 and M06 methods and different basis sets. Sky blue circles and orange circles represent NICS values which are different from the other data, page S-63.

Figure S-39. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in Sc_3^-. This plot includes all data, computed by B3LYP and BP86 and M06 methods and different basis sets. Sky blue circles and orange circles represent NICS values which are different from the other data, page S-63.

Figure S-40. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in Y_3^-. This plot includes all data, computed by B3LYP and BP86 and M06 methods and different basis sets, page S-64.

Figure S-41. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in La_3^-. This plot includes all data, computed by B3LYP and BP86 and M06 methods and different basis sets, page S-64.

Figure S-42. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in Al_4^{2-}. This plot includes all data, computed by B3LYP and BP86 and M06 methods and different basis sets, page S-65.

Figure S-43. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in Ga_4^{2-}. This plot includes all data, computed by B3LYP and BP86 and M06 methods and different basis sets, page S-65.

Figure S-44. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in Cu_4^{2-}. This plot includes all data, computed by B3LYP and BP86 and M06 methods and different basis sets. Sky blue circles and orange circles represent NICS values which are different from the other data, page S-66.

Figure S-45. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in Ag_4^{2-}. This plot includes all data, computed by B3LYP and BP86 and M06 methods and different basis sets, page S-66.

Figure S-46. $NICS(0)_{iso}$, dark blue circles, and $NICS(0)_{zz}$, red circle, in ppm versus bond length in Å in Au_4^{2-}. This plot includes all data, computed by B3LYP and BP86 and M06 methods and different basis sets. Orange circles represent NICS values which are different from the other data, page S-67.

Figure S-47A. NICS (0) values of Li_3^+ at different levels of theory. Numbers 1 to 8 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Lanl2DZ, (2) DZVP (DFT orbital), (3) Def2-TZVP, (4) Def2-TZVPP, (5) Def2-QZVP, (6) Def2-QZVPP, (7) 6-311G(d) and (8) 6-311+G(d) , page S-68.

Figure S-47B. NICS (1) values of Li_3^+ at different levels of theory. Numbers 1 to 8 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Lanl2DZ, (2) DZVP (DFT orbital), (3) Def2-TZVP, (4) Def2-TZVPP, (5) Def2-QZVP, (6) Def2-QZVPP, (7) 6-311G(d) and (8) 6-311+G(d) , page S-68.

Figure S-48A. NICS (0) values of Cu_3^+ at different levels of theory. Numbers 1 to 17 on the horizontal axis denote different basis sets which are employed for computation of NICS

values in geometry of molecule optimized by Aug-cc-pVQZ basis set, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) Lanl2TZ, (5) Lanl2TZ(f), (6) DZVP(DFT orbital), (7) cc-pVDZ-PP, (8) cc-pVTZ-PP, (9) Def2-TZVP, (10) Def2-TZVPP, (11) Def2-QZVP, (12) Def2-QZVPP, (13) 6-311G(d), (14) 6-311+G(d), (15) Aug-cc-pVDZ, (16) Aug-cc-pVTZ and (17) Aug-cc-pVQZ, page S-69.

Figure S-48B. NICS (1) values of Cu_3^+ at different levels of theory. Numbers 1 to 17 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Aug-cc-pVQZ basis set, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) Lanl2TZ, (5) Lanl2TZ(f), (6) DZVP(DFT orbital), (7) cc-pVDZ-PP, (8) cc-pVTZ-PP, (9) Def2-TZVP, (10) Def2-TZVPP, (11) Def2-QZVP, (12) Def2-QZVPP, (13) 6-311G(d), (14) 6-311+G(d), (15) Aug-cc-pVDZ, (16) Aug-cc-pVTZ and (17) Aug-cc-pVQZ, page S-69.

Figure S-49A. NICS (0) values of Ag_3^+ at different levels of theory. Numbers 1 to 14 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) Lanl2TZ, (5) Lanl2TZ(f), (6) DZVP(DFT orbital), (7) cc-pVDZ-PP, (8) cc-pVTZ-PP, (9) Def2-TZVP, (10) Def2-TZVPP, (11) Def2-QZVP and (12) Def2-QZVPP, page S-70.

Figure S-49B. NICS (1) values of Ag_3^+ at different levels of theory. Numbers 1 to 12 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) Lanl2TZ, (5) Lanl2TZ(f), (6) DZVP(DFT orbital), (7) cc-pVDZ-PP, (8) cc-pVTZ-PP, (9) Def2-TZVP, (10) Def2-TZVPP, (11) Def2-QZVP and (12) Def2-QZVPP, page S-70.

Figure S-50A. NICS (0) values of Au_3^+ at different levels of theory. Numbers 1 to 14 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) Lanl2TZ, (5) Lanl2TZ(f), (6) cc-pVDZ-PP, (7) cc-pVTZ-PP, (8) Def2-TZVP, (9) Def2-TZVPP, (10) Def2-QZVP and (11) Def2-QZVPP. At BP86/Aug-cc-pVTZ-PP levels of theory Self Consistent Field calculations did not converge, page S-71.

Figure S-50B. NICS (1) values of Au_3^+ at different levels of theory. Numbers 1 to 14 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) Lanl2TZ, (5) Lanl2TZ(f), (6) cc-pVDZ-PP, (7) cc-pVTZ-PP, (8) Def2-TZVP, (9) Def2-TZVPP, (10) Def2-QZVP and (11) Def2-QZVPP.
At BP86/Aug-cc-pVTZ-PP level of theory Self Consistent Field calculations did not converge, page S-71.

Figure S-51A. NICS (0) values of Sc_3^- at different levels of theory. Numbers 1 to 12 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Aug-cc-pVQZ basis set, (1) Lanl2DZ, (2) Lanl2TZ, (3) Lanl2TZ(f), (4) Def2-TZVP, (5) Def2-TZVPP, (6) Def2-QZVP, (7) Def2-QZVPP, (8) 6-311G(d), (9) 6-311+G(d), (10) Aug-cc-pVDZ, (11), Aug-cc-pVTZ and (12) Aug-cc-pVQZ, page S-72.

Figure S-51B. NICS (1) values of Sc_3^- at different levels of theory. Numbers 1 to 12 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Aug-cc-pVQZ basis set, (1) Lanl2DZ, (2) Lanl2TZ, (3) Lanl2TZ(f), (4) Def2-TZVP, (5) Def2-TZVPP, (6) Def2-QZVP, (7) Def2-QZVPP, (8) 6-311G(d), (9) 6-311+G(d), (10) Aug-cc-pVDZ, (11), Aug-cc-pVTZ and (12) Aug-cc-pVQZ, page S-72.

Figure S-52A. NICS (0) values of Y_3^- at different levels of theory. Numbers 1 to 14 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Lanl2DZ, (2) Lanl2TZ, (3) Lanl2TZ(f), (4) DZVP(DFT orbital), (5) Def2-TZVP, (6) Def2-TZVPP, (7) Def2-QZVP and (8) Def2-QZVPP, page S-73.

Figure S-52B. NICS (1) values of Y_3^- at different levels of theory. Numbers 1 to 14 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Lanl2DZ, (2) Lanl2TZ, (3) Lanl2TZ(f), (4) DZVP(DFT orbital), (5) Def2-TZVP, (6) Def2-TZVPP, (7) Def2-QZVP and (8) Def2-QZVPP, page S-73.

Figure S-53A. NICS (0) values of La_3^- at different levels of theory. Numbers 1 to 9 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Lanl2DZ, (2) Lanl2TZ, (3) Lanl2TZ(f), (4) Def2-TZVP, (5) Def2-TZVPP, (6) Def2-QZVP, (7) Def2-QZVPP, page S-74.

Figure S-53B. NICS (1) values of La_3^- at different levels of theory. Numbers 1 to 9 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Lanl2DZ, (2) Lanl2TZ, (3) Lanl2TZ(f), (4) Def2-TZVP, (5) Def2-TZVPP, (6) Def2-QZVP, (7) Def2-QZVPP, page S-74.

Figure S-54A. NICS (0) values of Al_4^{2-} at different levels of theory. Numbers 1 to 8 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Lanl2DZ, (2) DZVP(DFT orbital), (3) Def2-TZVP, (4) Def2-TZVPP, (5) Def2-QZVP and (6) Def2-QZVPP, (7) 6-311G(d) and (8) 6-311+G(d) , page S-75.

Figure S-54B. NICS (1) values of Al_4^{2-} at different levels of theory. Numbers 1 to 8 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Lanl2DZ, (2) DZVP(DFT orbital), (3) Def2-TZVP, (4) Def2-TZVPP, (5) Def2-QZVP and (6) Def2-QZVPP, (7) 6-311G(d) and (8) 6-311+G(d) , page S-75.

Figure S-55A. NICS (0) values of Ga_4^{2-} at different levels of theory. Numbers 1 to 12 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) DZVP(DFT orbital), (5) cc-pVDZ-PP, (6) cc-pVTZ-PP, (7) Def2-TZVP, (8) Def2-TZVPP, (9) Def2-QZVP, (10) Def2-QZVPP, (11) 6-311G(d) and (12) 6-311+G(d) , page S-76.

Figure S-55B. NICS (1) values of Ga_4^{2-} at different levels of theory. Numbers 1 to 12 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) DZVP(DFT orbital), (5) cc-pVDZ-PP, (6) cc-pVTZ-PP, (7) Def2-TZVP, (8) Def2-TZVPP, (9) Def2-QZVP, (10) Def2-QZVPP, (11) 6-311G(d) and (12) 6-311+G(d), page S-76.

Figure S-56A. NICS (0) values of Cu_4^{2-} at different levels of theory. Numbers 1 to 16 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) Lanl2TZ, (5) Lanl2TZ(f), (6) DZVP(DFT orbital), (7) cc-pVDZ-PP, (8) cc-pVTZ-PP, (9) Def2-TZVP, (10) Def2-TZVPP, (11) Def2-QZVP, (12) Def2-QZVPP, (13) 6-311G(d), (14) 6-311+G(d), (15) Aug-cc-pVDZ and (16) Aug-cc-pVTZ.
At M06/Aug-cc-pVTZ-PP, BP86/ cc-pVDZ-PP and B3LYP/cc-pVDZ-PP levels of theory Self Consistent Field calculations did not converge, page S-77.

Figure S-56B. NICS (1) values of Cu_4^{2-} at different levels of theory. Numbers 1 to 16 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) Lanl2TZ, (5) Lanl2TZ(f), (6) DZVP(DFT orbital), (7) cc-pVDZ-PP, (8) cc-pVTZ-PP, (9) Def2-TZVP, (10) Def2-TZVPP, (11) Def2-QZVP, (12) Def2-QZVPP, (13) 6-311G(d), (14) 6-311+G(d), (15) Aug-cc-pVDZ and (16) Aug-cc-pVTZ.
At M06/Aug-cc-pVTZ-PP, BP86/ cc-pVDZ-PP and B3LYP/cc-pVDZ-PP levels of theory Self Consistent Field calculations did not converge, page S-77.

Figure S-57A. NICS (0) values of Ag_4^{2-} at different levels of theory. Numbers 1 to 12 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) Lanl2TZ, (5) Lanl2TZ(f), (6) DZVP(DFT orbital),

(7) cc-pVDZ-PP, (8) cc-pVTZ-PP, (9) Def2-TZVP, (10) Def2-TZVPP, (11) Def2-QZVP and (12) Def2-QZVPP, page S-78.

Figure S-57B. NICS (1) values of Ag_4^{2-} at different levels of theory. Numbers 1 to 12 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) Lanl2TZ, (5) Lanl2TZ(f), (6) DZVP(DFT orbital), (7) cc-pVDZ-PP, (8) cc-pVTZ-PP, (9) Def2-TZVP, (10) Def2-TZVPP, (11) Def2-QZVP and (12) Def2-QZVPP, page S-78.

Figure S-58A. NICS (0) values of Au_4^{2-} at different levels of theory. Numbers 1 to 11 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) Lanl2TZ, (5) Lanl2TZ(f), (6) cc-pVDZ-PP, (7) cc-pVTZ-PP, (8) Def2-TZVP, (9) Def2-TZVPP, (10) Def2-QZVP and (11) Def2-QZVPP, page S-79.

Figure S-58B. NICS (1) values of Au_4^{2-} at different levels of theory. Numbers 1 to 11 on the horizontal axis denote different basis sets which are employed for computation of NICS values in geometry of molecule optimized by Def2-QZVPP basis set, (1) Aug-cc-pVDZ-PP, (2) Aug-cc-pVTZ-PP, (3) Lanl2DZ, (4) Lanl2TZ, (5) Lanl2TZ(f), (6) cc-pVDZ-PP, (7) cc-pVTZ-PP, (8) Def2-TZVP, (9) Def2-TZVPP, (10) Def2-QZVP and (11) Def2-QZVPP, page S-79.

Reference for Basis sets. see page S-80.

Table S-1

Li_3^+		BP86			B3LYP			M06		
Basis sets	Number of basis functions	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)
Lanl2DZ	27	-11.30 *-9.19*	-7.05 *-7.84*	-1.65 *-4.28*	-11.26 *-9.05*	-7.04 *-7.80*	-1.63 *-4.27*	-11.26 *-9.70*	-7.01 *-8.10*	-1.72 *-4.42*
DZVP(DFT orbital)	33	-12.21 *-10.91*	-7.71 *-9.07*	-2.03 *-4.92*	-12.35 *-11.05*	-7.69 *-9.17*	-1.96 *-4.93*	-11.85 *-10.52*	-7.69 *-8.80*	-2.15 *-4.86*
Def2-TZVP	42	-10.82 *-8.90*	-6.85 *-7.69*	-1.68 *-4.37*	-10.66 *-8.63*	-6.73 *-7.54*	-1.61 *-4.30*	-10.94 *-9.54*	-6.96 *-8.12*	-1.78 *-4.64*
Def2-TZVPP	57	-11.14 *-9.09*	-6.89 *-7.62*	-1.77 *-4.19*	-11.05 *-8.86*	-6.76 *-7.48*	-1.67 *-4.10*	-11.38 *-9.96*	-7.02 *-8.22*	-1.82 *-4.52*
Def2-QZVP	105	-11.16 *-8.95*	-6.84 *-7.42*	-1.74 *-3.94*	***-11.12*** *-8.81*	***-6.75*** *-7.32*	***-1.69*** *-3.88*	-11.39 *-10.33*	-7.01 *-8.37*	-1.89 *-4.49*
Def2-QZVPP	105	-11.16 *-8.95*	-6.84 *-7.42*	-1.74 *-3.94*	-11.12 *-8.81*	-6.75 *-7.32*	-1.69 *-3.88*	-11.39 *-10.33*	-7.01 *-8.37*	-1.89 *-4.49*
6-311G(d)	54	-11.21 *-9.02*	-6.93 *-7.49*	-1.72 *-4.05*	-11.07 *-8.74*	-6.79 *-7.32*	-1.61 *-3.96*	-11.41 *-9.72*	-7.00 *-7.97*	-1.70 *-4.31*
6-311+G(d)	66	-11.21 *-9.03*	-6.94 *-7.49*	-1.72 *-4.04*	-11.08 *-8.75*	-6.79 *-7.32*	-1.61 *-3.96*	-11.44 *-9.77*	-7.01 *-6.59*	-1.71 *-0.46*

Table S-2

Cu_3^+		BP86			B3LYP			M06		
Basis sets	Number of basis functions	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)
Aug-cc-pVDZ-PP	162	-42.60 *-28.58*	-17.07 *-28.16*	-2.67 *-14.18*	-34.86 *-16.26*	-14.47 *-23.34*	-2.37 *-13.24*	-34.55 *-14.78*	***-14.15*** *-22.94*	***-2.09*** *-13.12*
Aug-cc-pVTZ-PP	264	-42.27 *-28.32*	-16.93 *-28.29*	-2.65 *-14.35*	-34.17 *-15.70*	-14.14 *-23.19*	-2.28 *-13.28*	-34.55 *-15.55*	-14.22 *-23.34*	2.14 *-13.32*
Lanl2DZ	66	-32.507 *-13.07*	-13.79 *-21.78*	-1.99 *-13.19*	-28.27 *-7.46*	-12.31 *-18.98*	-1.83 *-12.42*	-29.07 *-7.45*	-12.22 *-19.31*	-1.57 *-12.45*
Lanl2TZ	105	-36.00 *-18.53*	-14.76 *-23.82*	-2.15 *-13.59*	-30.50 *-10.33*	-12.98 *-20.36*	-1.96 *-12.79*	-30.91 *-10.09*	-12.70 *-20.43*	-1.69 *-12.76*
Lanl2TZ(f)	126	-35.99 *-18.47*	-14.75 *-23.79*	-2.15 *-13.58*	-30.51 *-10.33*	-12.98 *-20.36*	-1.96 *-12.78*	-30.94 *-10.07*	-12.70 *-20.44*	-1.68 *-12.75*
DZVP(DFT orbital)	72	-33.07 *-15.01*	-15.40 *-24.10*	-2.72 *-13.68*	-28.29 *-8.25*	-13.56 *-20.67*	-2.49 *-12.88*	-29.75 *-8.80*	-14.14 *-21.43*	-2.47 *-13.06*
cc-pVDZ-PP	114	-43.52 *-30.52*	-17.23 *-29.29*	-2.91 *-14.62*	-34.91 *-16.72*	-14.36 *-23.89*	-2.52 *-13.52*	-34.60 *-15.39*	-14.08 *-23.49*	-2.29 *-13.43*
cc-pVTZ-PP	189	-41.66 *-27.33*	-17.09 *-28.03*	-2.68 *-14.32*	-33.66 *-14.80*	-14.27 *-22.92*	-2.30 *-13.23*	-33.96 *-14.40*	-14.34 *-22.94*	- 2.14 *-13.22*
Def2-TZVP	135	-33.63 *-14.53*	-13.94 *-22.08*	-1.66 *-12.77*	-28.13 *-6.92*	-12.09 *-18.67*	-1.52 *-12.05*	-28.94 *-7.06*	- 12.17 *-19.09*	-1.38 *-12.15*
Def2-TZVPP	192	-34.02 *-15.13*	-14.17 *-22.29*	-1.69 *-12.84*	-28.36 *-7.25*	-12.25 *-18.79*	-1.59 *-12.09*	-29.08 *-7.25*	-12.34 *-19.20*	-1.34 *-12.20*
Def2-QZVP	252	-34.19 *-15.20*	-13.98 *-22.42*	-2.09 *-12.86*	-28.41 *-7.17*	-12.09 *-18.89*	-1.92 -12.11	-29.11 *-7.12*	-12.28 *-19.26*	-1.80 *-12.21*
Def2-QZVPP	300	-34.02 *-15.13*	-14.17 *-22.29*	-1.69 *-12.84*	-28.36 *-7.25*	-12.25 *-18.79*	-1.59 -12.09	-29.06 *-6.91*	-12.16 *-19.16*	-1.71 *-12.18*
6-311G(d)	138	-30.26 *-9.80*	-8.59 *-14.79*	-0.94 *-8.47*	-23.98 *-2.91*	-7.98 *-14.42*	-1.13 *-10.36*	-23.47 *+5.06*	-7.69 *-14.81*	-0.83 *-10.75*
6-311+G(d)	174	-33.71 *-13.86*	-14.20 *-22.51*	-1.93 *-13.01*	-28.07 *-6.22*	-12.27 *-18.98*	-1.77 *-12.22*	-28.95 *-6.57*	-12.51 *-19.42*	-1.73 *-12.32*
Aug-cc-pVDZ	129	-34.67 *-16.81*	-14.4 *-22.87*	-1.96 *-12.92*	-28.56 *-7.96*	-12.34 *-19.11*	-1.80 *-12.16*	-29.42 *-8.08*	-12.49 *-19.51*	-1.68 *-12.29*
Aug-cc-pVTZ	279	-34.38 *-15.19*	-14.1 *-22.66*	-20.01 *-12.90*	-28.5 *-7.12*	-12.2 *-19.08*	-1.87 *-12.16*	-29.49 *-7.56*	-12.45 *-19.58*	-1.75 *-12.28*
Aug-cc-pVQZ	420	-34.3 *-15.11*	-14 *-22.56*	-20.24 *-12.88*	-28.47 *-7.1*	-12.12 *-19.01*	-1.89 *-12.15*	-29.15 *-7.08*	-12.25 *-19.34*	-1.71 *-12.23*

Table S-3

Ag_3^+		BP86			B3LYP			M06		
Basis sets	Number of basis functions	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)
Aug-cc-pVDZ-PP	162	-28.43 *-1.90*	-13.49 *-18.18*	-2.42 *-15.07*	-25.91 *+0.07*	-12.58 *-16.36*	-2.37 *-14.37*	-25.88 *+0.27*	-12.74 *-16.23*	-2.31 *-14.30*
Aug-cc-pVTZ-PP	264	-27.61 *-0.61*	-12.82 *-17.45*	-2.29 *-14.85*	-25.15 *+1.24*	-11.97 *-15.69*	-2.25 *-14.17*	-25.88 *+0.97*	-12.74 *-15.88*	-2.31 *-14.24*
Lanl2DZ	66	-25.36 *+1.12*	-12.51 *-16.08*	-2.04 *-14.59*	-23.51 *+2.38*	-11.85 *-14.65*	-2.06 *-13.96*	-24.02 *+2.04*	-12.06 *-14.94*	-1.99 *-14.02*
Lanl2TZ	105	-26.09 *-0.01*	-12.73 *-16.55*	-2.13 *-14.63*	-24.09 *+1.60*	-12.01 *-15.03*	-2.12 *-14.01*	-24.38 *+1.32*	-12.14 *-15.09*	-2.03 *-13.99*
Lanl2TZ(f)	126	-26.19 *-0.04*	-12.77 *-16.61*	-2.12 *-14.64*	-24.14 *+1.54*	-12.04 *-15.06*	-2.12 *-14.01*	-24.40 *+1.32*	-12.14 *-15.10*	-2.02 *-13.98*
DZVP(DFT orbital)	108	-22.61 *+4.28*	-11.82 *-14.08*	-2.47 *-14.13*	-20.98 *+5.11*	-11.16 *-12.75*	-2.42 *-13.51*	-22.45 *+4.08*	-11.90 *-13.69*	-2.49 *-13.83*
cc-pVDZ-PP	114	-27.83 *-1.77*	-13.29 *-17.72*	-2.43 *-14.93*	-25.25 *+0.52*	-12.31 *-15.79*	-2.34 *-14.18*	-25.37 *+0.43*	-12.46 *-15.76*	-2.27 *-14.15*
cc-pVTZ-PP	189	-27.67 *-1.29*	-13.05 *-17.59*	-2.40 *-14.92*	-25.21 *+0.68*	-12.14 *-15.76*	-2.32 *-14.20*	-25.27 *+0.47*	-12.43 *-15.82*	-2.21 *-14.18*
Def2-TZVP	120	-26.98 *-0.72*	-13.02 *-17.17*	-2.22 *-14.72*	-24.63 *+1.15*	-12.10 *-15.44*	-2.15 *-14.03*	-24.95 *+0.87*	-12.31 *-15.52*	-2.12 *-14.01*
Def2-TZVPP	168	-27.14 *-0.75*	-13.03 *-17.28*	-2.18 *-14.75*	-24.80 *+1.07*	-12.14 *-15.58*	-2.13 *-14.08*	-25.01 *+0.84*	-12.29 *-15.56*	-2.09 *-14.01*
Def2-QZVP	216	-27.45 *-0.85*	-12.70 *-17.33*	-2.34 *-14.79*	-25.07 *+0.90*	-11.90 *-15.61*	-2.29 *-14.12*	- 25.08 *+0.8*	-12.13 *-15.60*	-2.19 *-14.10*
Def2-QZVPP	264	-27.46 *-0.73*	-12.70 *-17.23*	-2.29 *-14.74*	-25.09 *+1.01*	-11.91 *-15.55*	-2.27 *-14.10*	-24.98 *+1.01*	-12.09 *-15.43*	-2.18 *-14.03*

Table S-4

Au_3^+		BP86			B3LYP			M06		
Basis sets	Number of basis functions	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)
Aug-cc-pVDZ-PP	162	-32.99 *-0.23*	-13.45 *-18.67*	-1.83 *-16.40*	-30.21 *+2.67*	-12.63 *-17.10*	-1.84 *-16.01*	-28.74 *+3.02*	-12.55 *-16.36*	-1.85 *-15.72*
Aug-cc-pVTZ-PP	264	*	*	*	-33.44 *-1.80*	-14.34 *-19.83*	-2.46 *-16.94*	-31.51 *-0.41*	-14.03 *-18.57*	-2.27 *-16.50*
Lanl2DZ	66	-35.89 *-6.10*	-15.94 *-21.86*	-2.78 *-17.96*	-33.07 *-3.25*	-14.97 *-20.08*	-2.70 *-17.40*	-32.05 *-3.26*	-15.01 *-19.69*	-2.80 *-17.23*
Lanl2TZ	105	-36.36 *-7.12*	-16.15 *-22.39*	-3.02 *-17.90*	-33.55 *-3.82*	-15.15 *-20.48*	-2.89 *-17.39*	-32.13 *-3.54*	-15.09 *-19.85*	-2.90 *-17.15*
Lanl2TZ(f)	126	-36.35 *-6.24*	-16.08 *-22.20*	-2.96 *-17.85*	-33.59 *-3.18*	-15.11 *-20.40*	-2.85 *-17.38*	-32.03 *-2.90*	-15.00 *-19.73*	-2.84 *-17.12*
cc-pVDZ-PP	114	-35.33 *-4.76*	-15.43 *-21.15*	-2.66 *-17.40*	-32.33 *-1.32*	-14.37 *-19.24*	-2.57 *-16.87*	-30.91 *-1.06*	-14.19 *-18.57*	-2.54 *-16.60*
cc-pVTZ-PP	189	-34.88 *-2.30*	-14.67 *-20.61*	-2.45 *-17.08*	-32.06 *+0.59*	-13.82 *-18.93*	-2.45 *-16.69*	-30.33 *+1.46*	- 13.67 *-17.97*	-2.30 *-16.35*
Def2-TZVP	120	-32.23 *+0.92*	-13.31 *-18.46*	-2.14 *-16.44*	-29.94 *+2.90*	-12.71 *-17.27*	-2.17 *-16.18*	-28.72 *+2.77*	-12.66 *-16.79*	- 2.15 *-15.94*
Def2-TZVPP	168	-32.52 *+1.06*	-13.15 *-18.52*	-2.05 *-16.42*	-30.20 *+3.07*	-12.60 *-17.35*	-2.10 *-16.20*	-28.82 *+3.10*	-12.51 *- 16.74*	-2.08 *-15.91*
Def2-QZVP	216	-34.39 *-1.56*	-14.19 *-19.91*	-2.29 *16.85*	-31.80 *+0.93*	-13.50 *-18.50*	-2.32 *-16.54*	-30.21 *+1.33*	-13.36 *-17.72*	-2.20 *-16.20*
Def2-QZVPP	264	-34.50 *-1.39*	-14.35 *-20.16*	-2.33 *-16.92*	-31.85 *+1.15*	-13.63 *-18.68*	-2.35 *-16.58*	-30.14 *+1.92*	-13.43 *-17.79*	-2.23 *-16.23*

*At this level of theory Self Consistent Field (SCF) calculations did not converge.

Table S-5

Sc_3^-		BP86			B3LYP			M06		
Basis sets	Number of basis functions	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)
Lanl2DZ	66	-15.88 *-50.17*	-11.25 *+15.73*	-2.06 *+29.52*	-27.82 *-49.98*	-18.49 *+16.26*	-4.66 *+29.64*	-38.59 *-62.91*	-32.81 *+35.26*	-10.03 *+49.21*
Lanl2TZ	105	-9.05 *-42.07*	-8.32 *+14.50*	-2.17 *+26.52*	-17.12 *-35.84*	-14.34 *+15.42*	-4.83 *+25.07*	-27.95 *-45.88*	-26.81 *+35.50*	-10.01 *+45.28*
Lanl2TZ(f)	126	-11.58 *-42.58*	-9.09 *+14.62*	-2.19 *+26.65*	-19.97 *-37.05*	-15.36 *+15.08*	-4.98 *+24.97*	-34.45 *-48.02*	-28.48 *+34.54*	-10.02 *+44.78*
Def2-TZVP	135	-9.16 *-50.32*	-14.12 *+9.80*	-6.62 *+25.17*	-17.58 *-44.94*	-21.84 *+8.32*	-10.21 *+21.80*	-20.56 *-44.69*	-33.10 *+16.39*	-16.66 *+28.56*
Def2-TZVPP	192	-14.03 *-51.15*	-15.28 *+10.81*	-5.60 *+25.66*	-22.64 *-46.68*	-22.93 *+9.01*	-9.23 *+22.30*	-20.70 *-47.19*	-32.30 *+16.93*	-15.01 *+28.87*
Def2-QZVP	252	-16.55 *-52.08*	-16.10 *+11.00*	-5.30 *+26.01*	-25.54 *-48.49*	-24.07 *+8.76*	-9.06 *+22.58*	-21.80 *-48.80*	-33.65 *+17.05*	-14.70 *+30.03*
Def2-QZVPP	279	-16.09 *-51.62*	-16.03 *+11.05*	-5.37 *+26.01*	-25.06 *-48.03*	-23.98 *+8.86*	-9.12 *+22.58*	-22.23 *-48.90*	-33.66 *+17.47*	-15 *+29.87*
6-311G(d)	138	-35.18 *-43.12*	-28.98 *+6.87*	-8.74 *+21.12*	-47.94 *-37.53*	-37.82 *+7.66*	-11.87 *+19.87*	-147.58 *-31.66*	-78.87 *+15.25*	-24.57 *+25.46*
6-311+G(d)	174	-15.89 *-51.92*	-15.61 *+10.43*	-5.18 *+25.67*	-25.07 *-48.13*	-23.29 *+8.75*	-8.67 *+22.59*	-22.18 *-49.22*	-33.58 *+15.96*	-14.67 *+29.29*
Aug-cc-pVDZ	129	-16.67 *-52.48*	-15.46 *+11.35*	-4.88 +26.17	-25.42 *-48.71*	-22.85 *+9.75*	-8.43 +23.23	-24.08 *-49.63*	-32.71 *+17.76*	-14.35 *+30.09*
Aug-cc-pVTZ	279	-16.25 *-51.7*	-15.88 *+11.01*	-5.45 +25.82	-25.06 *-47.97*	-23.67 *+8.79*	-9.15 *+22.30*	-22.58 *-47.65*	-33.18 *+17.02*	-15.04 *+29.20*
Aug-cc-pVQZ	420	-16.6 *-50.81*	-16.06 *+11.5*	-5.36 *+26.04*	-25.64 *-47.53*	-23.99 *+9.02*	-9.12 *+22.49*	-23.76 *-45.93*	-34.3 *+18*	-15.19 *+29.73*

Table S-6

Y_3^-		BP86			B3LYP			M06		
Basis sets	Number of basis functions	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)
Lanl2DZ	66	-11.98 *-22.60*	-14.43 *-0.29*	-6.50 *+12.39*	-13.13 *-18.52*	-16.72 *-0.40*	-8.26 *+10.11*	-11.40 *-11.31*	-20.29 *+5.65*	-11.38 *+14.62*
Lanl2TZ	105	-10.52 *-18.61*	-13.45 *+0.95*	-6.42 *+11.42*	-10.80 *-14.03*	-15.44 *+0.97*	-8.21 *+9.15*	-10.28 *-6.89*	-18.90 *+7.22*	-11.12 *+13.73*
Lanl2TZ(f)	126	-12.41 *-19.35*	-14.11 *+0.92*	-6.43 *+11.56*	-12.95 *-15.43*	-16.36 *+0.45*	-8.36 *+9.03*	-13.29 *-8.45*	-20.08 *+6.51*	-11.25 *+13.44*
DZVP (DFTorbital)	108	-6.79 *-16.46*	-11.22 *+5.07*	-6.48 *+15.34*	-7.15 *-12.63*	-13.62 *+3.63*	-8.61 *+11.89*	-6.72 *-6.89*	-18.08 *+6.41*	-12.56 *+12.76*
Def2-TZVP	120	-11.60 *-19.70*	-14.88 *-0.64*	-7.39 *+9.92*	-11.78 *-16.03*	-17.11 *-1.14*	-9.38 *+7.50*	-11.32 *-11.04*	-20.77 *+4.19*	-12.30 *+11.58*
Def2-TZVPP	168	-12.05 *-19.91*	-15.13 *- 0.71*	-7.37 *+9.88*	-12.22 *-16.34*	-17.36 *-1.32*	-9.46 *+7.38*	-12.07 *-11.67*	-21.12 *+3.71*	-12.48 *+11.59*
Def2-QZVP	216	-12.74 *-19.90*	-15.35 *-0.56*	-7.16 *+9.99*	-13.04 *-16.37*	-17.66 *-1.26*	-9.27 *+7.39*	-12.86 *-10.73*	-21.49 *+3.41*	-12.36 *+11.17*
Def2-QZVPP	243	-12.56 *-19.19*	-15.23 *-0.34*	-7.11 *+10.02*	-12.84 *-15.78*	-17.54 *-1.08*	-9.23 *+7.42*	-12.90 *-10.83*	-21.31 *+3.57*	-12.36 *+11.23*

Table S-7

La_3^-		BP86			B3LYP			M06		
Basis sets	Number of basis functions	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)
Lanl2DZ	66	-7.36 *-11.85*	-7.71 *+15.28*	-2.93 *+28.64*	-11.18 *-13.27*	-10.95 *+12.32*	-4.52 *+26.51*	-25.28 *+4.91*	-18.85 *+18.98*	-8.97 *+27.09*
Lanl2TZ	105	-7.70 *-11.51*	-7.99 *+14.15*	-2.96 *+26.95*	-11.04 *-11.80*	-11.00 *+11.48*	-4.63 *+24.44*	-26.38 *+8.49*	-18.14 *+20.08*	-7.99 *+25.91*
Lanl2TZ(f)	126	-10.51 *-9.75*	-8.41 *+17.17*	-2.30 *+29.27*	- 14.53 *-11.69*	-12.00 *+13.17*	-4.28 *+26.08*	-31.29 *+8.33*	-19.68 *+21.06*	-7.68 *+26.96*
Def2-TZVP	120	-11.08 *-10.50*	-10.13 *+13.67*	-3.70 *+25.08*	-14.78 *-11.84*	-13.69 *+9.67*	-5.79 *+21.47*	-27.72 *-0.66*	-20.69 *+14.25*	-9.33 *+22.73*
Def2-TZVPP	168	-15.90 *-11.91*	-13.69 *+10.30*	-5.57 *+22.01*	-12.07 *-9.94*	-10.09 *+14.72*	-3.34 *+25.79*	-29.06 *-1.84*	-20.52 *+14.09*	-9.02 *+22.88*
Def2-QZVP	216	-9.57 *-6.20*	-8.02 *+18.23*	-2.19 *+27.70*	-13.24 *-8.47*	-11.78 *+13.14*	-4.67 *+23.41*	-29.20 *-4.68*	-20.04 *+13.58*	-8.44 *+23.01*
Def2-QZVPP	243	-11.12 *-11.77*	-8.47 *+16.70*	-2.14 *+27.85*	-14.75 *-13.62*	-12.19 *+11.74*	-4.59 *+23.54*	-29.33 *-5.92*	-20.06 *+13.39*	-8.34 *+23.22*

Table S-8

Al_4^{2-}		BP86			B3LYP			M06		
Basis sets	Number of basis functions	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)
Lanl2DZ	32	-25.60 *-63.39*	-22.28 *-53.03*	-12.56 *-33.12*	-27.43 *-63.50*	-23.38 *-53.17*	-12.94 *-33.27*	-24.55 *-64.57*	-21.56 *-53.95*	-12.45 *-33.75*
DZVP (DFT orbital)	72	-31.26 *-66.69*	-25.81 *-55.80*	-13.68 *-34.47*	-33.55 *-67.09*	-27.16 *-56.12*	-14.19 *-34.68*	-33.65 *-65.86*	-26.96 *-55.20*	-13.93 *-34.23*
Def2-TZVP	148	-31.90 *-66.00*	-26.51 *-55.10*	-14.07 *-33.84*	-34.61 *-66.37*	-28.08 *-55.38*	-14.54 *-33.99*	-35.31 *-65.39*	-28.23 *-55.07*	-14.24 *-33.79*
Def2-TZVPP	168	-31.96 *-66.23*	-26.54 *-55.24*	-14.09 *-33.89*	-34.64 *-66.57*	-28.09 *-55.50*	-14.55 *-34.03*	-35.36 *-65.64*	-28.23 *-55.20*	-14.26 *-33.83*
Def2-QZVP	280	-33.30 *-66.35*	-26.94 *-55.28*	-14.35 *-33.99*	-36.24 *-66.56*	-28.57 *-55.41*	-14.91 *-34.09*	-35.90 *-63.55*	-27.95 *-53.45*	-14.66 *-33.22*
Def2-QZVPP	280	-33.30 *-66.35*	-26.94 *-55.28*	-14.35 *-33.99*	-36.24 *-66.56*	-28.57 *-55.41*	-14.91 *-34.09*	-35.90 *-63.55*	-27.95 *-53.45*	-14.66 *-33.22*
6-311G(d)	104	-30.65 *-65.98*	-25.46 *-55.15*	-13.83 *-34.19*	-32.77 *-66.18*	-26.69 *-55.27*	-14.32 *-34.30*	-33.09 *-65.53*	-26.55 *-54.50*	-14.12 *-33.83*
6-311+G(d)	120	-32.21 *-66.01*	-26.07 *-54.81*	-14.42 *-33.71*	-34.46 *-66.18*	-27.39 *-54.88*	-15.03 *-33.74*	-34.46 *-66.04*	-27.17 *-54.62*	-15.06 *-33.33*

Table S-9

Ga_4^{2-}		BP86			B3LYP			M06		
Basis sets	Number of basis functions	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)
Aug-cc-pVDZ-PP	128	-37.05 *-67.43*	-29.29 *-59.96*	-15.72 *-38.19*	-38.45 *-66.90*	-30.22 *-59.50*	-16.24 *-38.07*	-33.91 *-63.42*	-27.98 *-56.89*	-16.13 *-36.84*
Aug-cc-pVTZ-PP	220	-38.95 *-70.79*	-30.15 *-61.72*	-15.81 *-38.79*	-40.34 *-69.99*	-31.05 *-61.12*	-16.33 *-38.62*	-30.72 *-66.63*	-26.44 *-58.59*	-16.15 *-37.61*
Lanl2DZ	32	-25.19 *-64.32*	-22.39 *-53.62*	-12.73 *-33.32*	-26.65 *-64.35*	-23.28 *-53.75*	-13.11 *-33.49*	-26.27 *-64.30*	-22.64 *-53.73*	-12.66 *-33.60*
DZVP(DFT orbital)	108	-33.70 *-62.23*	-27.80 *-57.57*	-14.47 *-37.67*	-35.40 *-62.29*	-28.86 *-57.57*	-14.95 *-37.79*	-32.19 *-60.17*	-27.39 *-56.16*	-14.93 *-37.37*
cc-pVDZ-PP	92	-34.01 *-66.57*	-28.27 *-60.00*	-14.77 *-38.32*	-35.47 *-66.56*	-29.23 *-59.97*	-15.16 *-38.39*	-34.61 *-66.01*	-28.84 *-59.69*	-15.22 *-38.46*
cc-pVTZ-PP	156	-36.30 *-68.87*	-29.13 *-60.59*	-15.38 *-38.41*	-37.78 *-68.81*	-30.12 *-60.52*	-15.82 *-38.46*	-34.49 *-66.16*	-28.27 *-58.48*	-15.64 *-37.66*
Def2-TZVP	192	-33.61 *-63.46*	-27.62 *-57.73*	-14.47 *-37.14*	-35.38 *-63.76*	-28.76 *-57.89*	-14.93 *-37.29*	-34.86 *-63.68*	-28.56 *-57.82*	-15.13 *-37.34*
Def2-TZVPP	192	-33.61 *-63.46*	-27.62 *-57.73*	-14.47 *-37.14*	-35.38 *-63.76*	-28.76 *-57.89*	-14.93 *-37.29*	-34.86 *-63.68*	- 28.56 *-57.82*	-15.13 *-37.34*
Def2-QZVP	300	-34.91 *-63.39*	-28.12 *-57.60*	-14.75 *-37.27*	-36.76 *-63.57*	-29.27 *-57.63*	-15.23 *-37.36*	-34.01 *-61.48*	-27.76 *-55.91*	-15.23 *-36.68*
Def2-QZVPP	356	-34.93 *-63.39*	-28.13 *-57.61*	-14.76 *-37.28*	-36.77 *-63.58*	-29.28 *-57.64*	-15.24 *-37.37*	-34.04 *-61.53*	-27.78 *-55.95*	-15.24 *- 36.70*
6-311G(d)	176	-33.69 *-62.58*	-27.59 *-57.45*	-14.62 *-37.42*	-35.26 *-62.45*	-28.55 *-57.27*	-15.05 *-37.45*	-32.12 *-60.35*	-26.87 *-55.60*	-14.96 *-36.89*
6-311+G(d)	192	-42.40 *-76.86*	-32.17 *-67.62*	-15.95 *-41.90*	-39.18 *-63.39*	-29.86 *-57.68*	-15.12 *-37.29*	-31.44 *-57.68*	-26.39 *-53.40*	-15.15 *-35.51*

Table S-10

Cu_4^{2-}		BP86			B3LYP			M06		
Basis sets	Number of basis functions	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)
Aug-cc-pVDZ-PP	216	-27.43 *-36.09*	-15.38 *-33.59*	-6.28 *-22.21*	-19.86 *-25.75*	-11.90 *-29.13*	-5.53 *-21.61*	-18.67 *-20.88*	-11.28 *-26.25*	-5.42 *-20.63*
Aug-cc-pVTZ-PP	352	-26.03 *-34.68*	-14.55 *-32.68*	-5.80 *-21.79*	-18.17 *-24.10*	-10.80 *-28.01*	-4.98 *-21.16*	*	*	*
Lanl2DZ	88	-19.39 *-24.37*	-11.25 *-28.31*	-5.36 *-21.65*	-14.56 *-18.81*	-8.84 *-25.47*	-4.69 *-21.00*	- 14.96 *-16.29*	-9.14 *-24.17*	-5.08 *-20.58*
Lanl2TZ	140	-22.01 *-27.06*	-12.56 *-29.77*	-5.50 *-21.89*	-16.17 *-20.07*	-9.64 *-26.41*	-4.73 *-21.22*	-16.72 *-17.63*	-10.11 *-25.05*	-5.21 *-20.75*
Lanl2TZ(f)	168	-21.98 *-27.00*	-12.54 *-29.74*	-5.49 *-21.88*	-16.15 *-20.05*	- 9.63 *-26.40*	-4.73 *-21.22*	-16.70 *-17.70*	-10.09 *-25.03*	-5.20 *-20.74*
DZVP(DFT orbital)	96	-19.05 *-24.10*	-13.47 *-27.46*	-6.48 *-20.44*	-16.37 *-20.82*	-12.12 *-25.32*	-6.32 *-19.92*	-16.74 *-20.81*	-12.33 *-25.95*	-6.40 *-20.23*
cc-pVDZ-PP	154	*	*	*	*	*	*	-17.68 *- 24.16*	-10.70 *-28.60*	-5.71 *-21.65*
cc-pVTZ-PP	352	-24.83 *-34.18*	-14.52 *-33.07*	-5.85 *-22.07*	-17.57 *-24.24*	-10.88 *-28.35*	-5.06 *-21.26*	-16.94 *-21.59*	-10.64 *-26.92*	-5.09 *-20.82*
Def2-TZVP	180	-21.06 *-24.82*	-13.06 *-27.38*	-6.02 *-20.47*	-16.96 *-19.50*	-11.40 *-24.77*	-5.89 *-20.09*	-16.13 *- 17.66*	-10.93 *-24.05*	-5.85 *-20.01*
Def2-TZVPP	256	-20.00 *-24.92*	-12.19 *-27.69*	-5.68 *-20.66*	-15.53 *-19.41*	-10.26 *-25.04*	-5.50 *-20.30*	-14.54 *-17.39*	-9.64 *-24.31*	-5.44 *-20.25*
Def2-QZVP	336	-19.24 *-25.17*	-11.52 *-28.37*	-5.16 *-20.94*	-14.04 *-19.28*	-9.04 *-25.43*	-4.64 *-20.52*	- 13.71 *-16.42*	-8.98 *-24.20*	- 4.87 *-20.25*
Def2-QZVPP	400	-19.11 *-25.12*	-11.50 *-28.31*	-5.13 *-20.93*	-13.92 *-19.23*	-9.05 *-25.42*	-4.64 *-20.53*	-13.58 *- 16.34*	-8.86 *-23.98*	-4.81 *-20.19*
6-311G(d)	184	-9.84 *-19.15*	-5.27 *-18.88*	-3.67 *-12.94*	-13.91 *-11.56*	-8.58 *-20.28*	-5.09 *-16.98*	-13.60 *-10.21*	-8.12 *-19.47*	-4.86 *-16.51*
6-311+G(d)	232	-19.65 *-24.97*	-12.00 *-28.53*	-4.97 *-20.94*	-14.25 *-19.02*	-9.32 *-25.52*	-4.47 *-20.50*	-13.38 *-14.88*	-8.93 *-22.80*	-4.39 *-19.35*
Aug-cc-pVDZ	172	-19.81 *-26.47*	-11.67 *-28.6*	-5.29 *-20.94*	-14.37 *-20.07*	-9.11 *-25.61*	-4.91 *-20.61*	-13.68 *-17.89*	-8.86 *-24.59*	-4.89 *-20.37*
Aug-cc-pVTZ-PP	372	-19.82 *-25.76*	-11.68 *-28.68*	-5.09 *-20.89*	-14.28 *-19.56*	-9.12 *-25.77*	-4.62 *-20.59*	-12.8 *-14.63*	-8.23 *-22.74*	-4.43 *-19.48*

*****At these levels of theory Self Consistent Field (SCF) calculations did not converge.

Table S-11

Ag_4^{2-}		BP86			B3LYP			M06		
Basis sets	Number of basis functions	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)
Aug-cc-pVDZ-PP	216	-14.98 *-10.83*	-10.22 *-21.07*	-5.29 *-21.37*	-13.07 *-10.34*	-9.22 *-20.04*	-5.05 *-20.78*	-12.74 *-8.57*	-9.08 *- 18.99*	-5.01 *-20.38*
Aug-cc-pVTZ-PP	352	-14.34 *-9.61*	-9.72 *-20.31*	-5.03 *-21.04*	-12.46 *-9.29*	-8.74 *-19.40*	-4.82 *-20.53*	-11.95 *-9.00*	-8.70 *-19.65*	-5.01 *-20.94*
Lanl2DZ	88	-13.38 *-8.50*	-9.28 *-19.06*	-5.00 *-20.70*	-11.88 *-8.60*	-8.45 *-18.39*	-4.73 *-20.13*	-12.60 *-7.11*	-9.04 *-17.86*	- 5.10 *- 20.11*
Lanl2TZ	140	-14.13 *-9.84*	-9.72 *-20.08*	-5.00 *-21.05*	-12.35 *-9.35*	-8.73 *-19.06*	-4.73 *-20.41*	-12.91 *-7.90*	-9.28 *-18.36*	-5.23 *- 20.33*
Lanl2TZ(f)	168	-14.09 *-9.74*	-9.70 *-20.06*	-4.99 *-21.05*	-12.30 *-9.26*	-8.69 *-19.04*	-4.71 *-20.41*	-12.85 *-7.78*	-9.24 *-18.31*	-5.21 *-20.32*
DZVP(DFT orbital)	144	-12.37 *-9.11*	-9.74 *-18.86*	-6.01 *-20.42*	-11.39 *-9.04*	-9.24 *-17.83*	-5.94 *-19.61*	-11.30 *-7.80*	- 9.20 *-18.06*	-6.06 *-20.26*
cc-pVDZ-PP	152	-14.42 *-10.90*	-9.99 *-20.76*	-5.19 *-21.15*	-12.46 *-10.27*	-8.90 *-19.66*	-4.93 *-20.47*	-12.96 *-9.66*	-9.40 *-19.53*	- 5.18 *-20.61*
cc-pVTZ-PP	252	-14.45 *-10.70*	-10.12 *-20.89*	-5.18 *-21.22*	-12.58 *-10.24*	-9.08 *-19.87*	-4.91 *-20.61*	-12.71 *-9.63*	-9.32 *-19.76*	-5.18 *-20.85*
Def2-TZVP	160	-14.04 *-10.95*	-9.75 *-20.62*	-5.11 *-21.05*	-12.28 *-10.45*	-8.81 *-19.61*	-4.95 *-20.43*	-12.65 *-9.67*	-9.22 *-19.48*	- 5.21 *-20.70*
Def2-TZVPP	224	-14.00 *-10.83*	-9.69 *-20.66*	-5.07 *-21.09*	-12.27 *-10.43*	-8.77 *-19.70*	-4.92 *-20.50*	-12.57 *-9.51*	-9.14 *-19.49*	-5.16 *-20.74*
Def2-QZVP	288	-14.16 *-10.13*	-9.82 *-20.52*	-5.09 *-21.10*	-12.40 *-9.82*	-8.90 *-19.60*	-4.87 *-20.55*	-12.33 *-8.55*	-9.01 *-19.11*	-5.07 *-20.66*
Def2-QZVPP	352	-14.08 *-10.05*	-9.80 *-20.56*	-5.11 *-21.14*	-12.38 *-9.78*	-8.90 *-19.66*	-4.90 *-20.61*	-12.15 *-8.47*	-8.95 *-19.01*	-5.06 *-20.56*

Table S-12

Au_4^{2-}		BP86			B3LYP			M06		
Basis sets	Number of basis functions	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)	NICS(0)	NICS(1)	NICS(2)
Aug-cc-pVDZ-PP	216	-16.54 *-4.69*	-10.57 *-18.00*	-4.65 *-20.53*	-15.23 *-4.95*	-10.01 *-17.75*	-4.67 *-20.46*	- 14.05 *-4.28*	-9.47 *-16.74*	-4.56 *-20.02*
Aug-cc-pVTZ-PP	352	-19.45 *-9.84*	-12.58 *-21.55*	-5.60 *-22.32*	-18.06 *-9.93*	-11.96 *-21.23*	-5.61 *-22.26*	- 15.87 *-6*	-10.79 *-17.97*	-5.20 *-20.70*
Lanl2DZ	88	-17.46 *-5.27*	-11.69 *-17.58*	-5.25 *-20.55*	-16.19 *-5.63*	-11.10 *-17.38*	-5.25 *-20.41*	-16.42 *- 6.74*	-11.46 *-18.18*	-5.55 *-20.89*
Lanl2TZ	140	-18.75 *-6.85*	-12.44 *-18.91*	-5.45 *-21.08*	-17.30 *-6.78*	-11.74 *-18.55*	-5.44 *-21.00*	-16.94 *-7.76*	-11.76 *- 18.89*	-5.68 *-21.26*
Lanl2TZ(f)	168	-18.65 *-6.32*	-12.36 *-18.80*	-5.39 *-21.09*	-17.21 *-6.31*	-11.66 *-18.48*	-5.38 *-21.04*	-16.76 *-7.25*	-11.62 *-18.72*	-5.61 *-21.25*
cc-pVDZ-PP	152	-18.01 *-6.85*	-11.82 *-18.93*	-5.28 *-20.98*	-16.48 *-6.68*	-11.09 *-18.50*	-5.23 *-20.83*	-15.87 *-6.65*	-10.99 *-18.17*	-5.36 *-20.74*
cc-pVTZ-PP	252	-18.12 *-6.41*	-11.85 *-19.36*	-5.37 *-21.22*	-16.75 *-6.77*	-11.26 *-19.19*	-5.38 *-21.21*	-15.65 *- 5.81*	-10.75 *-17.85*	-5.27 *-20.60*
Def2-TZVP	160	-17.11 *-5.37*	-11.27 *-18.32*	-5.11 *-20.79*	-15.77 *-5.76*	-10.69 *-18.14*	-5.14 *-20.75*	-15.33 *-5.60*	-10.55 *-17.48*	-5.20 *-20.44*
Def2-TZVPP	224	-17.05 *-5.13*	-11.19 *-18.31*	-5.05 *-20.82*	-15.74 *-5.60*	-10.65 *-18.18*	-5.11 *-20.81*	-15.23 *-5.28*	-10.47 *-17.43*	-5.15 *-20.47*
Def2-QZVP	288	-17.59 *-5.67*	-11.56 *-18.95*	-5.19 *-21.18*	-16.28 *-6.04*	-11.00 *-18.79*	-5.22 *-21.19*	-15.25 *-5.38*	-10.52 *-17.55*	-5.08 *-20.44*
Def2-QZVPP	352	-17.73 *-6.19*	-11.61 *-19.27*	-5.19 *-21.22*	-16.44 *-6.56*	-11.05 *-19.10*	-5.22 *-21.25*	-15.17 *-5.69*	-10.53 *-17.85*	-5.12 *-20.58*

Table S-13

Li_3^+	BP86				B3LYP				M06			
	Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)	
Basis sets	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$
Lanl2DZ	0.02	-0.08	0.02	-0.03	0.02	-0.08	0.01	-0.03	0	0.01	0	0.01
DZVP(DFT orbital)	0.13	-0.03	0.05	0.01	0.12	-0.03	0.04	0	0.03	0	0	0
Def2-TZVP	0.01	-0.12	-0.01	-0.05	0.01	-0.14	-0.01	-0.06	0.01	-0.02	0	-0.01
Def2-TZVPP	0.02	-0.05	-0.01	-0.02	0.01	-0.05	-0.01	-0.03	-0.05	0.06	0.01	0.03
Def2-QZVP	0	0	0	0	0	0	0	0	0	0	0	0
Def2-QZVPP	0	0	0	0	0	0	0	0	0	0	0	0
6-311G(d)	0	-0.02	0	-0.01	0.01	-0.02	-0.01	-0.01	-0.04	0.13	0	0.08
6-311+G(d)	0.01	-0.02	0	0.29	0.01	-0.02	-0.01	0	-0.04	0.15	0.01	1.5

Table S-14

Cu_3^+	BP86				B3LYP				M06			
	Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)	
Basis sets	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$
Aug-cc-pVDZ-PP	-0.7	-0.28	-0.13	-0.36	-0.79	-0.16	-0.15	-0.46	-0.56	0.02	-0.08	-0.32
Aug-cc-pVTZ-PP	-1.35	-0.91	-0.34	-0.75	-1.34	-0.74	-0.36	-0.83	0.87	0.42	0.22	0.54
Lanl2DZ	0.513	0.12	0.12	0.32	0.06	0.01	0.02	0.04	-0.14	-0.02	-0.03	-0.1
Lanl2TZ	0.24	0.1	0.06	0.14	-0.31	-0.1	-0.09	-0.2	-0.19	-0.05	-0.06	-0.12
Lanl2TZ(f)	0.23	0.1	0.06	0.14	-0.3	-0.09	-0.08	-0.19	-0.21	-0.04	-0.06	-0.13
DZVP(DFT orbital)	1.06	0.13	0.31	0.72	0.69	-0.01	0.23	0.53	0.35	-0.04	0.11	0.25
cc-pVDZ-PP	-1.55	-0.92	-0.4	-0.88	-1.61	-0.79	-0.44	-1.02	-1.18	-0.44	-0.31	-0.75
cc-pVTZ-PP	-0.78	-0.5	-0.21	-0.44	-0.92	-0.48	-0.26	-0.58	-0.57	-0.24	-0.15	-0.36
Def2-TZVP	0.6	0.25	0.26	0.38	0.37	0.07	0.11	0.25	0.28	0.03	0.08	0.19
Def2-TZVPP	0.49	0.19	0.13	0.31	0.32	0.06	0.09	0.22	0.24	0.02	0.07	0.18
Def2-QZVP	0.19	0.07	0.05	0.11	0.09	0.02	0.03	0.06	0.07	-0.01	0.02	0.05
Def2-QZVPP	0.3	-0.05	-0.26	0.13	0.1	-0.21	-0.2	0.1	0.05	0	0.01	0.03
6-311G(d)	-1.21	0.94	-0.04	-0.48	-1.81	-4.66	-0.15	-0.93	-1.83	1.02	-0.2	-1.02
6-311+G(d)	0.23	0.09	0.06	0.13	0.13	0.02	0.03	0.08	0.12	0.01	0.03	0.08
Aug-cc-pVDZ	0.74	0.33	0.2	0.45	0.48	0.13	0.14	0.33	0.35	0.06	0.1	0.23
Aug-cc-pVTZ	-0.74	-0.27	-0.17	-0.43	0.69	0.11	0.17	0.45	0	0	0.01	0.01
Aug-cc-pVQZ	0	0	0	0	0	0	0	0	0	0	0	0

Table S-15

Ag_3^+	BP86				B3LYP				M06			
	Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)	
Basis sets	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$
Aug-cc-pVDZ-PP	0.08	-0.01	0.03	0.06	0.06	-0.02	0.02	0.05	-0.04	0.02	-0.02	-0.03
Aug-cc-pVTZ-PP	-0.12	0.01	-0.04	-0.07	-0.09	0.02	-0.03	-0.06	-0.79	0.03	-0.51	-0.05
Lanl2DZ	1.18	-0.09	0.37	0.87	0.89	-0.2	0.29	0.68	0.5	-0.17	0.16	0.38
Lanl2TZ	1.25	-0.07	0.43	0.9	0.87	-0.18	0.3	0.64	0.62	-0.21	0.21	0.45
Lanl2TZ(f)	1.18	-0.09	0.41	0.85	0.86	-0.2	0.29	0.63	0.6	-0.22	0.21	0.43
DZVP(DFT orbital)	2.94	-1.18	1.04	2.24	2.49	-1.43	0.89	1.94	1.81	-1.21	0.67	1.39
cc-pVDZ-PP	0.51	0.02	0.17	0.35	0.34	-0.05	0.1	0.24	0.14	-0.04	0.05	0.1
cc-pVTZ-PP	0.22	-0.01	0.06	0.15	0.15	-0.03	0.05	0.11	0.12	-0.04	0.03	0.09
Def2-TZVP	0.73	-0.03	0.25	0.51	0.52	-0.1	0.19	0.36	0.27	-0.1	0.09	0.19
Def2-TZVPP	0.47	-0.04	0.15	0.33	0.33	-0.08	0.11	0.23	0.17	-0.07	0.06	0.13
Def2-QZVP	0.04	0	0.01	0.03	0.03	-0.01	0.01	0.03	0	0	0	0
Def2-QZVPP	0	0	0	0	0	0	0	0	0	0	0	0

Table S-16

Au_3^+	BP86				B3LYP				M06			
	Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)	
Basis sets	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$
Aug-cc-pVDZ-PP	0.17	0.02	0.04	0.1	0.15	0	0.04	0.09	0.15	-0.01	0.03	0.09
Aug-cc-pVTZ-PP	-	-	-	-	-0.02	0	0	-0.01	-0.05	0	-0.01	-0.02
Lanl2DZ	2.06	1.14	0.6	1.32	1.76	0.86	0.52	1.14	1.23	0.56	0.38	0.8
Lanl2TZ	1.24	0.35	0.33	0.74	1.01	0.29	0.28	0.62	0.83	0.21	0.24	0.54
Lanl2TZ(f)	0.67	0.12	0.17	0.4	0.5	0.09	0.13	0.31	0.46	0.07	0.13	0.28
cc-pVDZ-PP	0.74	0.18	0.22	0.47	0.61	0.1	0.17	0.4	0.47	0.04	0.14	0.32
cc-pVTZ-PP	0.09	-0.01	0.02	0.05	0.11	-0.01	0.02	0.06	0.09	-0.03	0.02	0.06
Def2-TZVP	0.5	0.01	0.12	0.33	0.43	-0.04	0.1	0.28	0.3	-0.06	0.08	0.2
Def2-TZVPP	0.15	0	0.04	0.1	0.12	-0.02	0.03	0.08	0.09	-0.02	0.02	0.06
Def2-QZVP	0.11	0	0.03	0.06	0.07	-0.01	0.02	0.05	0.09	-0.02	0.02	0.05
Def2-QZVPP	0	0	0	0	0	0	0	0	0	0	0	0

Table S-17

Sc_3^-	BP86				B3LYP				M06			
	Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)	
Basis sets	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$
Lanl2DZ	0.01	-0.46	-0.11	-0.45	-0.17	-0.34	-0.21	-0.3	1.51	1.64	2.19	1.11
Lanl2TZ	0	-2.22	-0.46	-2.12	-0.71	-1.84	-0.92	-1.68	-1.07	-1.05	-1.41	-0.74
Lanl2TZ(f)	0.01	-2.04	-0.44	-2.02	-0.63	-1.6	-0.85	-1.53	-0.98	-0.8	-1.14	-0.58
Def2-TZVP	0.09	-0.16	-0.02	-0.18	0	0.05	0.04	0.06	-0.01	0.16	0.3	0.12
Def2-TZVPP	0.06	-0.15	-0.02	-0.18	-0.01	-0.02	-0.02	-0.02	-0.02	0.08	0.13	0.07
Def2-QZVP	0.03	-0.08	-0.02	-0.1	-0.01	-22.96	-0.02	-0.02	-0.02	0.25	0.31	0.18
Def2-QZVPP	0.04	-0.11	-0.02	-0.13	-0.01	-22.97	-0.02	-0.02	-0.01	0.2	0.27	0.16
6-311G(d)	4.96	2.21	2.73	2.34	12.21	22.62	6.77	2.11	-569.51	1.78	-137.27	1.17
6-311+G(d)	0.12	-0.37	-0.09	-0.44	-0.07	-0.2	-0.19	-0.24	0.01	-0.24	-10.47	-0.18
Aug-cc-pVDZ	0.07	-0.25	-0.07	-0.29	-0.06	-0.17	-0.15	-0.2	-0.01	-0.06	-10.02	-0.05
Aug-cc-pVTZ	0.01	-0.05	-0.01	-0.06	0	0	0	0	0	0	-9.51	0
Aug-cc-pVQZ	0	0	0	0	0	0	0	0	0	0	0	0

Table S-18

Y_3^-	BP86				B3LYP				M06			
	Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)	
Basis sets	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	*-0.13*	$NICS_{zz}$
Lanl2DZ	-0.03	-0.14	-0.06	-0.13	-0.03	-0.09	-0.05	-0.07	-0.04	-0.12	-0.42	-0.07
Lanl2TZ	-0.08	-0.49	-0.19	-0.43	-0.12	-0.41	-0.22	-0.32	-0.1	-0.44	-0.28	-0.26
Lanl2TZ(f)	-0.05	-0.31	-0.12	-0.29	-0.06	-0.26	-0.16	-0.22	-0.07	-0.27	-0.65	-0.15
DZVP(DFT orbital)	-0.01	-0.11	-0.04	-0.09	-0.03	-0.25	-0.13	-0.21	0.11	-0.89	0	-0.51
Def2-TZVP	0.02	-0.08	-0.02	-0.08	0.01	-0.05	-0.02	-0.04	0	-0.01	-0.01	0
Def2-TZVPP	0.01	-0.08	-0.02	-0.07	0.01	-0.04	-0.03	-0.04	0	-0.01	0	0
Def2-QZVP	0	-0.02	-0.01	-0.02	0	-0.01	-0.01	-0.01	0	0	0	0
Def2-QZVPP	0	0	0	0	0	0	0	0	0	0	-0.13	0

Table S-19

La_3^-	BP86				B3LYP				M06			
	Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)	
Basis sets	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$
Lanl2DZ	-0.9	-3.1	-1.36	-3.26	-1.76	-3.07	-0.89	-3.13	-2.3	13.3	4.13	-3.32
Lanl2TZ	-0.89	-2.76	-1.36	-3.28	-1.16	-2.77	-1.6	-3.18	-2.28	20.08	5.96	-3.03
Lanl2TZ(f)	-0.32	-1.09	-0.5	-1.27	-0.53	-1.42	2	-1.62	-0.91	18.08	10.7	-1.39
Def2-TZVP	-0.12	-0.57	-0.25	-0.7	-0.1	-0.38	0.99	-0.45	-0.14	-0.27	6.89	-0.29
Def2-TZVPP	-3.89	-2.26	-3.72	-4.77	3.81	1.86	3.55	4.29	-0.05	-0.1	8.48	-0.1
Def2-QZVP	-0.01	-0.02	-0.019	-0.02	-0.01	-0.03	1.45	-0.03	0.01	0	9.17	0.01
Def2-QZVPP	0	0	0	0	0	0	0	0	0	0	0	0

Table S-20

Al_4^{2-}	BP86				B3LYP				M06			
	Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)	
Basis sets	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$
Lanl2DZ	0.13	1.73	0.04	1.06	0.14	1.66	0.01	1.01	-0.91	2.7	-0.44	1.67
DZVP(DFT orbital)	0.11	0.38	0.06	0.26	0.11	0.38	0.05	0.26	0.05	0.32	0.04	0.22
Def2-TZVP	-0.01	-0.04	-0.01	-0.03	-0.04	-0.11	-0.02	-0.07	-0.05	-0.23	-0.03	-0.16
Def2-TZVPP	-0.02	-0.05	-0.01	-0.03	-0.04	-0.11	-0.02	-0.07	-0.06	-0.25	-0.04	-0.17
Def2-QZVP	-0.01	0	0	0	0	0	0	0	0	0	0	0
Def2-QZVPP	0	0	0	0	0	0	0	0	0	0	0	0
6-311G(d)	0.07	0.26	0.04	0.17	0.07	0.26	0.04	0.17	0.03	0.19	0.01	0.12
6-311+G(d)	0.08	0.26	0.04	0.17	0.07	0.25	0.03	0.17	0.08	0.32	0.04	0.22

Table S-21

Ga_4^{2-}	BP86				B3LYP				M06			
	Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)	
Basis sets	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$
Aug-cc-pVDZ-PP	0.46	0.92	0.3	0.94	0.41	0.85	0.26	0.89	0.43	0.42	0.24	0.49
Aug-cc-pVTZ-PP	0.28	0.63	0.15	0.52	0.26	0.61	0.14	0.51	0.63	0.65	0.33	0.54
Lanl2DZ	0.22	2.27	0.16	1.52	0.22	1.89	0.13	1.27	-0.37	1.88	-0.14	1.26
DZVP(DFT orbital)	0.31	0.43	0.19	0.55	0.26	0.36	0.15	0.46	0.21	0.28	0.13	0.34
cc-pVDZ-PP	0.31	0.52	0.2	0.55	0.23	0.35	0.13	0.37	-0.01	-0.02	0	-0.01
cc-pVTZ-PP	0.13	0.23	0.08	0.21	0.08	0.13	0.05	0.13	0.07	0.1	0.04	0.09
Def2-TZVP	-0.08	-0.11	-0.05	-0.12	-0.12	-0.16	-0.07	-0.18	-0.4	-0.4	-0.21	-0.49
Def2-TZVPP	-0.08	-0.12	-0.05	-0.12	-0.12	-0.16	-0.07	-0.18	-0.4	-0.4	-0.21	-0.49
Def2-QZVP	0.01	0	0	0	0	0	0	0	0	0.01	0	0
Def2-QZVPP	0	0	0	0	0	0	0	0	0	0	0	0
6-311G(d)	0.15	0.24	0.09	0.28	0.13	0.22	0.08	0.26	0.19	0.27	0.11	0.32
6-311+G(d)	1.2	4.09	0.94	3.17	0.02	0.61	0.07	0.64	0.37	0.34	0.2	0.43

Table S-22

Cu_4^{2-}	BP86				B3LYP				M06			
	Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)	
Basis sets	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$
Aug-cc-pVDZ-PP	-0.81	-0.76	-0.21	-0.56	-0.71	-0.51	-0.14	-0.65	-0.31	-0.09	-0.03	-0.23
Aug-cc-pVTZ-PP	-1.25	-1.28	-0.45	-1.02	-1.02	-1	-0.34	-1.1	-	-	-	-
Lanl2DZ	0.1	0.08	0.02	0.08	-0.15	-0.1	-0.01	-0.19	-0.22	-0.11	-0.03	-0.24
Lanl2TZ	-0.58	-0.49	-0.18	-0.5	-0.67	-0.5	-0.16	-0.77	-0.56	-0.35	-0.13	-0.58
Lanl2TZ(f)	-0.59	-0.48	-0.18	-0.5	-0.67	-0.5	-0.16	-0.77	-0.57	6.75	-0.13	-0.58
DZVP(DFT orbital)	1.62	1.4	0.85	2.05	1.12	0.84	0.62	1.65	0.73	0.52	0.41	1.15
cc-pVDZ-PP	-	-	-	-	-	-	-	-	-0.61	-0.67	-0.16	-0.75
cc-pVTZ-PP	-0.74	-0.81	-0.29	-0.68	-0.58	-0.55	-0.21	-0.68	-0.26	-0.24	-0.08	-0.33
Def2-TZVP	0.59	0.49	0.23	0.53	0.36	0.21	0.14	0.39	0.43	0.23	0.17	0.51
Def2-TZVPP	0.23	0.21	0.08	0.22	0.08	0.05	0.03	0.09	0.16	0.07	0.04	0.2
Def2-QZVP	0.03	0.02	0.01	0.03	0.01	0.01	0.01	0.03	0.01	0	-0.01	0.02
Def2-QZVPP	0	0	0	0	0	0	0	0	0	0	0	0
6-311G(d)	-7.33	0.53	-3.12	-2.2	-3.59	1.33	-1.41	-2.02	-3.98	1.26	-1.53	-2.09
6-311+G(d)	-0.12	-0.11	-0.05	-0.14	-0.09	-0.05	-0.03	-0.15	0.01	7.94	0	0.02
Aug-cc-pVDZ	0.42	0.43	0.14	0.43	0.25	0.21	0.07	0.36	0.27	0.24	0.05	0.49
Aug-cc-pVTZ	-0.23	-0.18	-0.07	-0.24	-0.16	-0.1	-0.04	-0.25	-0.02	0	0	-0.03

Table S-23

Ag_4^{2-}	BP86				B3LYP				M06			
	Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)	
Basis sets	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$
Aug-cc-pVDZ-PP	-0.06	0.02	-0.02	-0.07	-0.05	0.02	-0.01	-0.06	-0.03	0.02	-0.01	-0.06
Aug-cc-pVTZ-PP	-0.15	0.05	-0.05	-0.18	-0.11	0.07	-0.04	-0.15	-0.02	0.03	0.01	-0.05
Lanl2DZ	0	0	0	0	0.3	-0.24	0.08	0.47	0.11	-0.13	0.03	0.16
Lanl2TZ	0.3	-0.02	0.13	0.39	0.19	-0.08	0.07	0.3	0.13	-0.08	0.04	0.16
Lanl2TZ(f)	0.26	-0.03	0.1	0.33	0.16	-0.07	0.06	0.26	-1.14	-0.07	0.03	0.14
DZVP(DFT orbital)	1.1	-0.82	0.51	1.83	0.93	-0.98	0.44	1.77	0.41	-0.71	0.19	1.05
cc-pVDZ-PP	0.16	0.01	0.07	0.22	0.11	-0.02	0.05	0.18	0.06	-0.01	0.03	0.12
cc-pVTZ-PP	0.06	-0.01	0.03	0.08	0.05	-0.02	0.02	0.06	0.03	-0.02	0.01	0.05
Def2-TZVP	0.31	0.02	0.13	0.44	0.24	-0.06	0.08	0.38	0.14	-0.03	0.06	0.25
Def2-TZVPP	0.2	-0.01	0.08	0.27	0.16	-0.05	0.06	0.26	0.06	-0.03	0.02	0.12
Def2-QZVP	0.01	0	0.01	0.01	0.01	-0.01	0	0.01	-0.01	0.01	0	0
Def2-QZVPP	0	0	0	0	0	0	0	0	0	0	0	0

Table S-24

Au_4^{2-}	BP86				B3LYP				M06			
	Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)		Δ NICS (0)		Δ NICS (1)	
Basis sets	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$	$NICS_{iso}$	$NICS_{zz}$
Aug-cc-pVDZ-PP	-0.01	0	0	-0.01	0	0	0	0.01	-0.03	0.02	-0.01	-0.04
Aug-cc-pVTZ-PP	-0.13	-0.04	-0.06	-0.15	-0.1	-0.03	-0.04	-0.11	-0.05	0.04	-0.02	-0.07
Lanl2DZ	1.37	0.46	0.65	1.32	1.21	0.3	0.59	1.23	0.46	0	0.23	0.45
Lanl2TZ	-6.06	0.17	0.25	0.5	0.47	0.11	0.23	0.47	0.21	0	0.1	0.2
Lanl2TZ(f)	0.17	0.04	0.08	0.17	0.16	0.02	0.08	0.16	0.02	0	0.01	0.02
cc-pVDZ-PP	0.33	0.09	0.16	0.32	0.28	0.04	0.13	0.29	0.11	-0.04	0.05	0.11
cc-pVTZ-PP	0	0	0	0.01	0.03	-0.01	0.01	0.03	0.01	0	0	0.01
Def2-TZVP	0.29	-0.03	0.12	0.29	0.26	-0.06	0.11	0.28	0.17	-0.09	0.07	0.17
Def2-TZVPP	0.12	-0.02	0.05	0.13	0.13	-0.05	0.05	0.14	0.07	-0.04	0.03	0.06
Def2-QZVP	0.01	0	0.01	0.01	0.02	-0.01	0.01	0.03	0.03	-0.02	0.01	0.02
Def2-QZVPP	0	0	0	0	0	0	0	0	0	0	0	0

Table S-25

Li_3^+	BP86	B3LYP	M06
Lanl2DZ	0.03	0.027	-0.007
DZVP(DFT orbital)	0.063	0.057	0.003
Def2-TZVP	0.044	0.044	0.007
Def2-TZVPP	0.022	0.018	-0.043
Def2-QZVP	0	-0.001	0
Def2-QZVPP	0	0	0
6-311G(d)	0.008	0.005	-0.055
6-311+G(d)	0.008	0.005	-0.059

Table S-26

Cu_3^+	BP86	B3LYP	M06
Aug-cc-pVDZ-PP	-0.02	-0.029	-0.024
Aug-cc-pVTZ-PP	-0.03	-0.036	-0.029
Lanl2DZ	0.017	0.002	-0.006
Lanl2TZ	0.007	-0.01	-0.006
Lanl2TZ(f)	0.007	-0.01	-0.007
DZVP(DFT orbital)	0.037	0.029	0.014
cc-pVDZ-PP	-0.035	-0.044	-0.035
cc-pVTZ-PP	-0.017	-0.025	-0.017
Def2-TZVP	0.018	0.014	0.01
Def2-TZVPP	0.015	0.012	0.009
Def2-QZVP	0.006	0.004	0.002
Def2-QZVPP	0.003	0.002	0.001
6-311G(d)	-0.048	-0.081	-0.08
6-311+G(d)	0.007	0.005	0.004
Aug-cc-pVDZ	0.021	0.017	0.012
Aug-cc-pVTZ	0	0	0
Aug-cc-pVQZ	0	0	0

Table S-27

Ag_3^+	BP86	B3LYP	M06
Aug-cc-pVDZ-PP	0.003	0.004	0
Aug-cc-pVTZ-PP	-0.005	-0.003	-0.004
Lanl2DZ	0.049	0.043	0.026
Lanl2TZ	0.049	0.04	0.03
Lanl2TZ(f)	0.047	0.04	0.03
DZVP(DFT orbital)	0.14	0.138	0.106
cc-pVDZ-PP	0.018	0.015	0.008
cc-pVTZ-PP	0.008	0.008	0.008
Def2-TZVP	0.028	0.024	0.014
Def2-TZVPP	0.018	0.015	0.01
Def2-QZVP	0.048	-0.045	0.002
Def2-QZVPP	0	0	0

Table S-28

Au_3^+	BP86	B3LYP	M06
Aug-cc-pVDZ-PP	0.005	0.005	0.005
Aug-cc-pVTZ-PP	-0.01	-0.001	-0.002
Lanl2DZ	0.046	0.042	0.032
Lanl2TZ	0.032	0.027	0.025
Lanl2TZ(f)	0.019	0.014	0.014
cc-pVDZ-PP	0.02	0.018	0.015
cc-pVTZ-PP	0.003	0.004	0.003
Def2-TZVP	0.016	0.014	0.011
Def2-TZVPP	0.005	0.004	0.003
Def2-QZVP	0.003	0.002	0.003
Def2-QZVPP	0	0	0

Table S-29

Sc_3^-	BP86	B3LYP	M06
Lanl2DZ	0.007	0.006	-0.016
Lanl2TZ	0.036	0.036	0.013
Lanl2TZ(f)	0.035	0.033	0.01
Def2-TZVP	0.004	-0.001	-0.004
Def2-TZVPP	0.004	0.001	-0.002
Def2-QZVP	0.002	0.001	-0.004
Def2-QZVPP	0.003	0.001	-0.004
6-311G(d)	-0.078	-0.088	-0.075
6-311+G(d)	0.009	0.007	0.006
Aug-cc-pVDZ	0.006	0.006	0.002
Aug-cc-pVTZ	0.001	0	0
Aug-cc-pVQZ	0	0	0

Table S-30

Y_3^-	BP86	B3LYP	M06
Lanl2DZ	0.005	0.003	0.004
Lanl2TZ	0.017	0.019	0.017
Lanl2TZ(f)	0.012	0.014	0.012
DZVP(DFT orbital)	0.003	0.007	0.024
Def2-TZVP	0.005	0.004	0
Def2-TZVPP	0.004	0.003	0
Def2-QZVP	0.002	0.001	0
Def2-QZVPP	0	0	0

Table S-31

La_3^-	BP86	B3LYP	M06
Lanl2DZ	0.03	0.031	0.03
Lanl2TZ	0.037	0.039	0.035
Lanl2TZ(f)	0.014	0.019	0.014
Def2-TZVP	0.009	0.007	0.004
Def2-TZVPP	0.005	0.002	0
Def2-QZVP	0.001	0.001	0
Def2-QZVPP	0	0	0

Table S-32

Al_4^{2-}	BP86	B3LYP	M06
Lanl2DZ	0.082	0.081	0.109
DZVP(DFT orbital)	0.019	0.019	0.015
Def2-TZVP	-0.003	-0.005	-0.01
Def2-TZVPP	-0.003	-0.006	-0.011
Def2-QZVP	0	0	0
Def2-QZVPP	0	0	0
6-311G(d)	0.012	0.012	0.008
6-311+G(d)	0.012	0.014	0.015

Table S-33

Ga_4^{2-}	BP86	B3LYP	M06
Aug-cc-pVDZ-PP	0.038	0.036	0.024
Aug-cc-pVTZ-PP	0.019	0.02	0.02
Lanl2DZ	0.105	0.09	0.07
DZVP(DFT orbital)	0.025	0.021	0.015
cc-pVDZ-PP	0.023	0.016	0
cc-pVTZ-PP	0.01	0.005	0.004
Def2-TZVP	-0.006	-0.009	-0.024
Def2-TZVPP	-0.006	-0.009	-0.024
Def2-QZVP	0	0	0.001
Def2-QZVPP	0	0	0
6-311G(d)	0.013	0.012	0.016
6-311+G(d)	0.019	0.022	0.022

Table S-34

Cu_4^{2-}	BP86	B3LYP	M06
Aug-cc-pVDZ-PP	-0.03	-0.044	-0.023
Aug-cc-pVTZ-PP	-0.041	-0.053	–
Lanl2DZ	0.005	-0.013	-0.017
Lanl2TZ	-0.024	-0.045	-0.035
Lanl2TZ(f)	-0.024	-0.045	-0.035
DZVP(DFT orbital)	0.095	0.09	0.062
cc-pVDZ-PP	–	–	-0.036
cc-pVTZ-PP	-0.024	-0.031	-0.016
Def2-TZVP	0.025	0.023	0.031
Def2-TZVPP	0.011	0.006	0.013
Def2-QZVP	0.002	0.001	0.001
Def2-QZVPP	0	0	0
6-311G(d)	-0.119	-0.147	-0.145
6-311+G(d)	-0.007	-0.01	0.002
Aug-cc-pVDZ	0.02	0.02	0.028
Aug-cc-pVTZ-PP	-0.013	-0.016	-0.004

Table S-35

Ag_4^{2-}	BP86	B3LYP	M06
Aug-cc-pVDZ-PP	-0.006	-0.006	-0.006
Aug-cc-pVTZ-PP	-0.015	-0.016	-0.005
Lanl2DZ	0.05	0.047	0.019
Lanl2TZ	0.028	0.025	0.016
Lanl2TZ(f)	0.025	0.023	0.014
DZVP(DFT orbital)	0.157	0.175	0.104
cc-pVDZ-PP	0.014	0.015	0.009
cc-pVTZ-PP	0.006	0.005	0.004
Def2-TZVP	0.03	0.032	0.02
Def2-TZVPP	0.02	0.022	0.01
Def2-QZVP	0.001	0	-0.001
Def2-QZVPP	0	0	0

Table S-36

Au_4^{2-}	BP86	B3LYP	M06
Aug-cc-pVDZ-PP	0	0.001	-0.002
Aug-cc-pVTZ-PP	-0.007	-0.006	-0.005
Lanl2DZ	0.067	0.069	0.032
Lanl2TZ	0.026	0.026	0.015
Lanl2TZ(f)	0.01	0.01	0.002
cc-pVDZ-PP	0.017	0.017	0.009
cc-pVTZ-PP	0.001	0.003	0.001
Def2-TZVP	0.018	0.019	0.015
Def2-TZVPP	0.008	0.01	0.006
Def2-QZVP	0.001	0.002	0.003
Def2-QZVPP	0	0	0

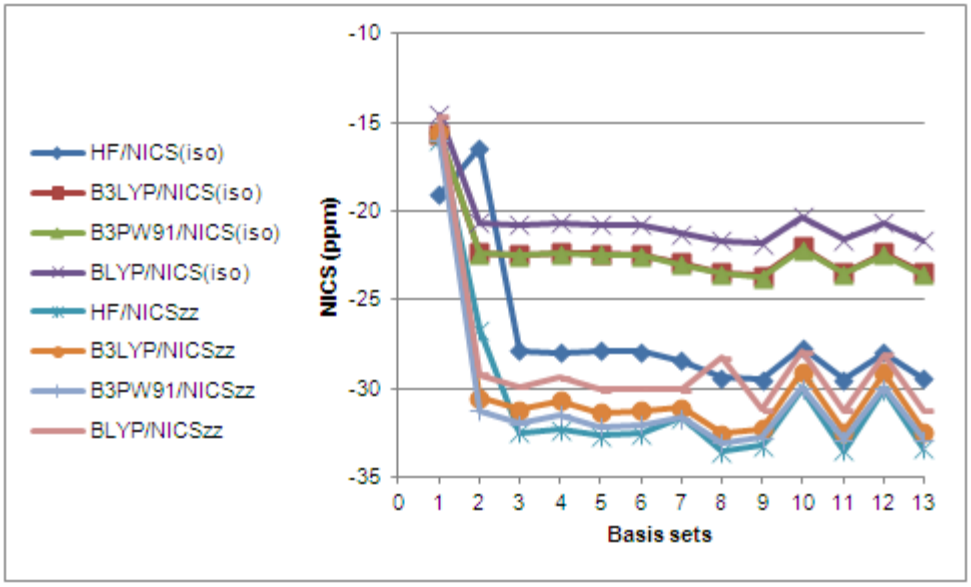


Figure S-1A

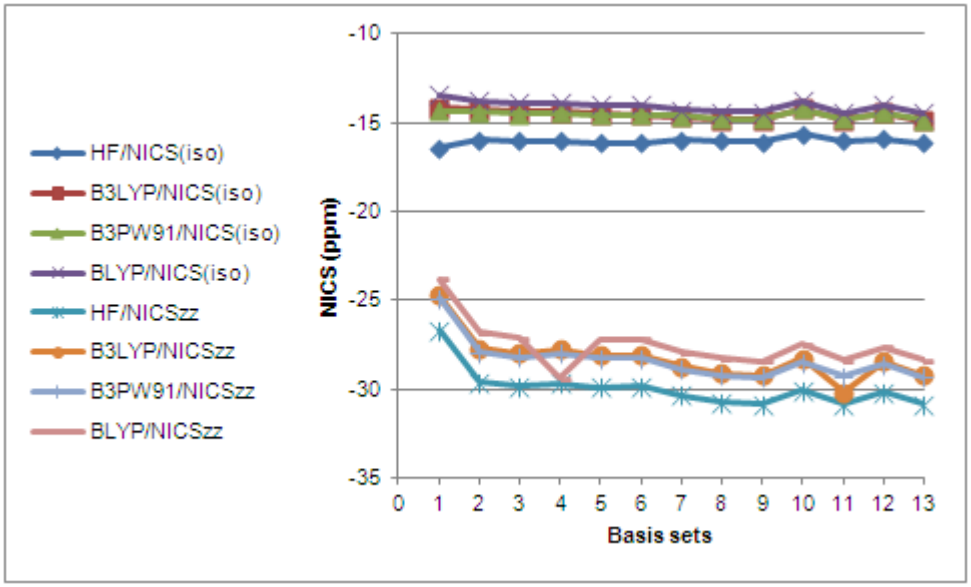


Figure S-1B

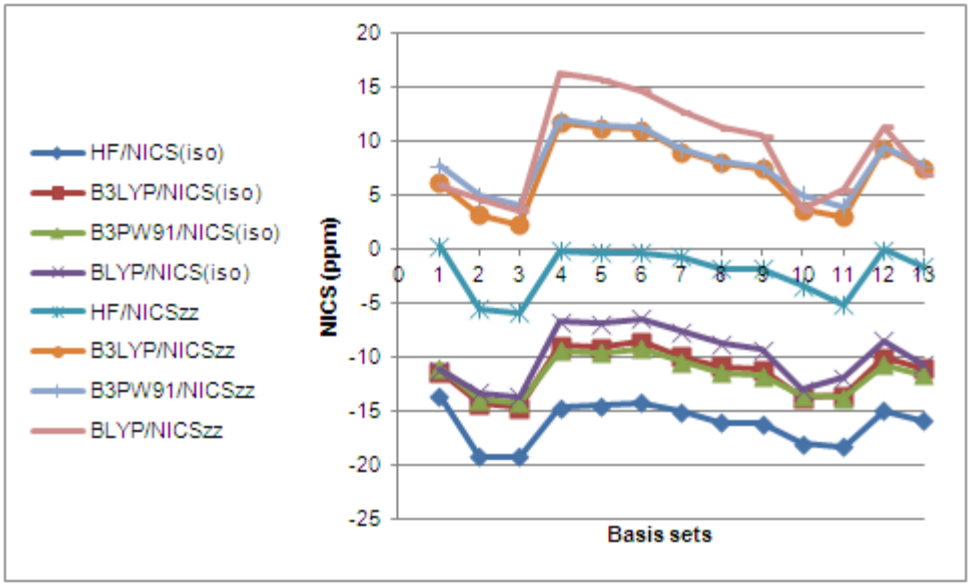


Figure S-2A

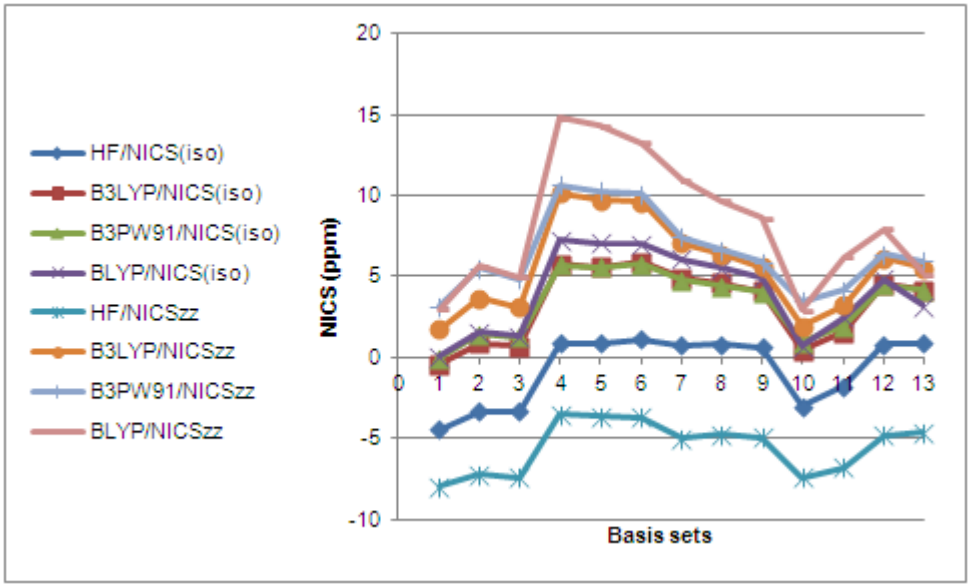


Figure S-2B

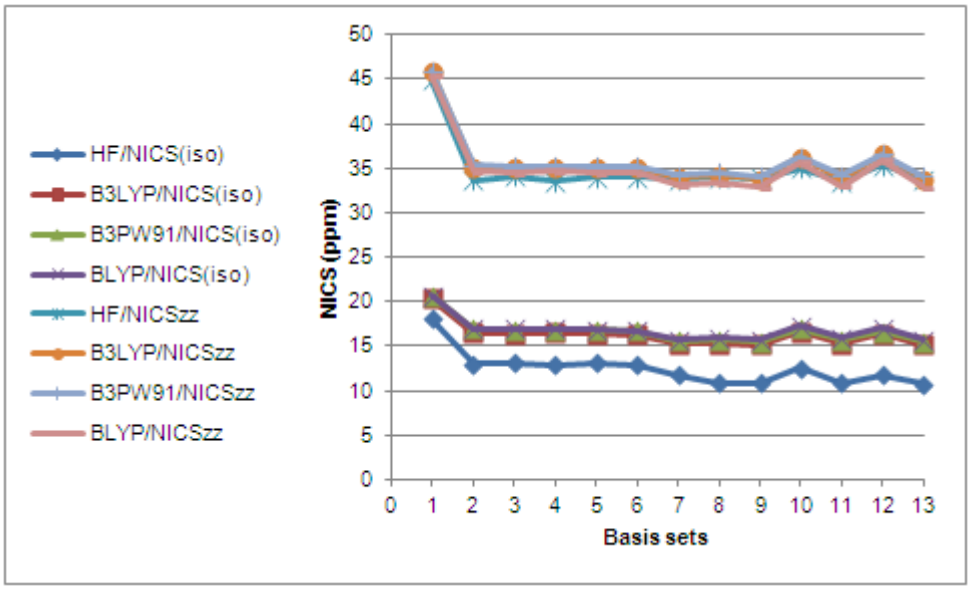


Figure S-3A

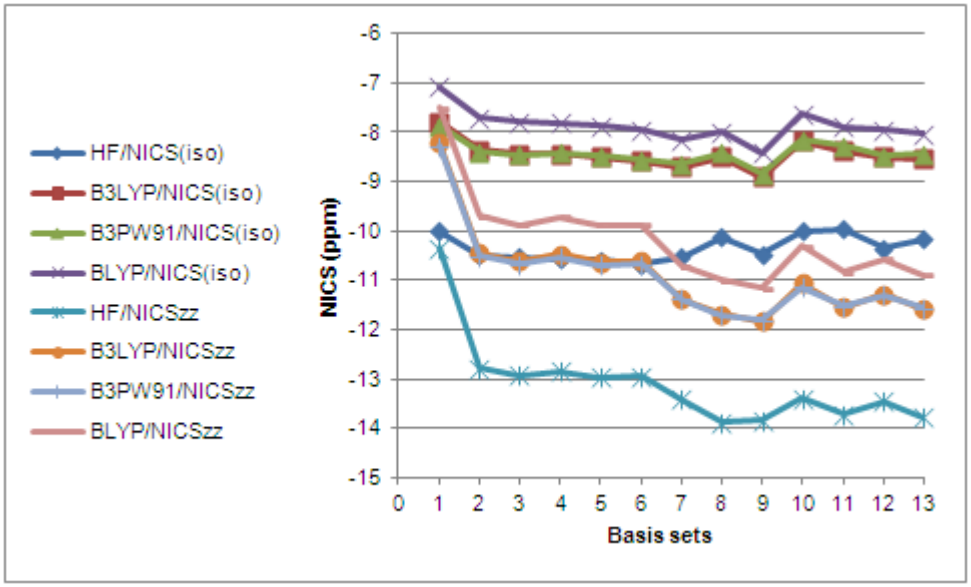


Figure S-3B

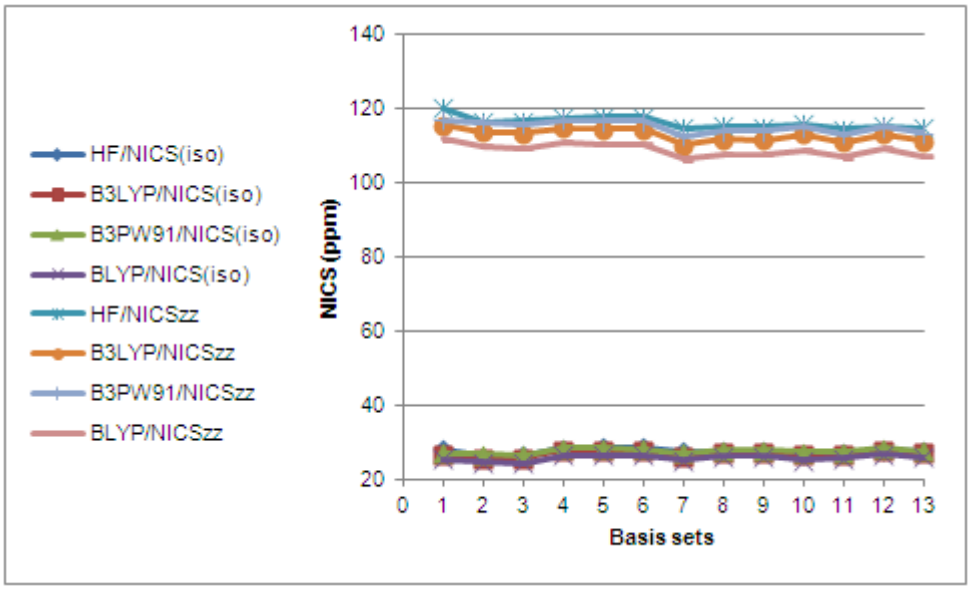


Figure S-4A

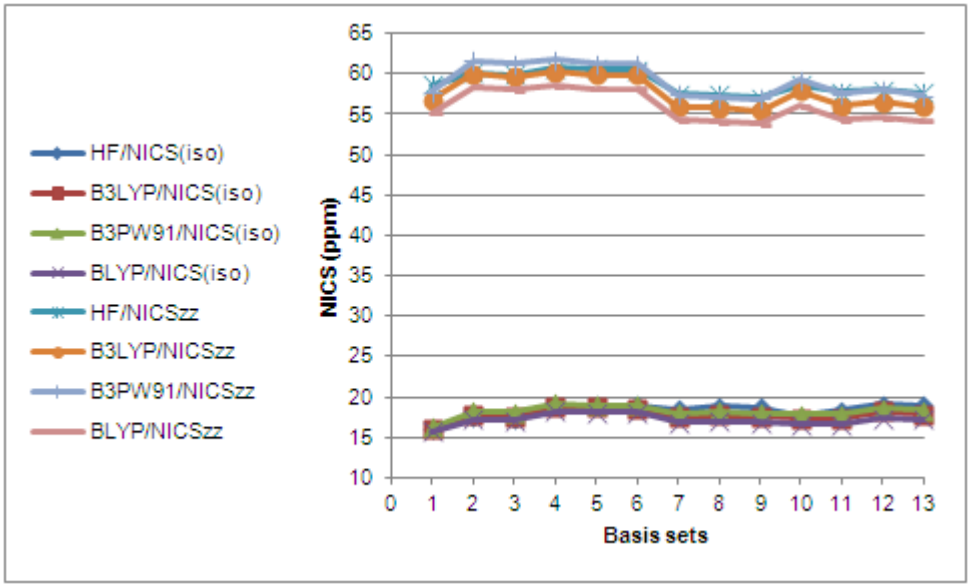


Figure S-4B

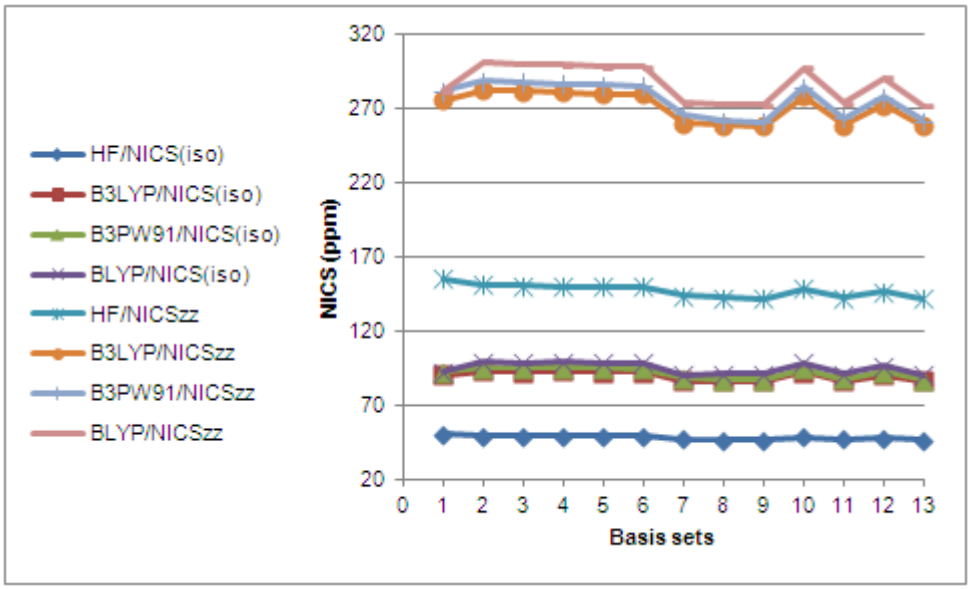


Figure S-5A

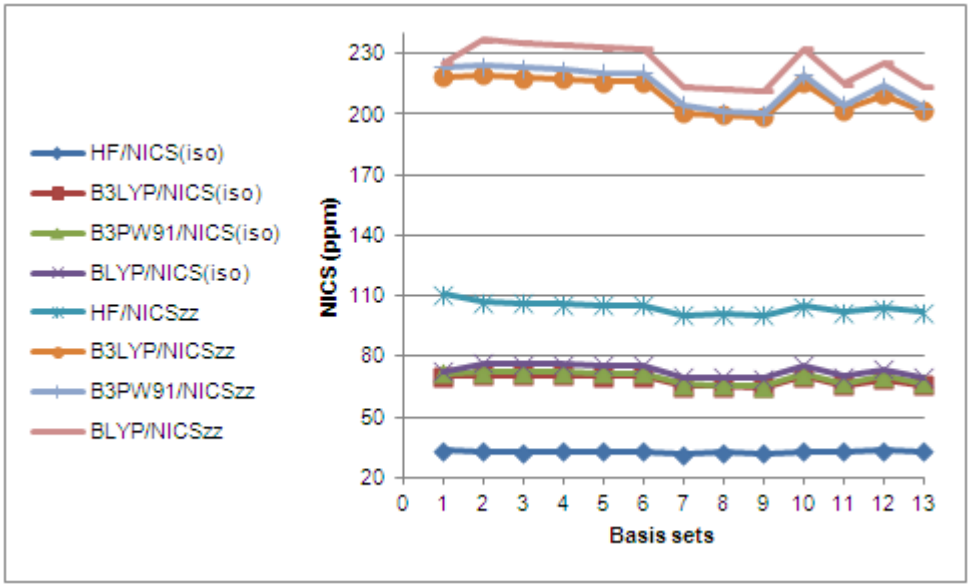


Figure S-5B

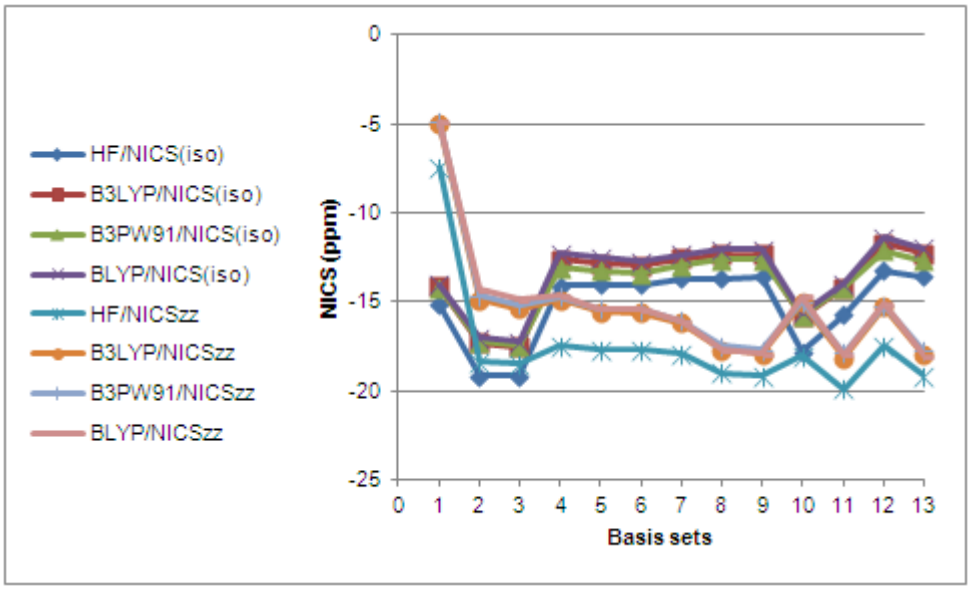


Figure S-6A

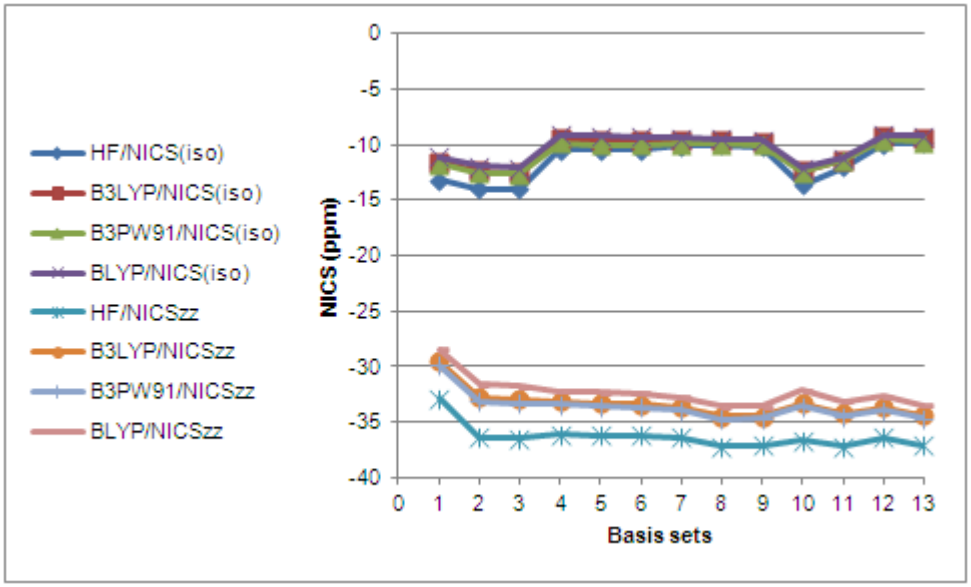


Figure S-6B

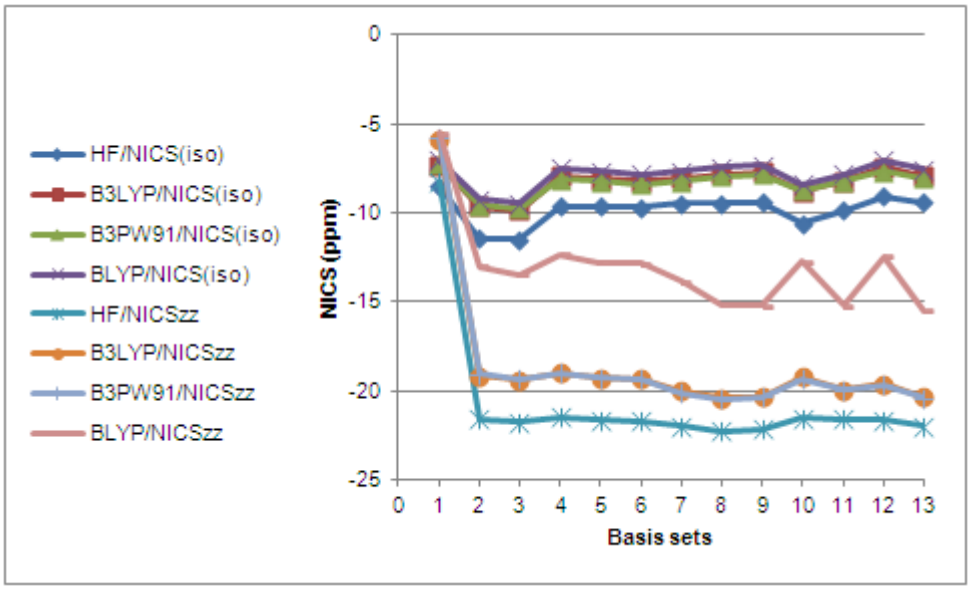


Figure S-7A

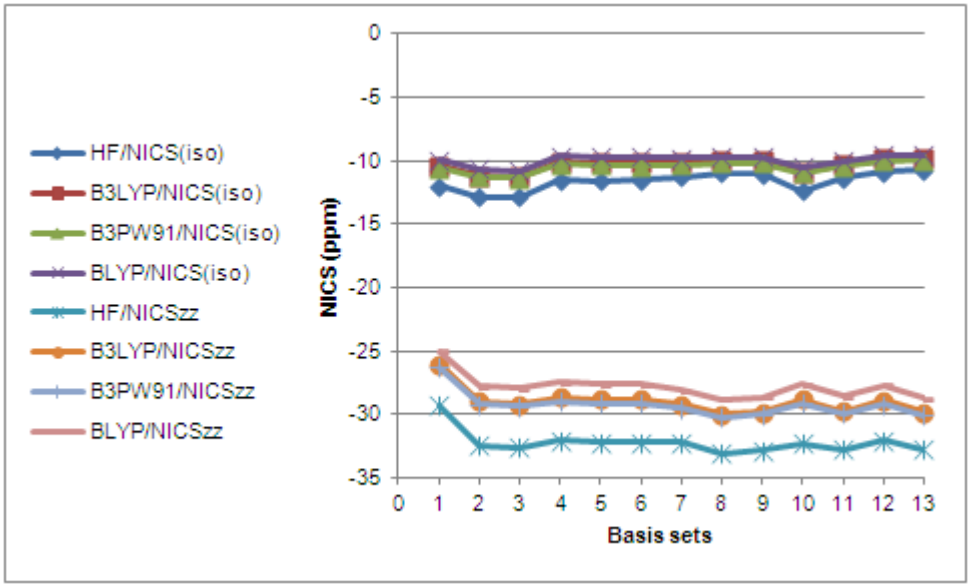


Figure S-7B

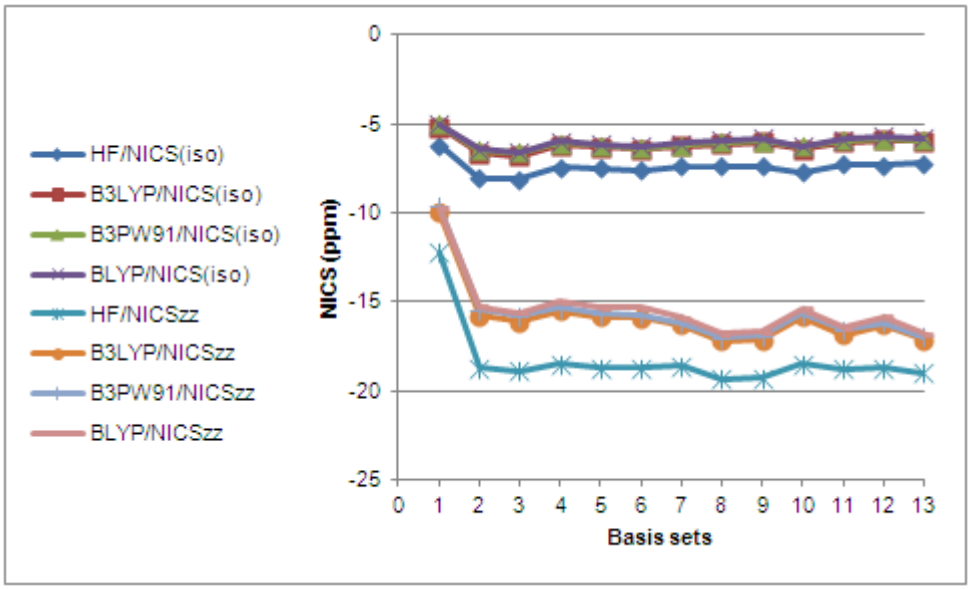


Figure S-8A

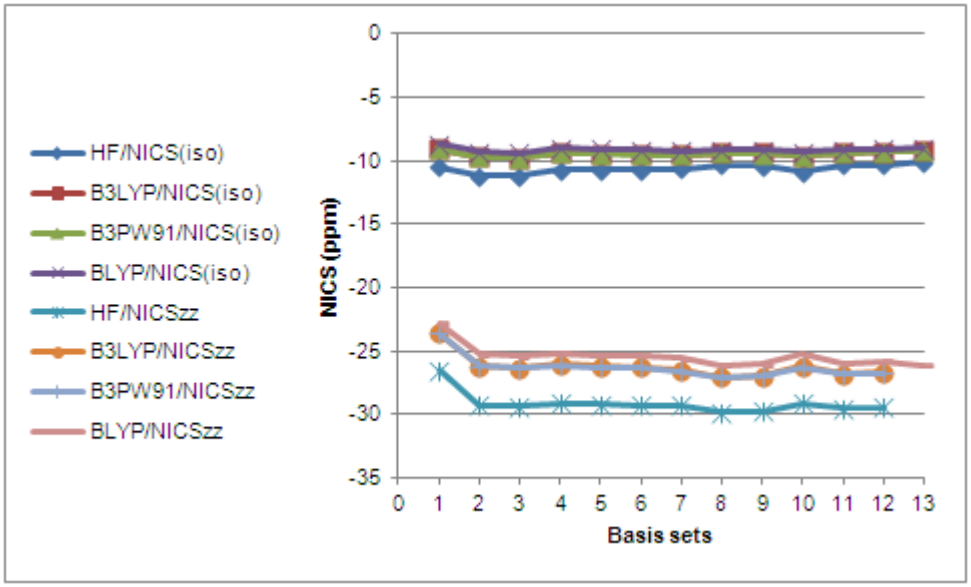


Figure S-8B

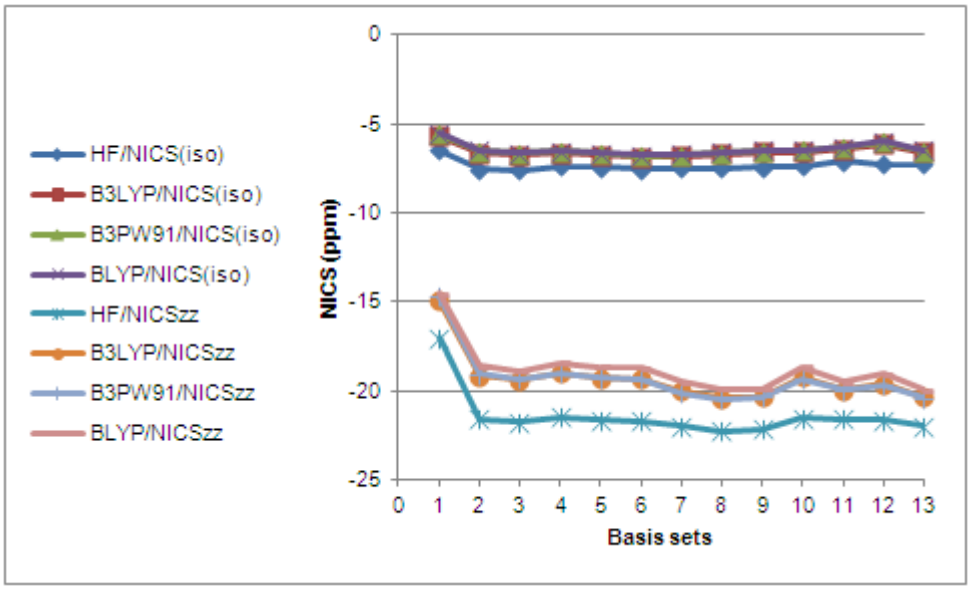


Figure S-9A

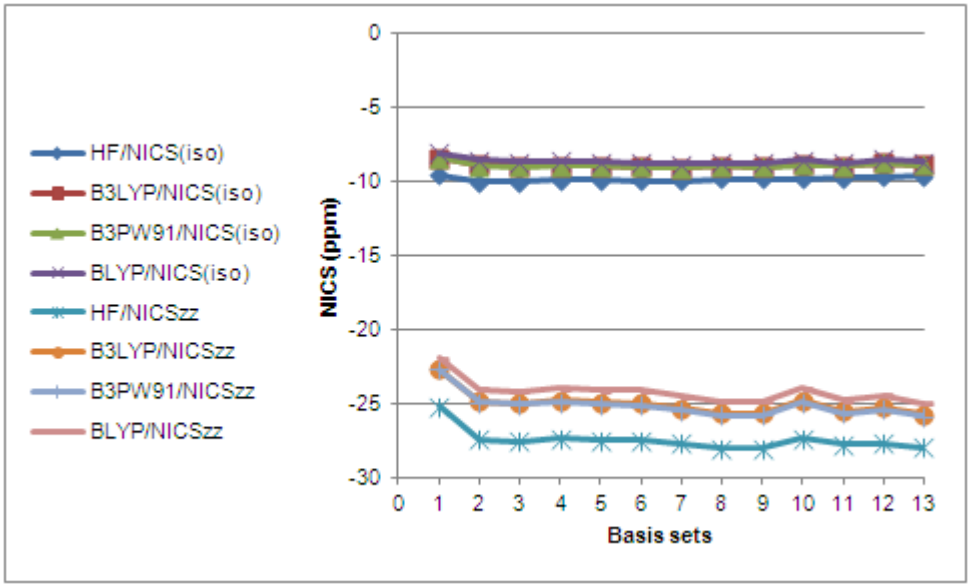


Figure S-9B

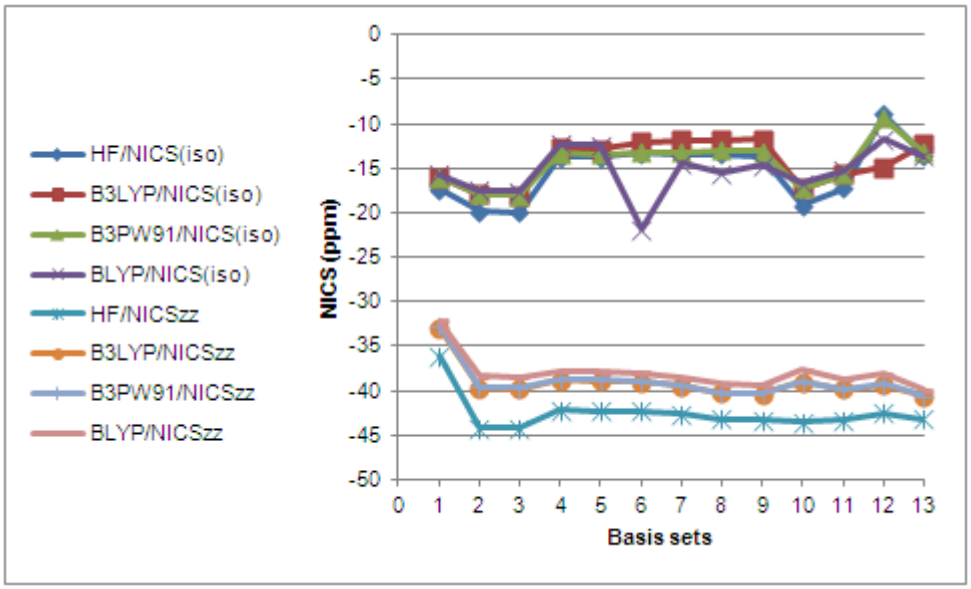


Figure S-10A

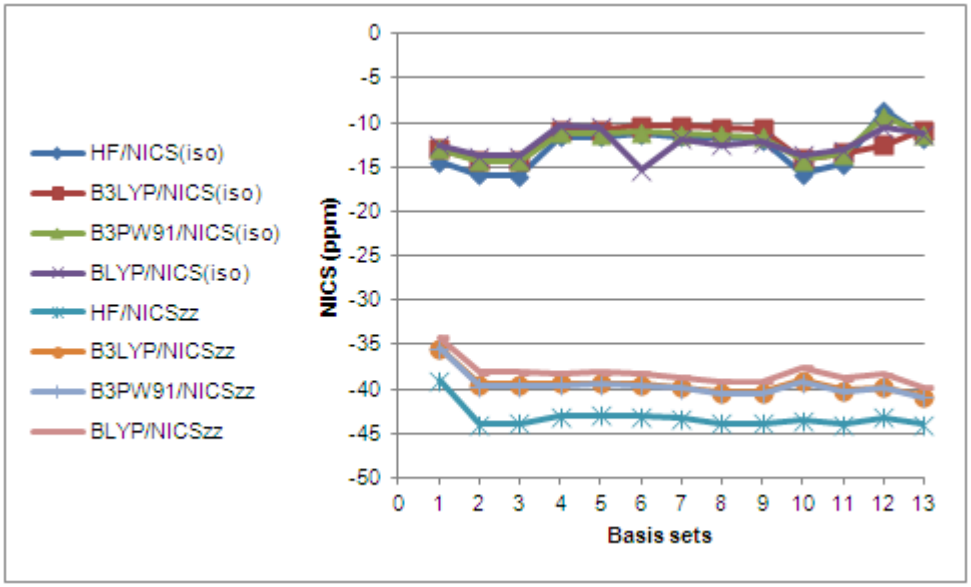


Figure S-10B

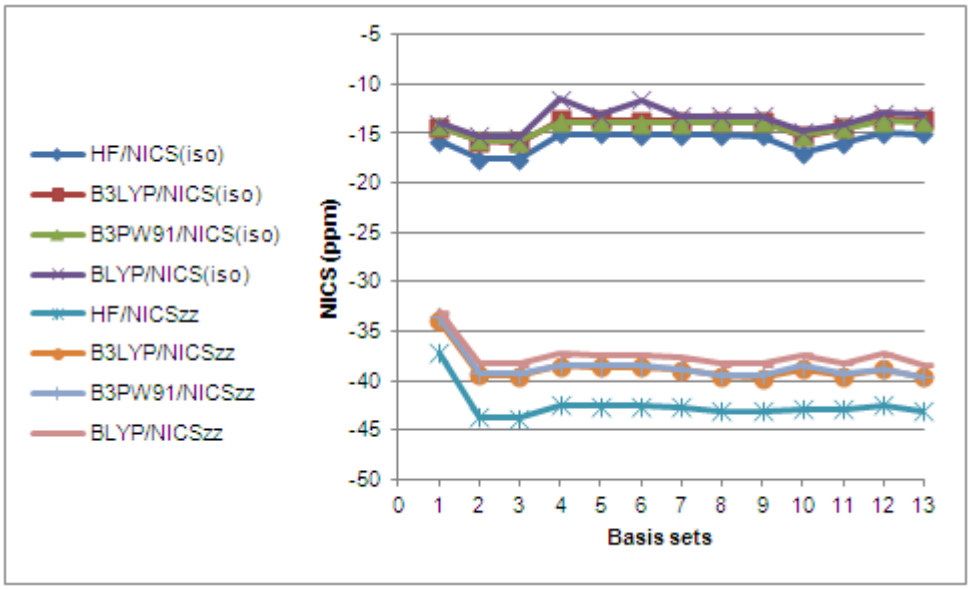


Figure S-11A

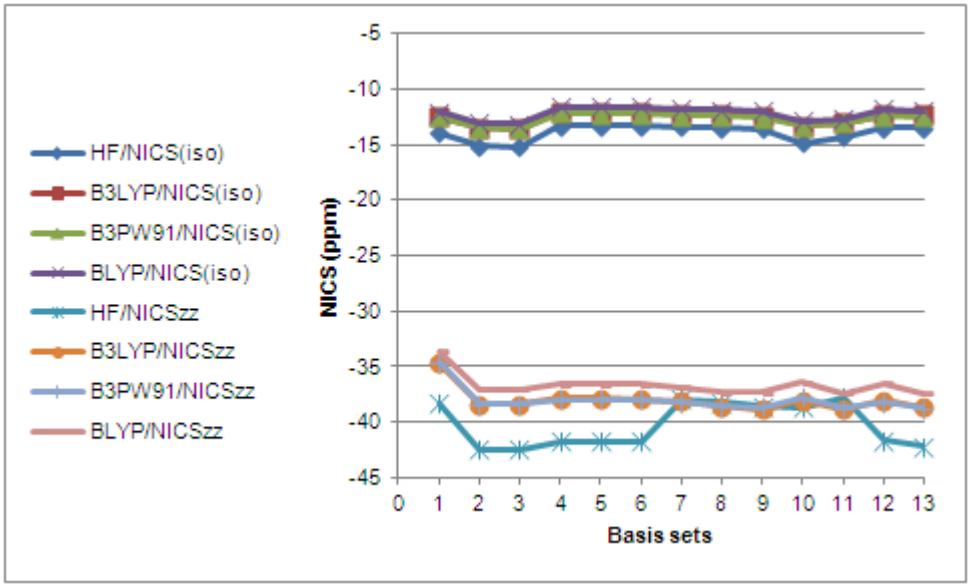


Figure S-11B

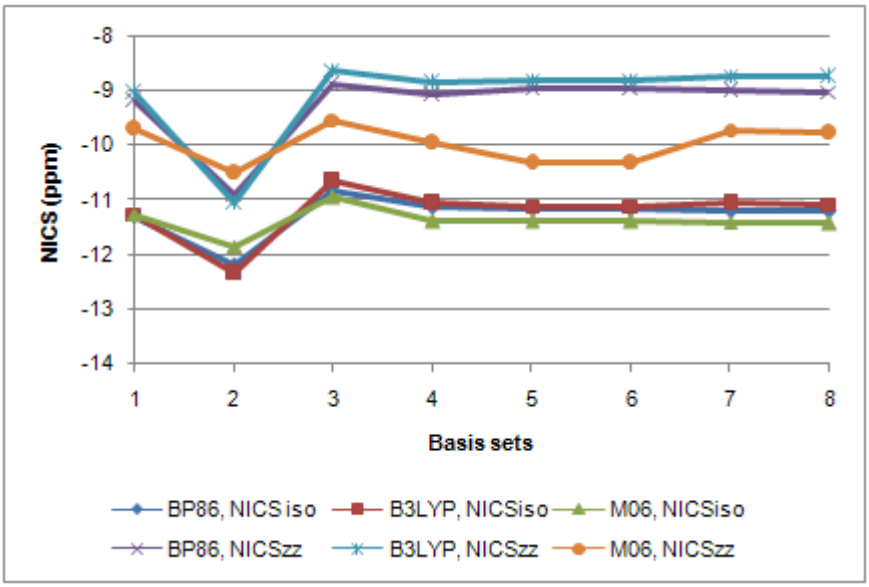


Figure S-12A

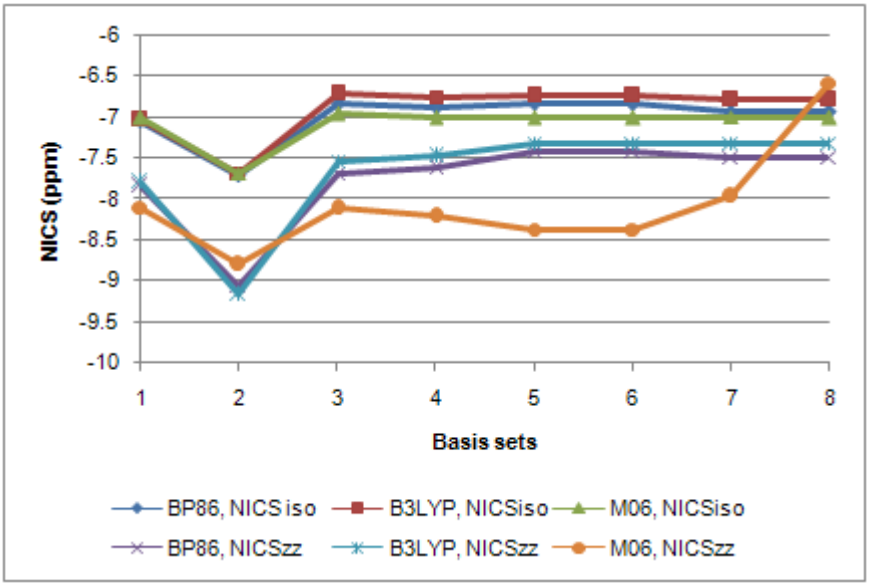
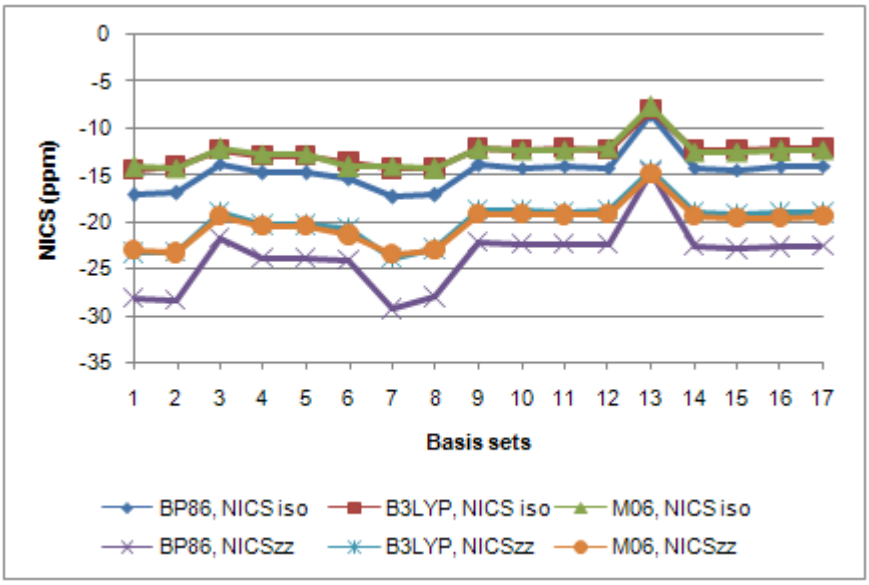


Figure S-12B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-5
-10
-15
-20
-25
-30
-35
NICS (ppm)
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
Basis sets
BP86, NICS iso
B3LYP, NICS iso
M06, NICS iso
BP86, NICSzz
B3LYP, NICSzz
M06, NICSzz

Figure S-13

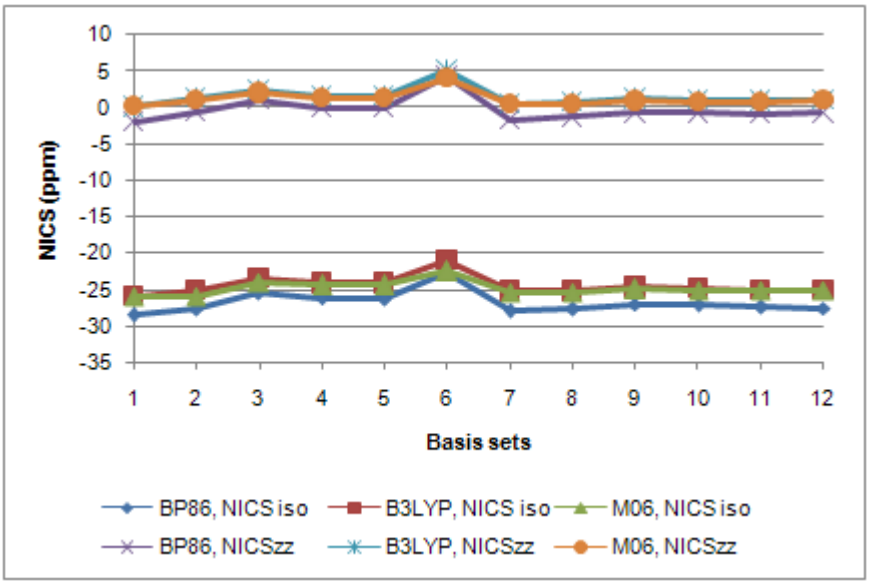


Figure S-14A

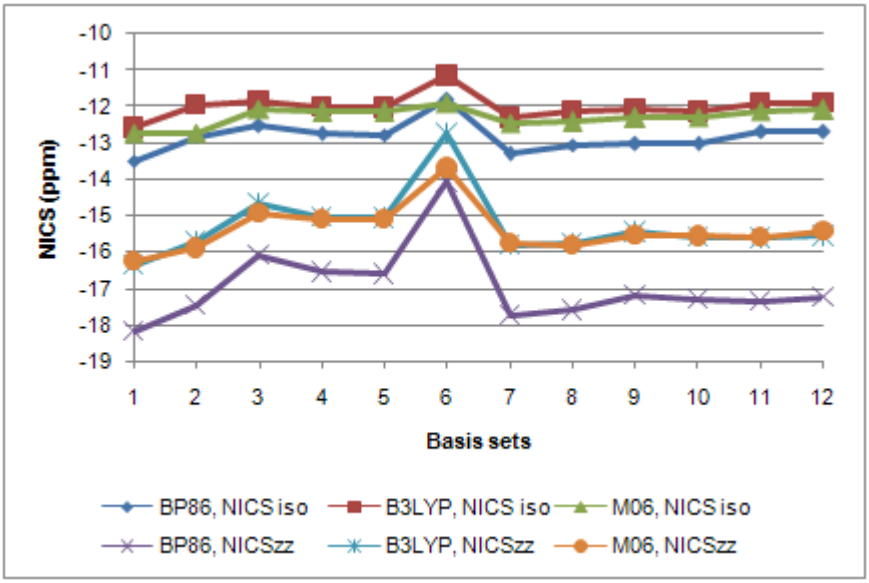


Figure S-14B

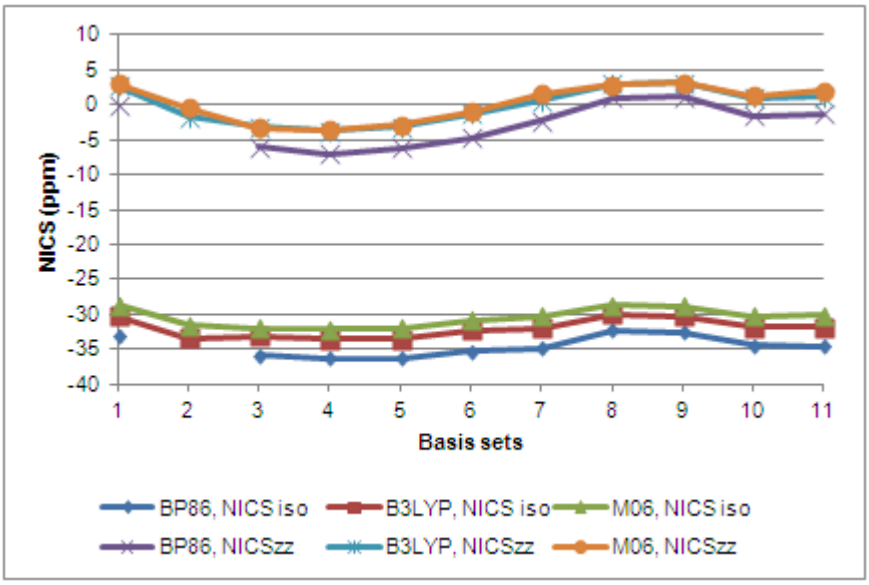


Figure S-15A

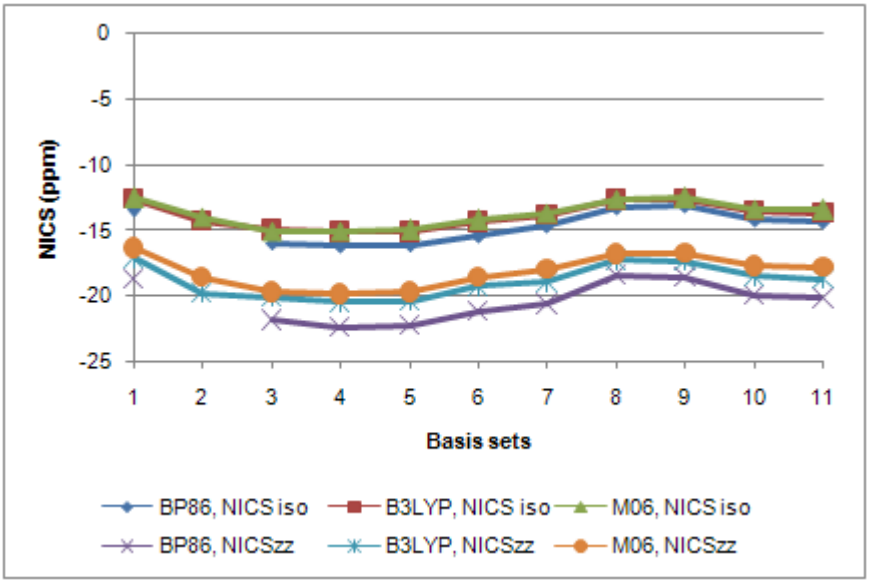
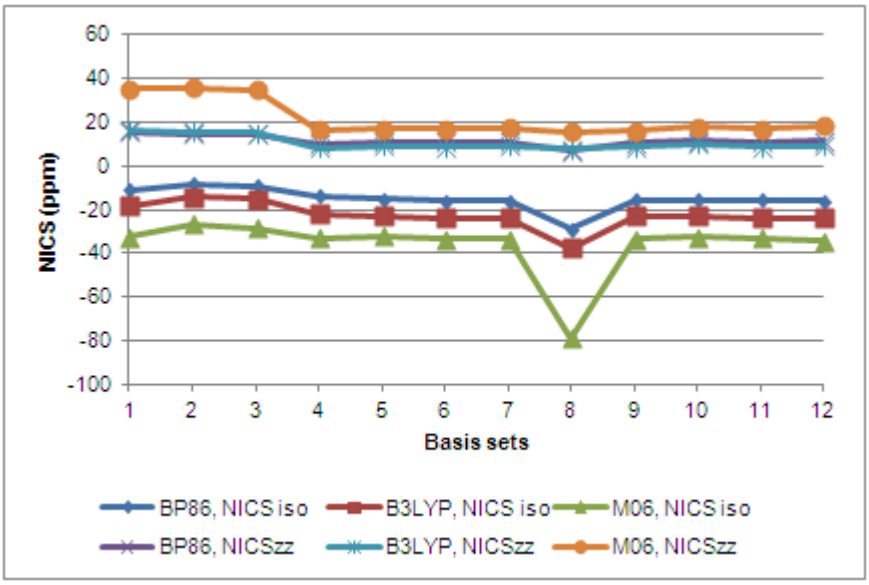


Figure S-15B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-20
-40
-60
-80
-100
NICS (ppm)
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2
3
4
5
6
7
8
9
10
11
12
Basis sets
BP86, NICS iso
B3LYP, NICS iso
M06, NICS iso
BP86, NICSzz
B3LYP, NICSzz
M06, NICSzz

Figure S-16

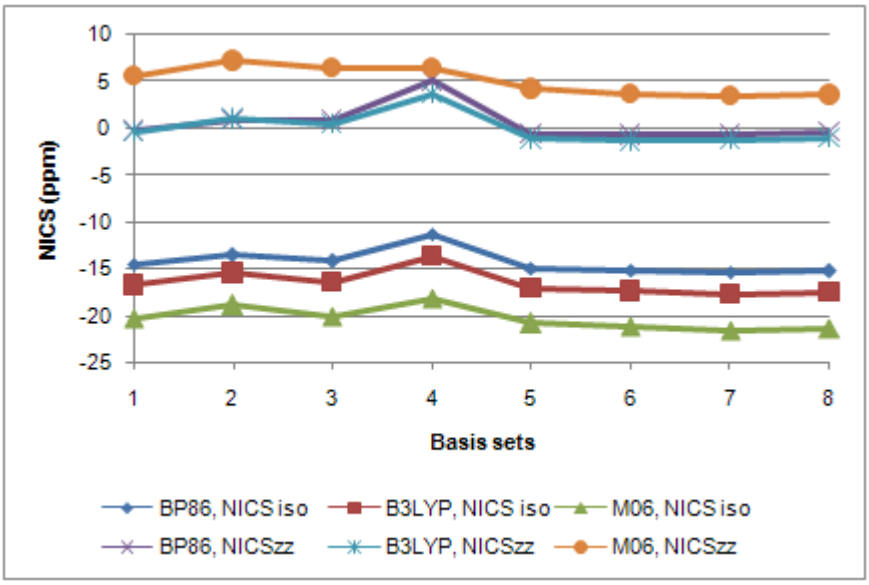
10
5
0
-5
-10
-15
-20
-25
NICS (ppm)
1
2
3
4
5
6
7
8
Basis sets
BP86, NICS iso
B3LYP, NICS iso
M06, NICS iso
BP86, NICSzz
B3LYP, NICSzz
M06, NICSzz

Figure S-17

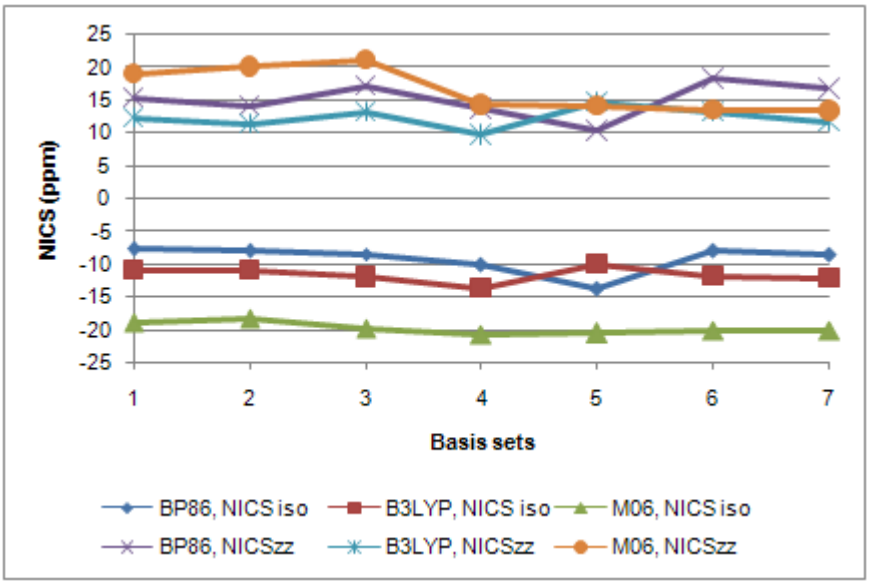
NICS (ppm)
25
20
15
10
5
0
-5
-10
-15
-20
-25
1
2
3
4
5
6
7
Basis sets
BP86, NICS iso
B3LYP, NICS iso
M06, NICS iso
BP86, NICSzz
B3LYP, NICSzz
M06, NICSzz

Figure S-18

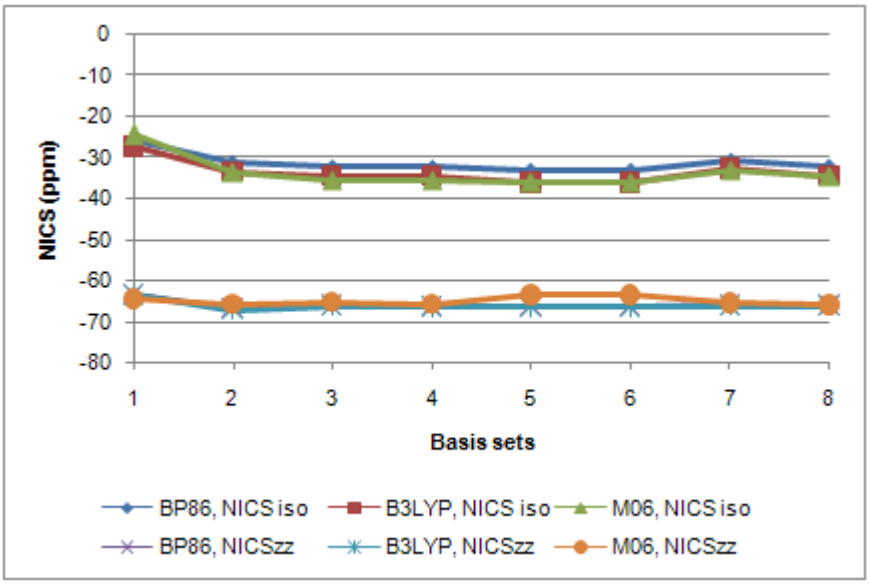

Figure S-19A

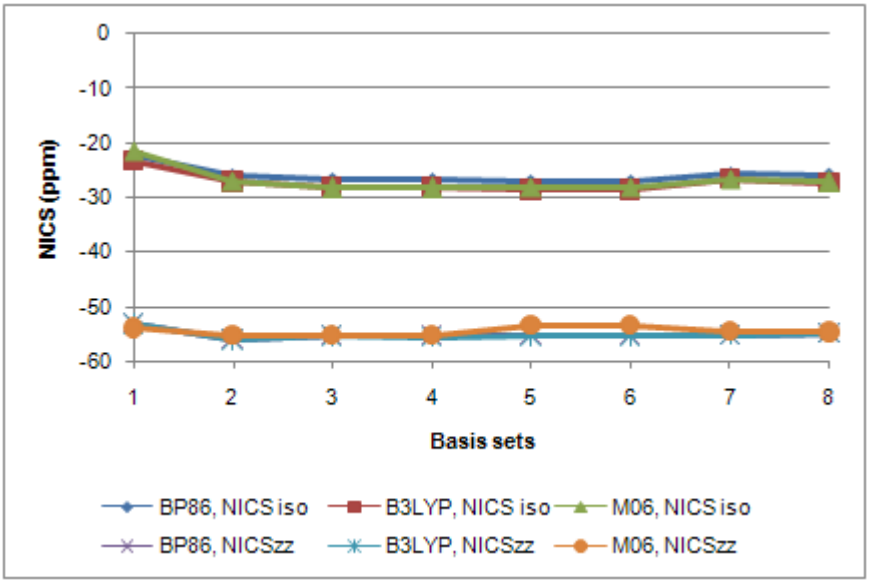

Figure S-19B

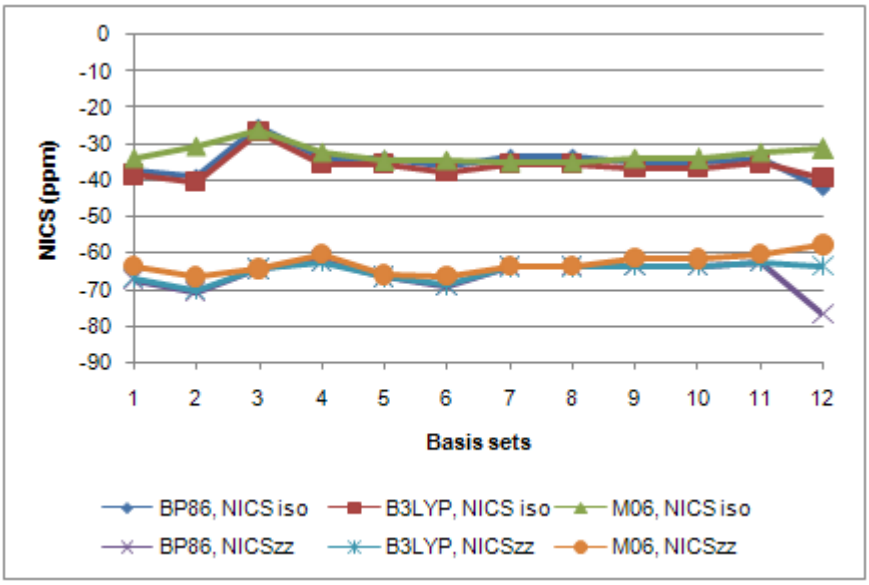

Figure S-20A

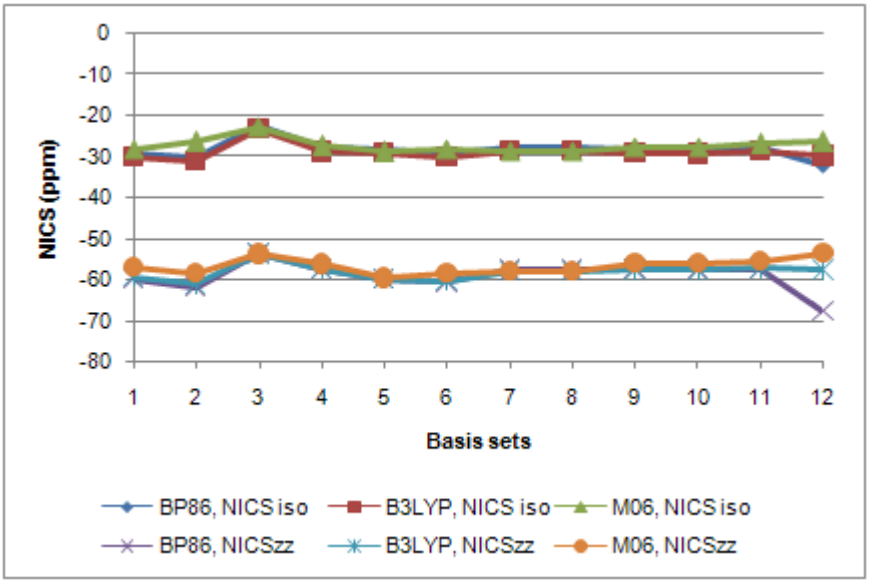

Figure S-20B

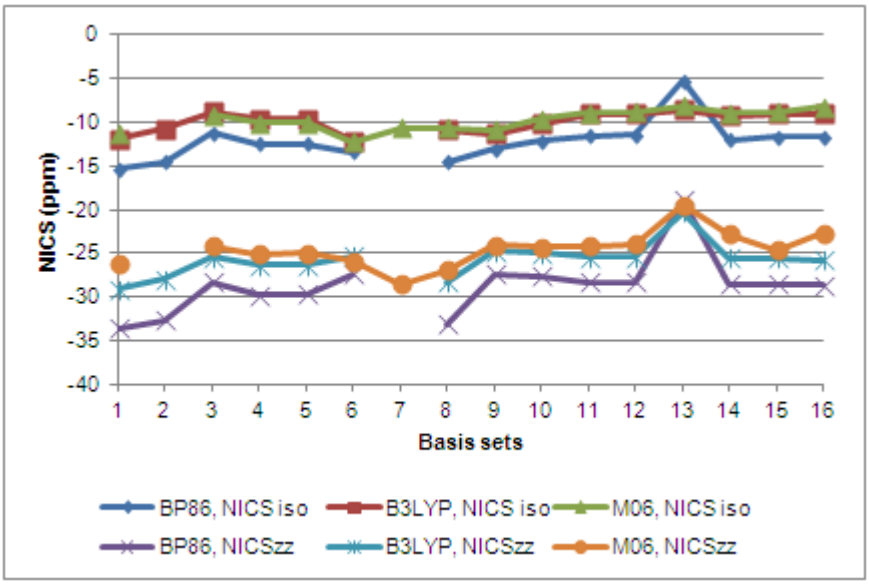
0
-5
-10
-15
-20
-25
-30
-35
-40
NICS (ppm)
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
Basis sets
BP86, NICS iso
B3LYP, NICS iso
M06, NICS iso
BP86, NICSzz
B3LYP, NICSzz
M06, NICSzz

Figure S-21

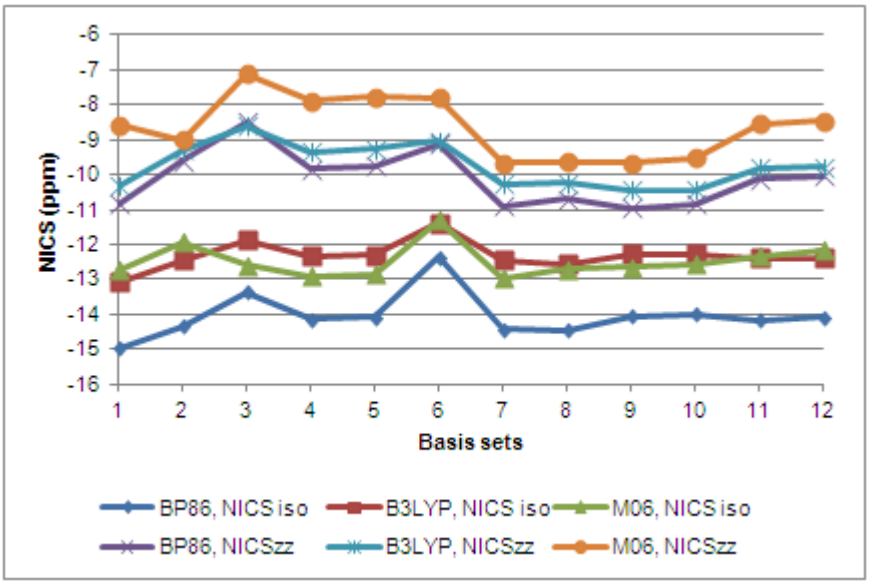

Figure S-22A

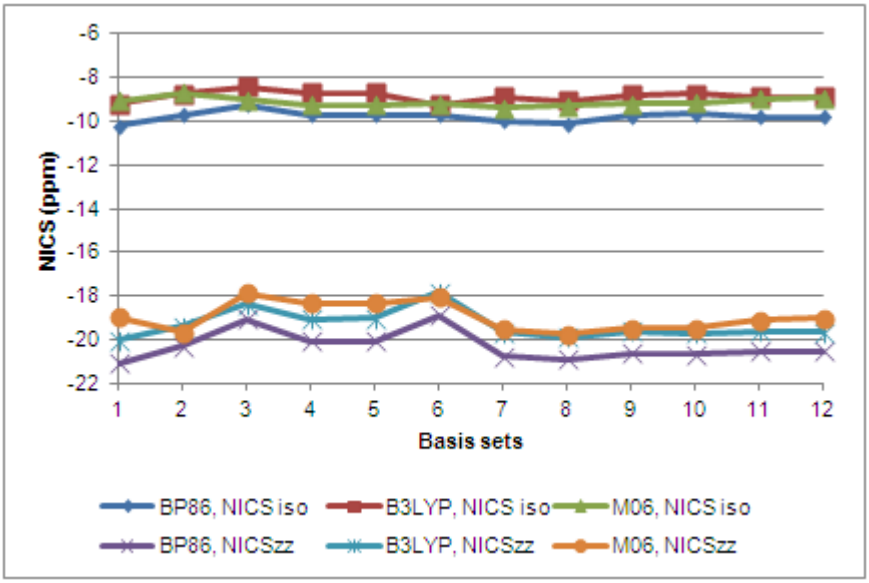

Figure S-22B

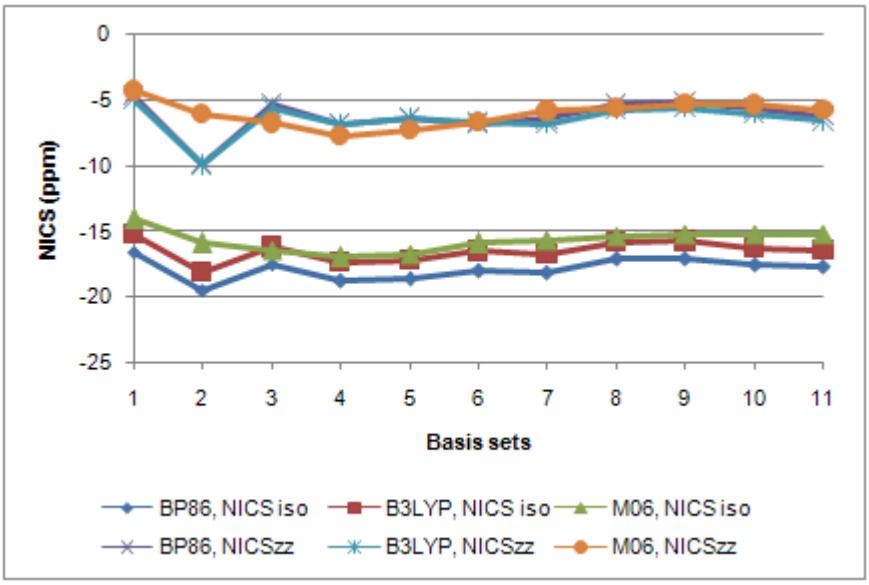

Figure S-23A

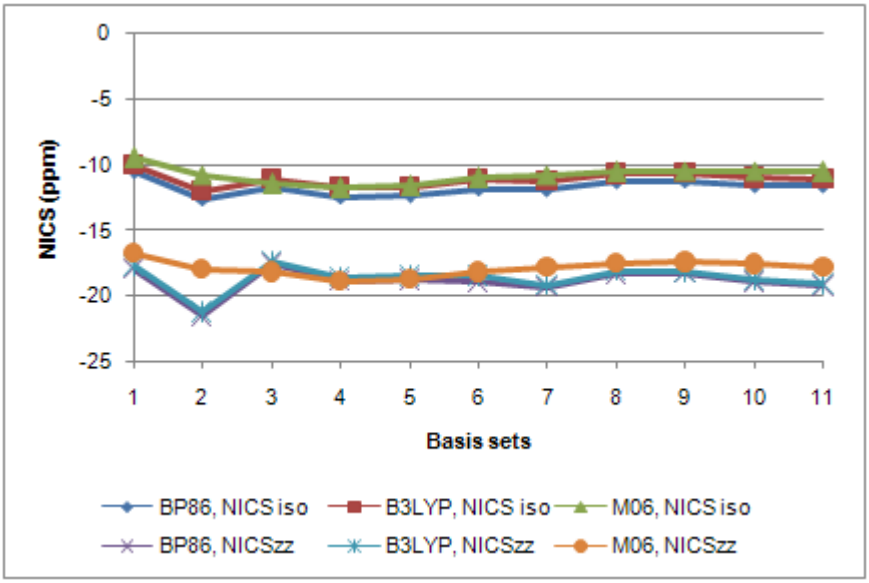

Figure S-23B

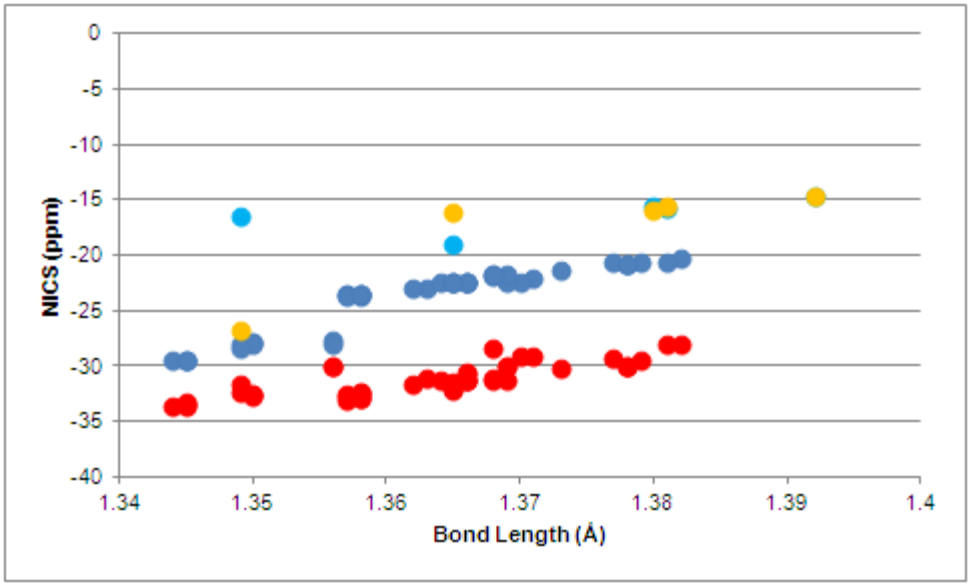

Figure S-24

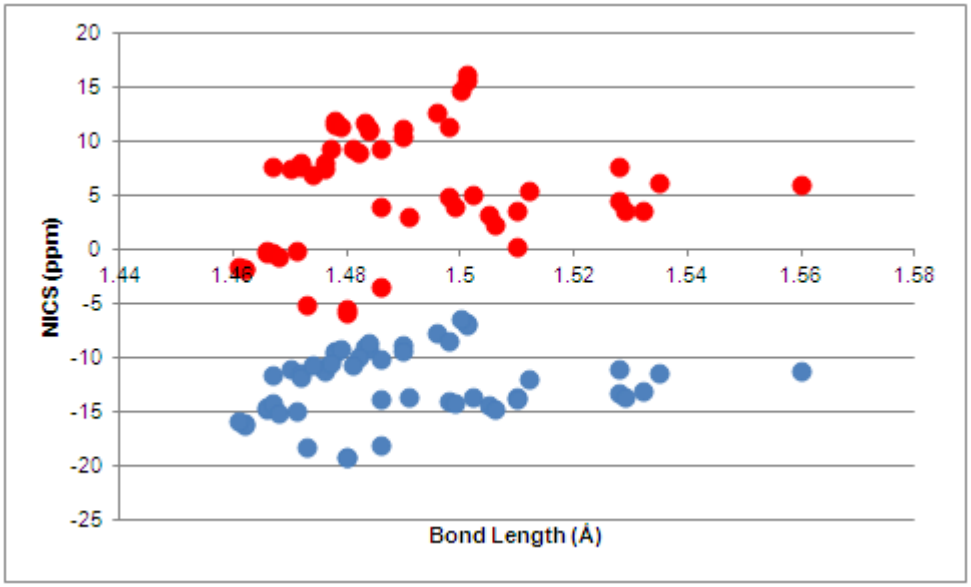

Figure S-25

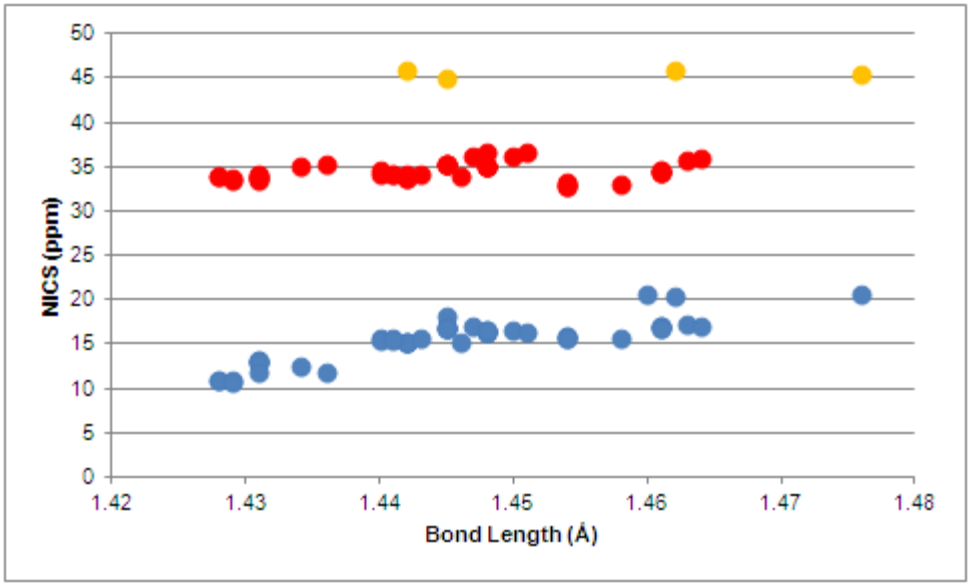

Figure S-26

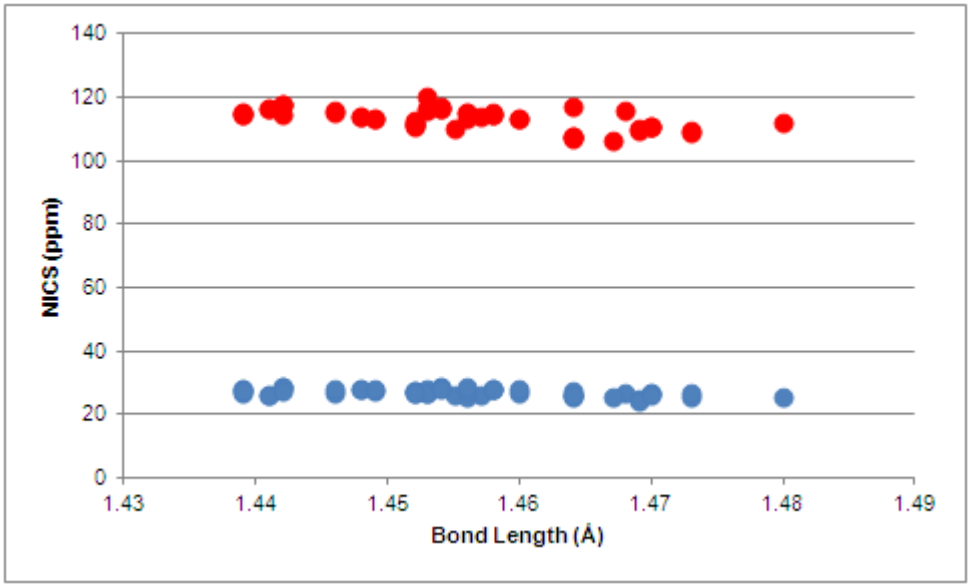

Figure S-27

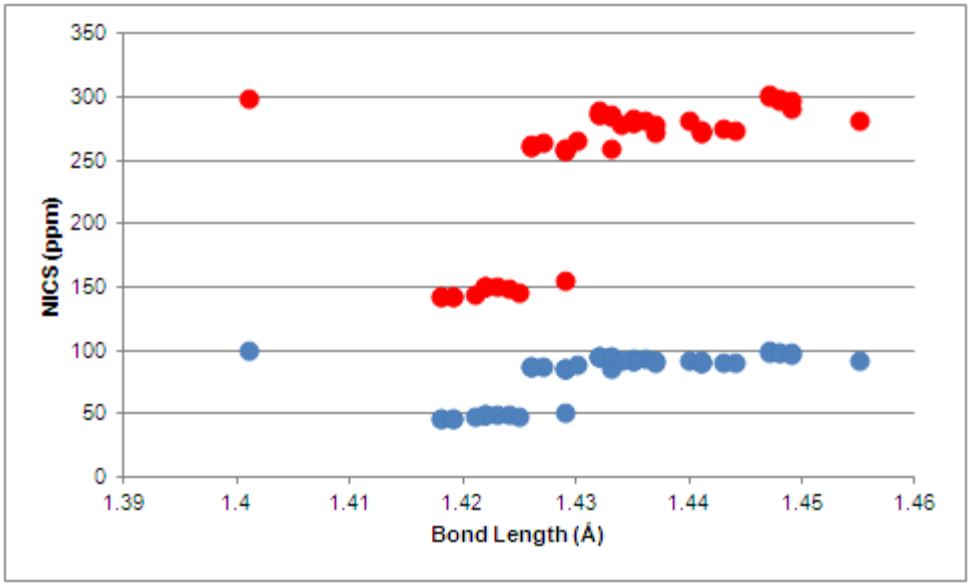

Figure S-28

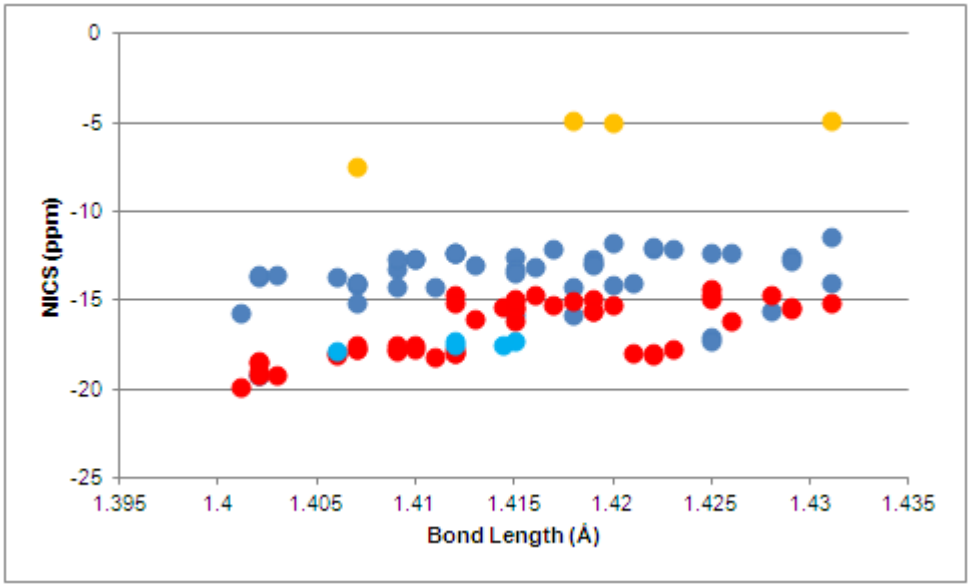

Figure S-29

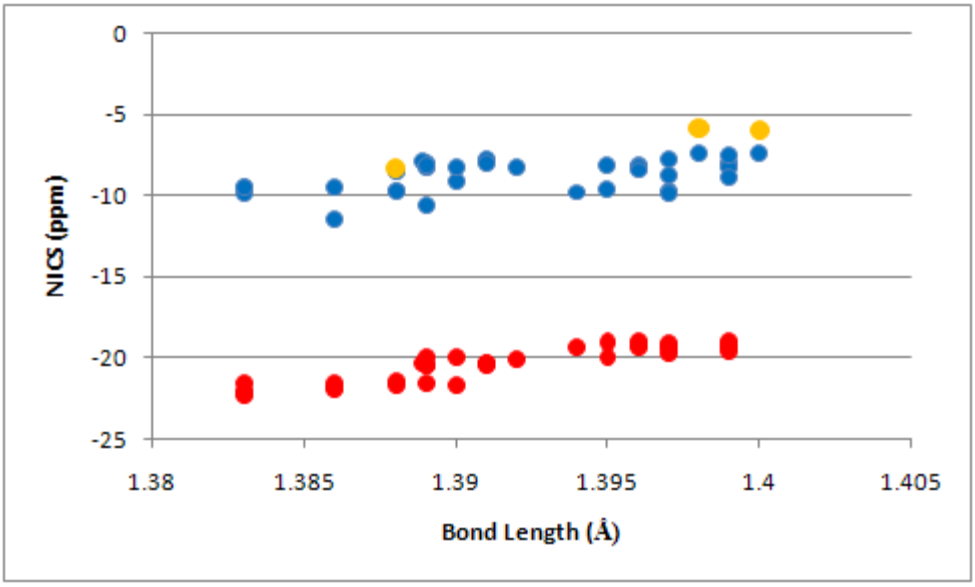

Figure S-30

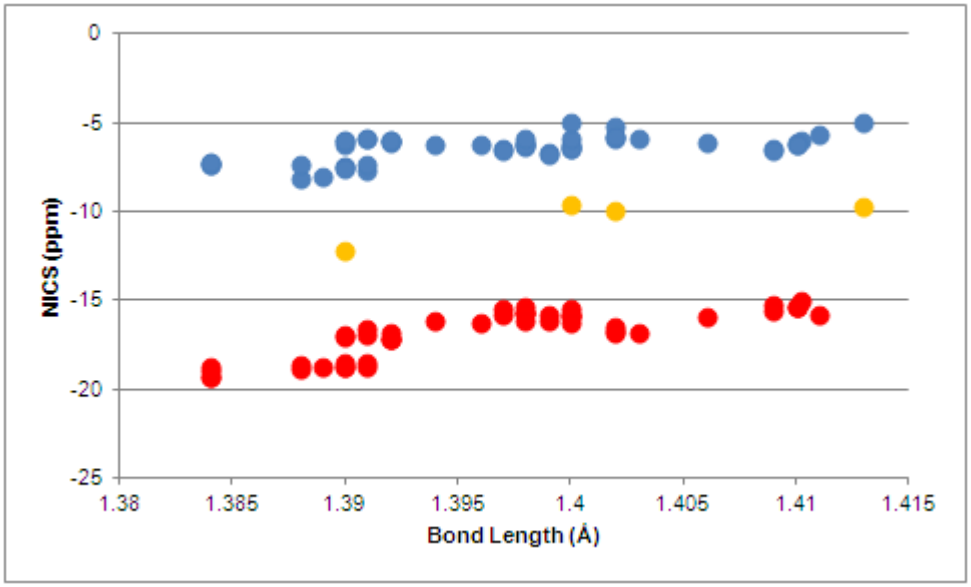

Figure S-31

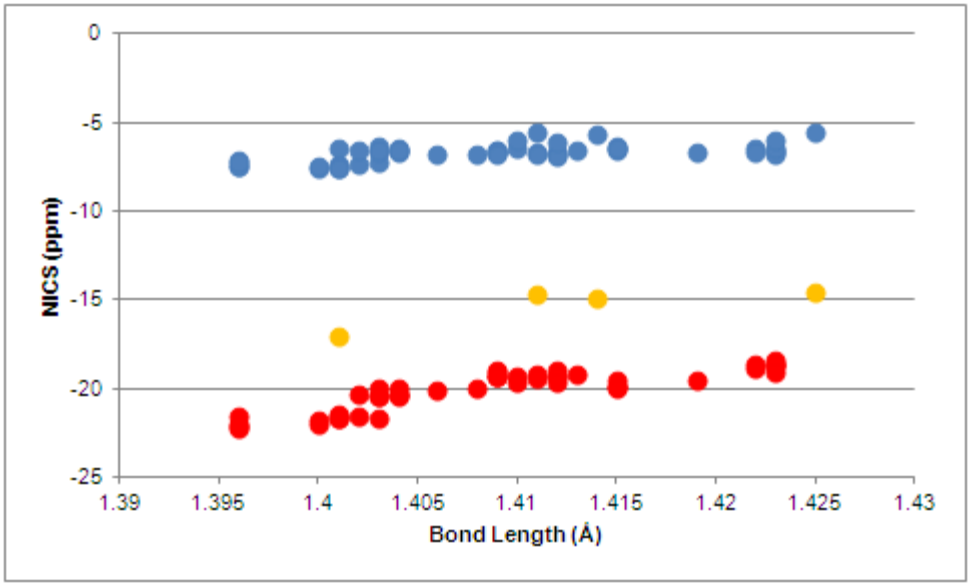

Figure S-32

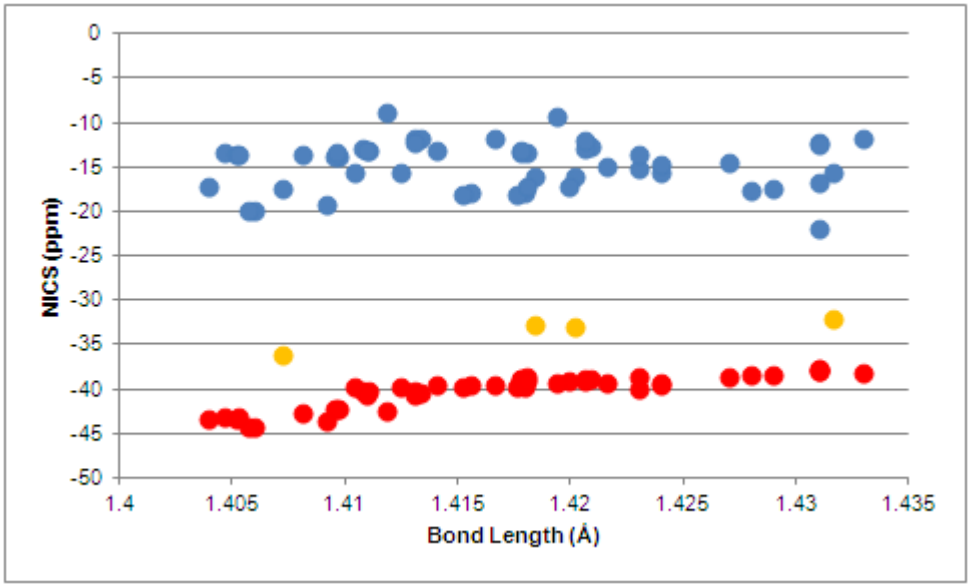

Figure S-33

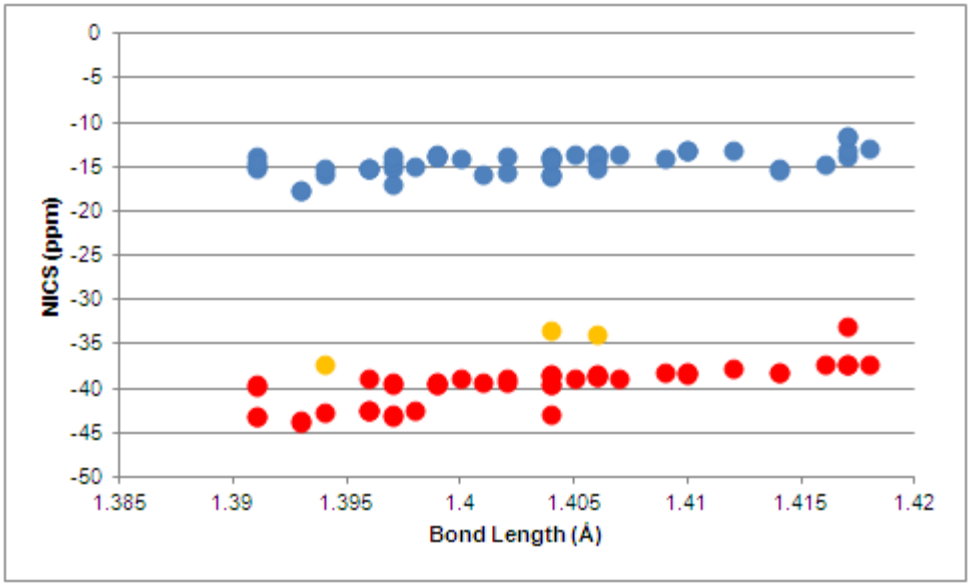

Figure S-34

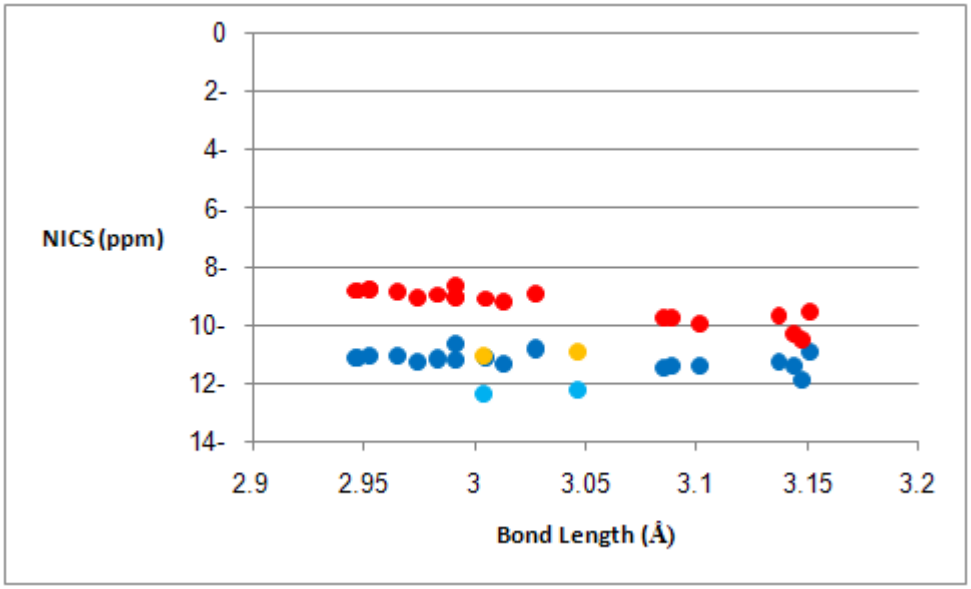

Figure S-35

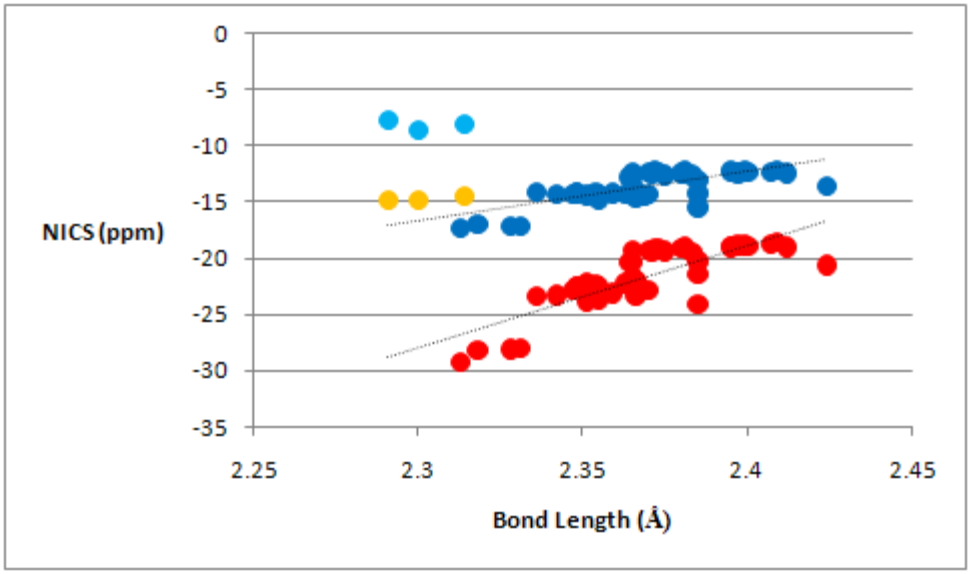

Figure S-36

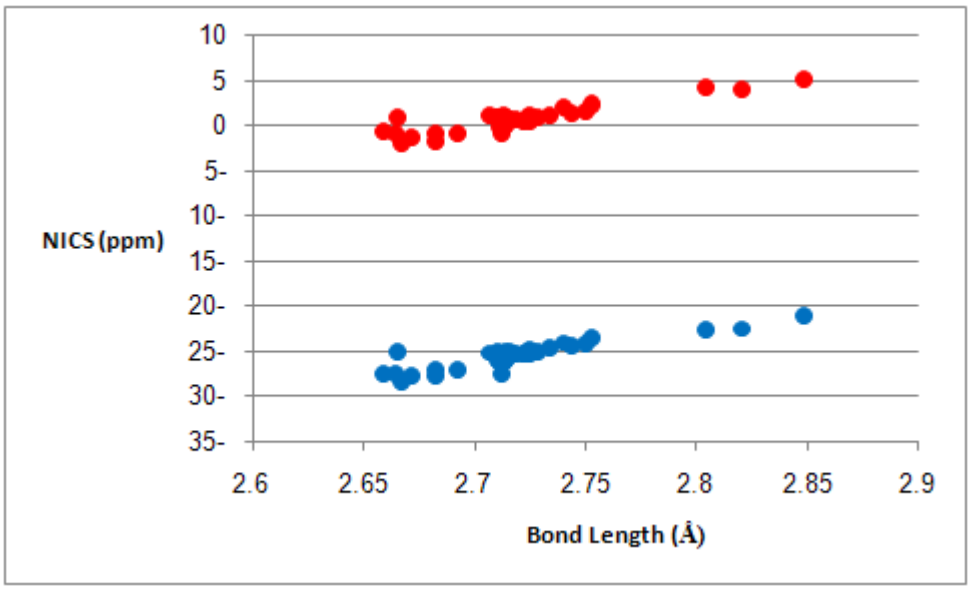

Figure S-37

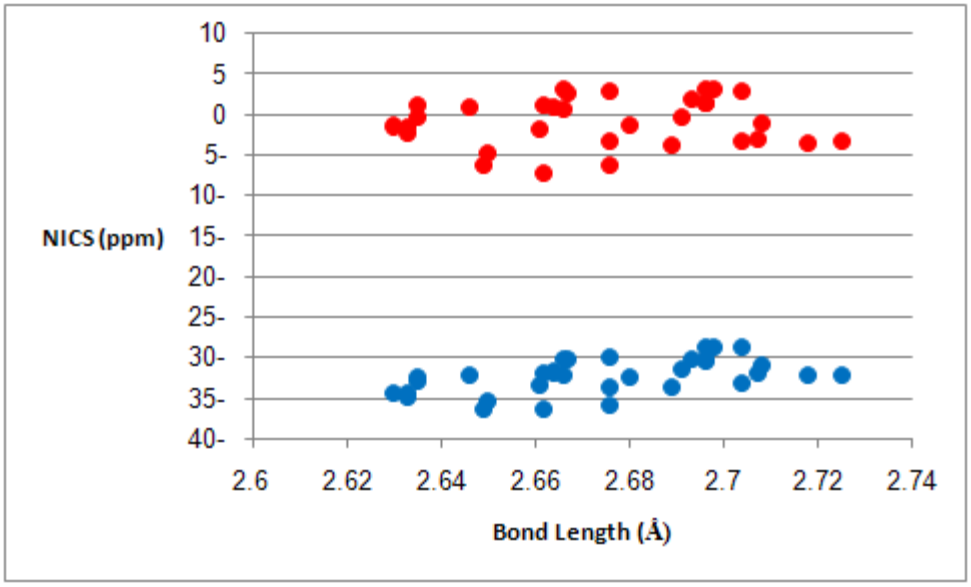

Figure S-38

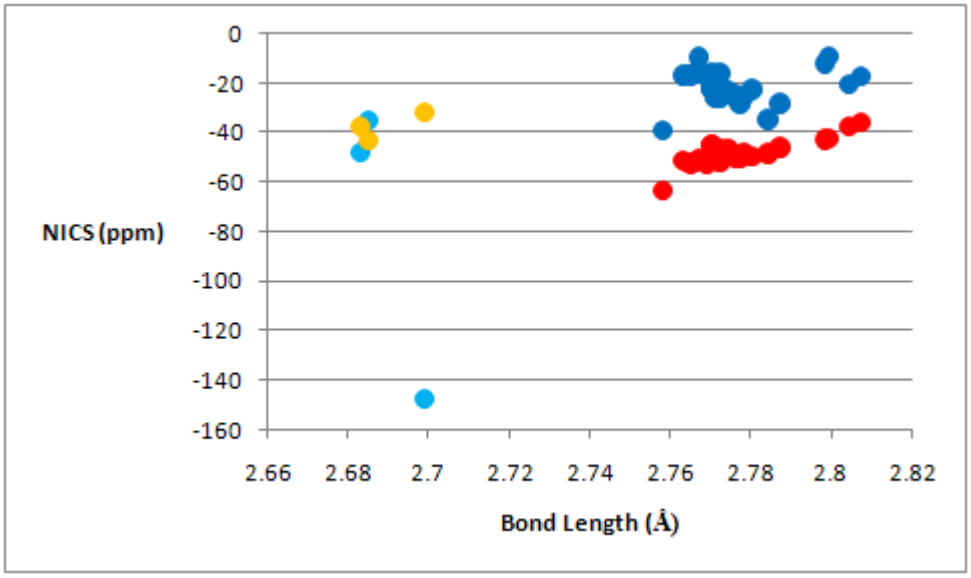

Figure S-39

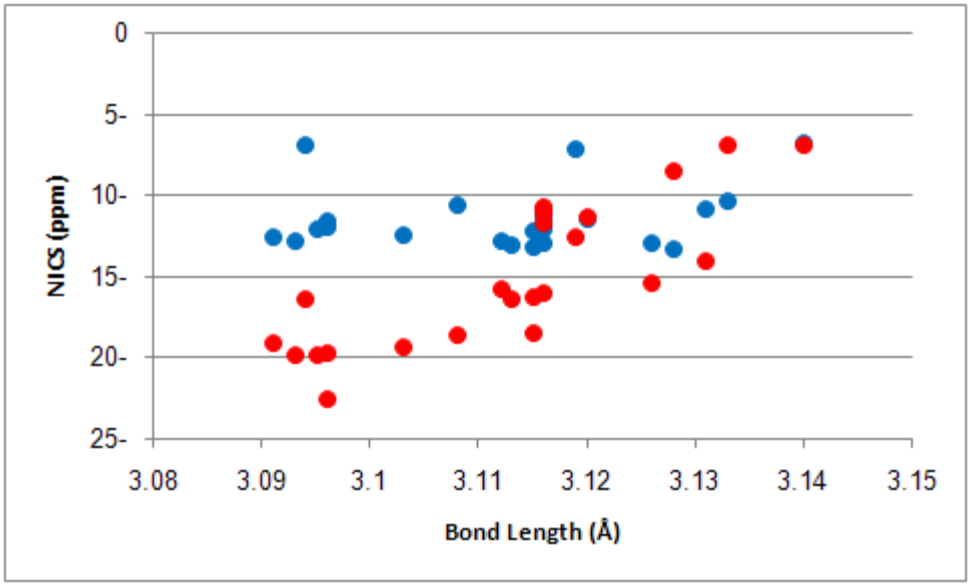

Figure S-40

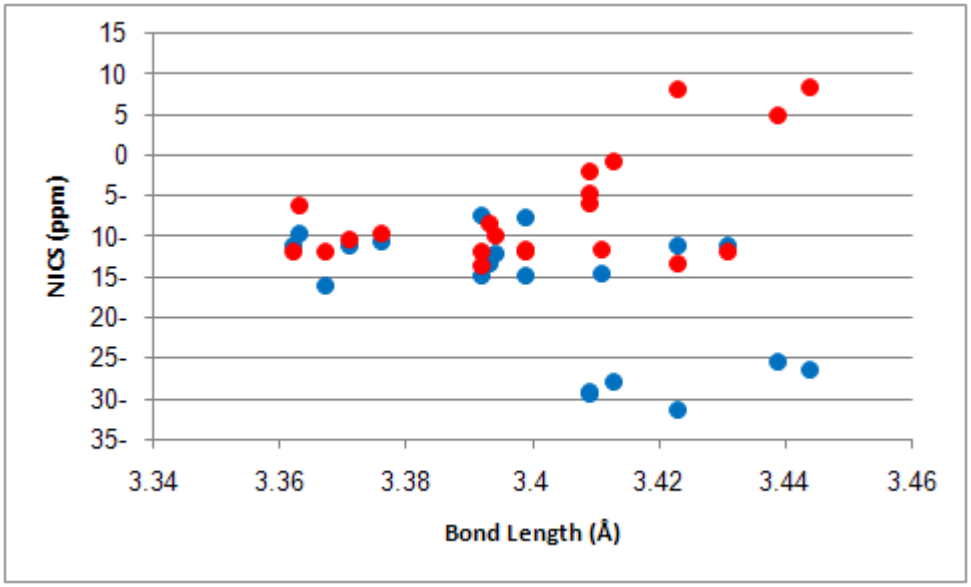

Figure S-41

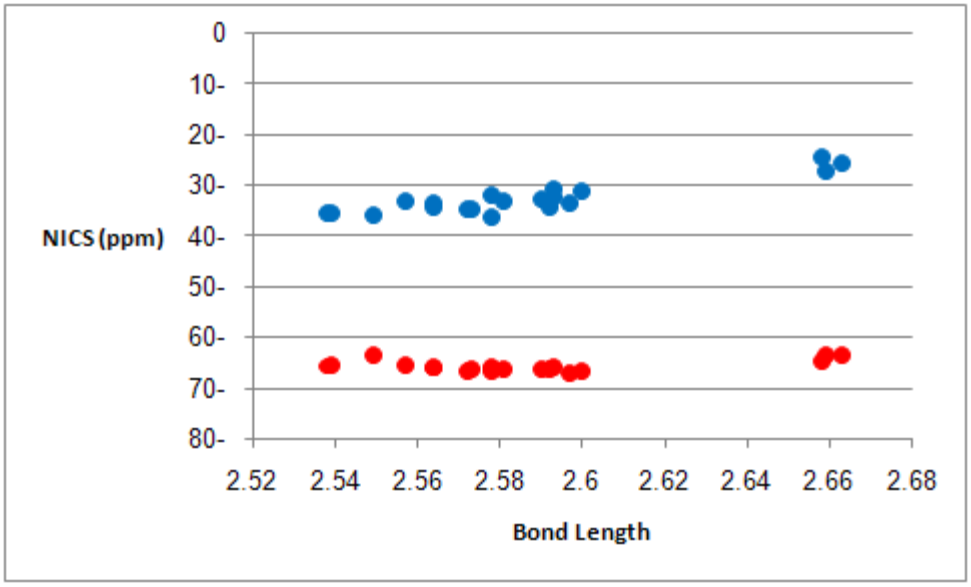

Figure S-42

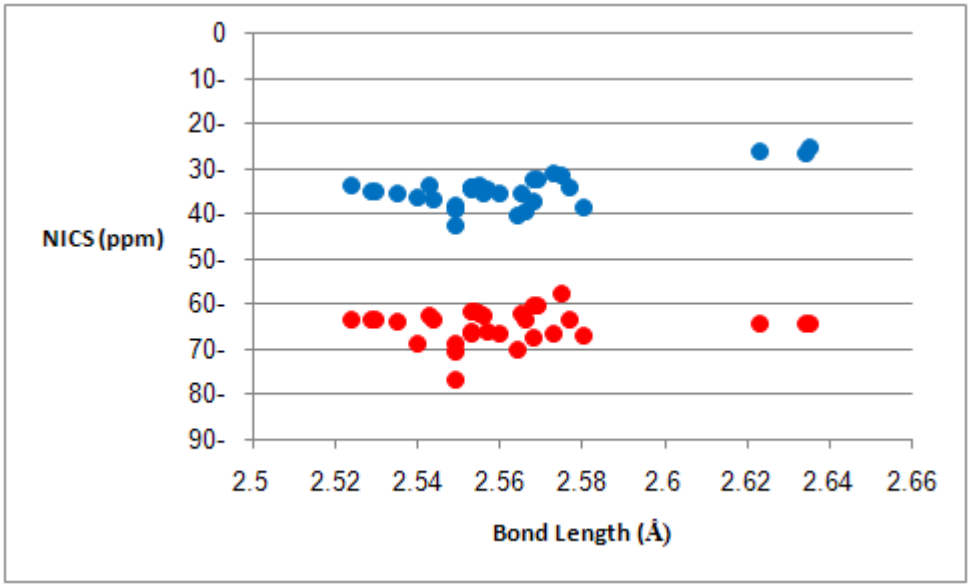

Figure S-43

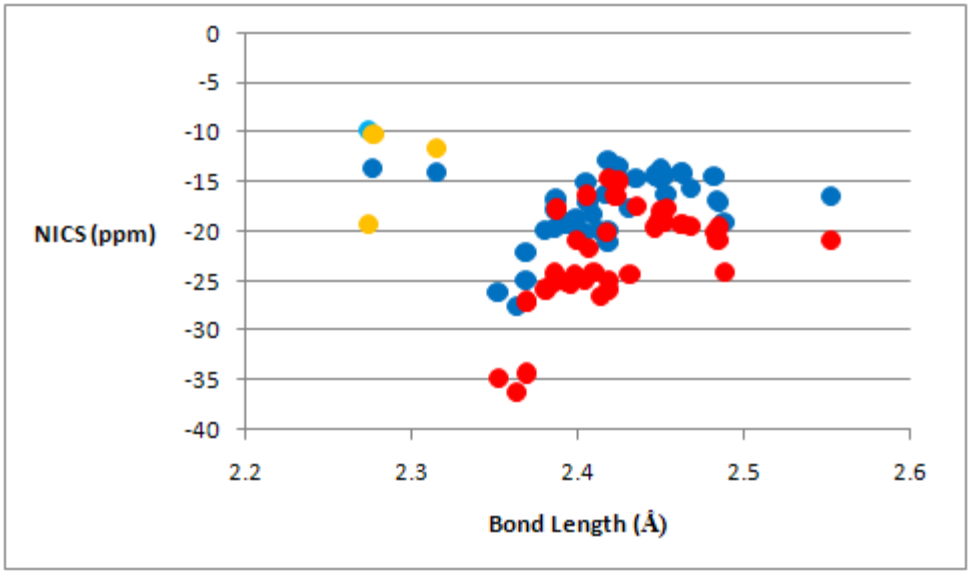

Figure S-44

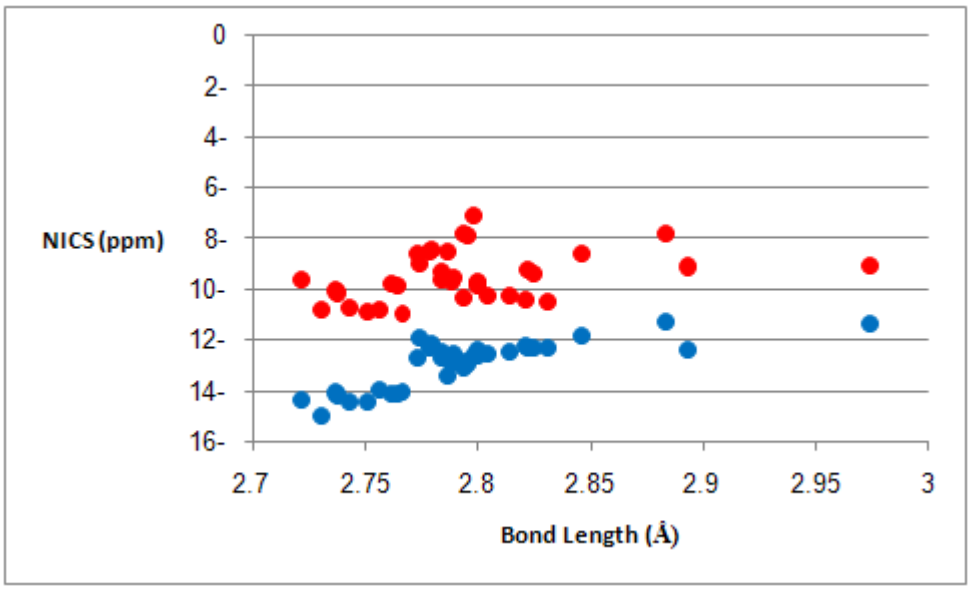

Figure S-45

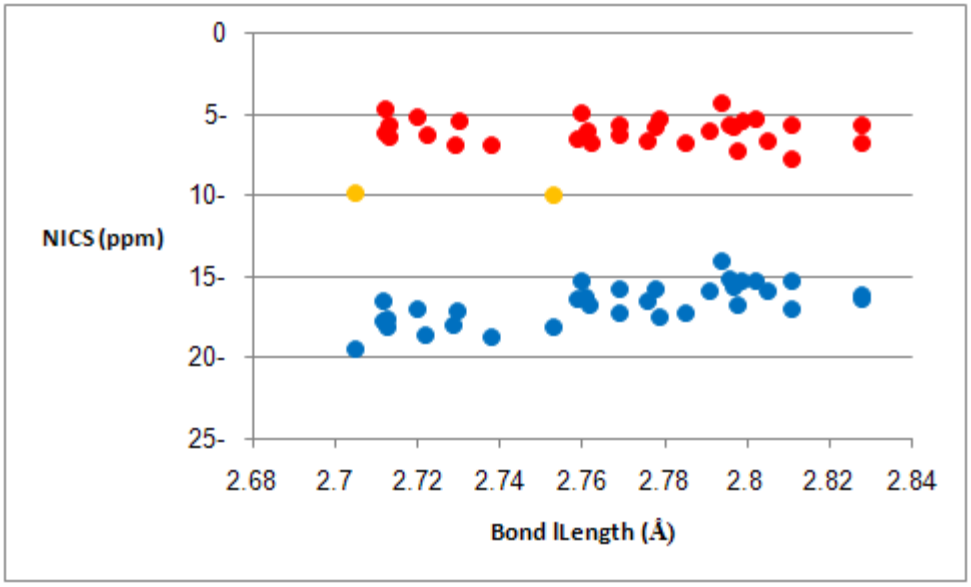
0
5-
10-
15-
20-
25-
NICS (ppm)
2.68
2.7
2.72
2.74
2.76
2.78
2.8
2.82
2.84
Bond lLength (Å)

Figure S-46

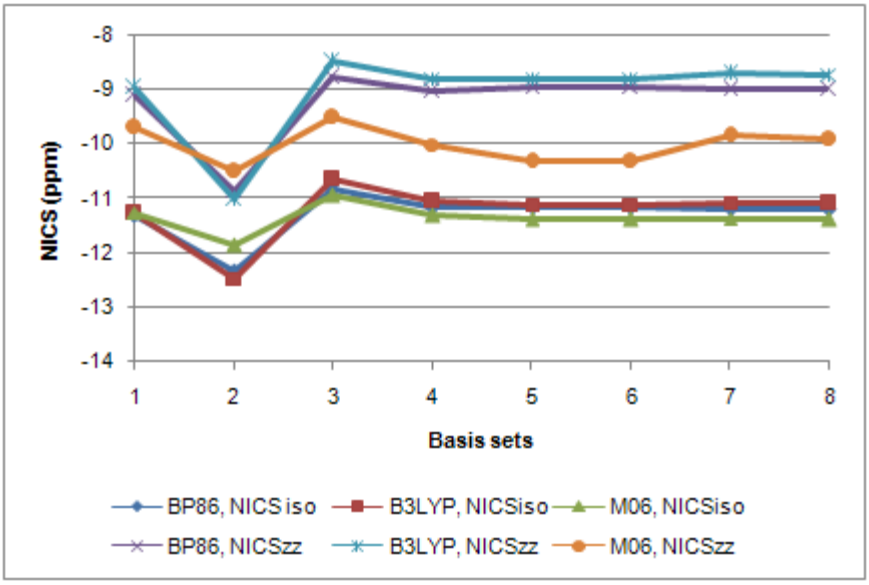

Figure S-47A

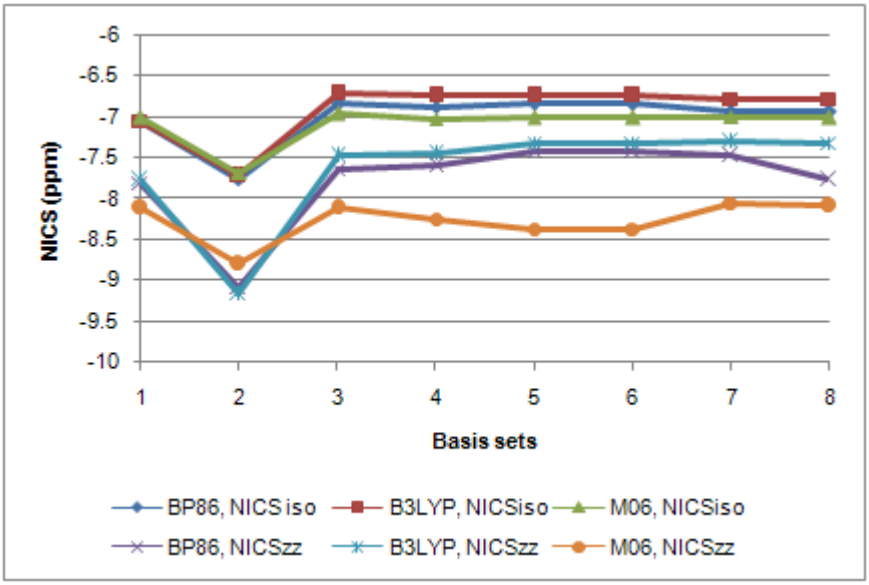

Figure S-47B

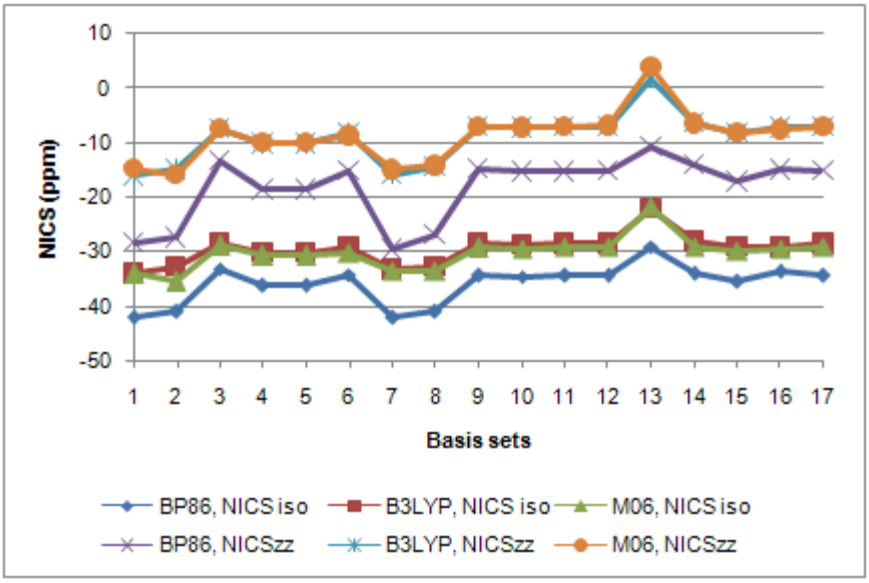

Figure S-48A

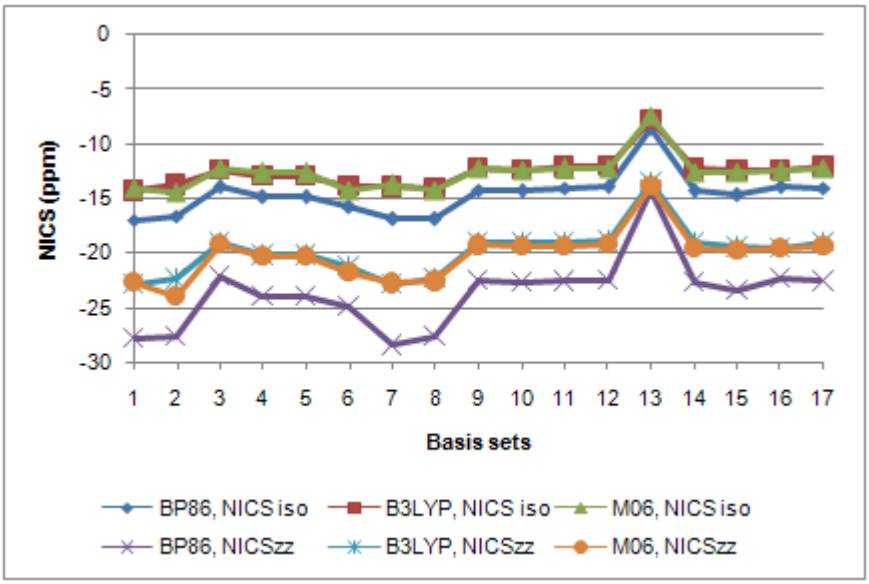

Figure S-48B

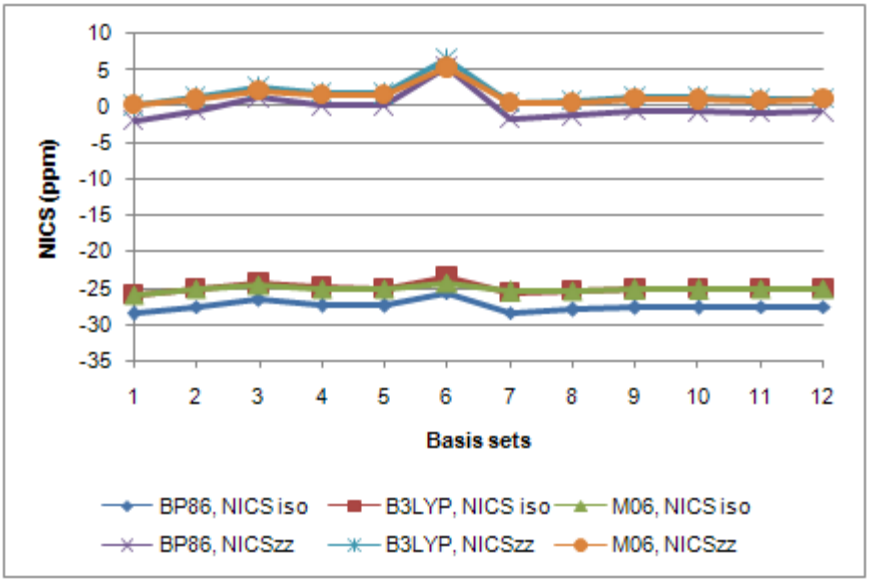

Figure S-49A

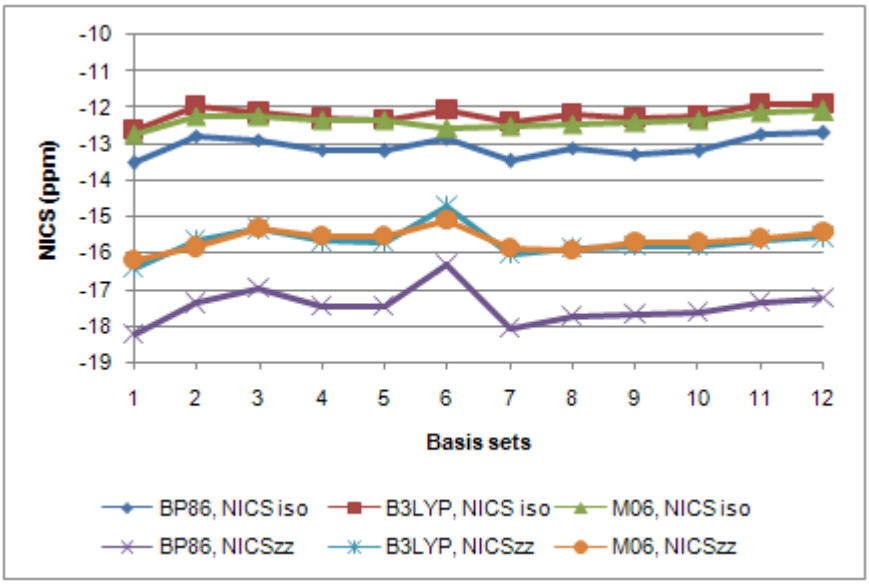

Figure S-49B

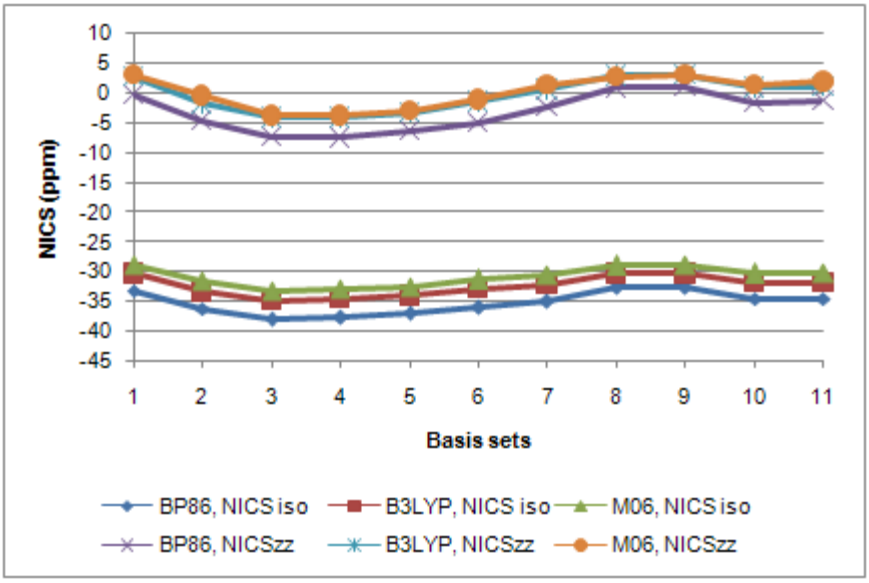

Figure S-50A

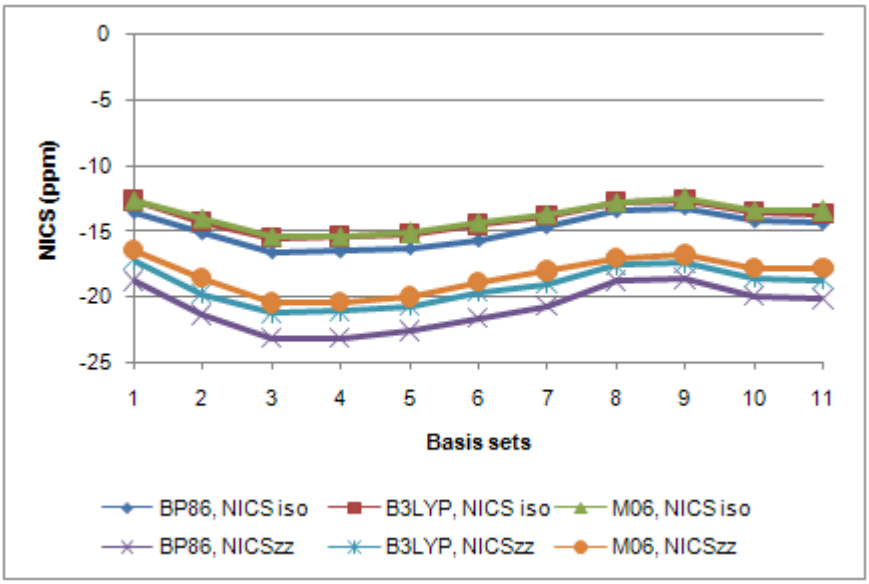

Figure S-50B

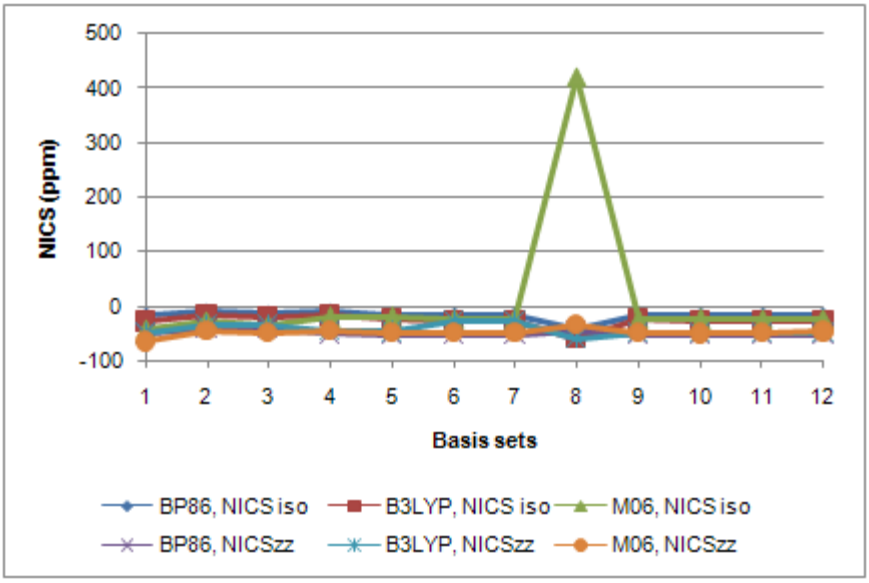

Figure S-51A

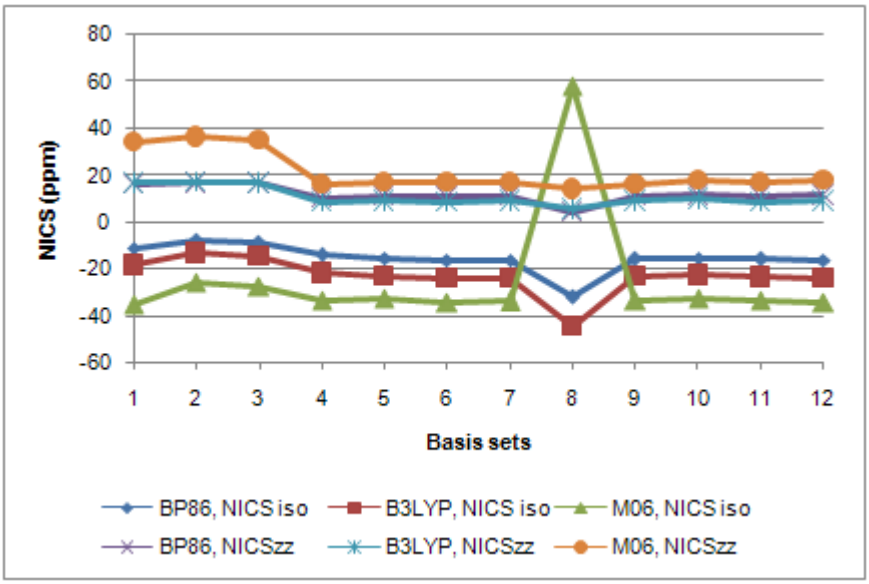

Figure S-51B

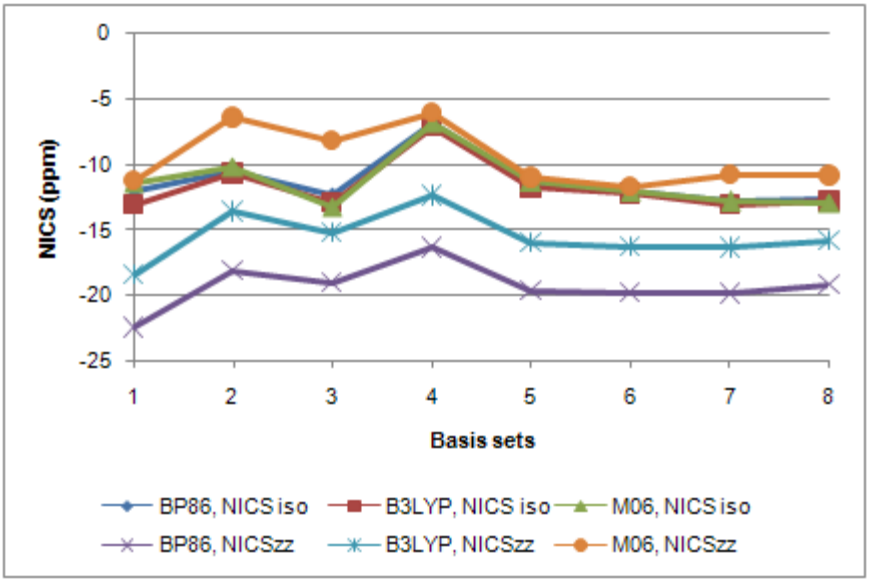

Figure S-52A

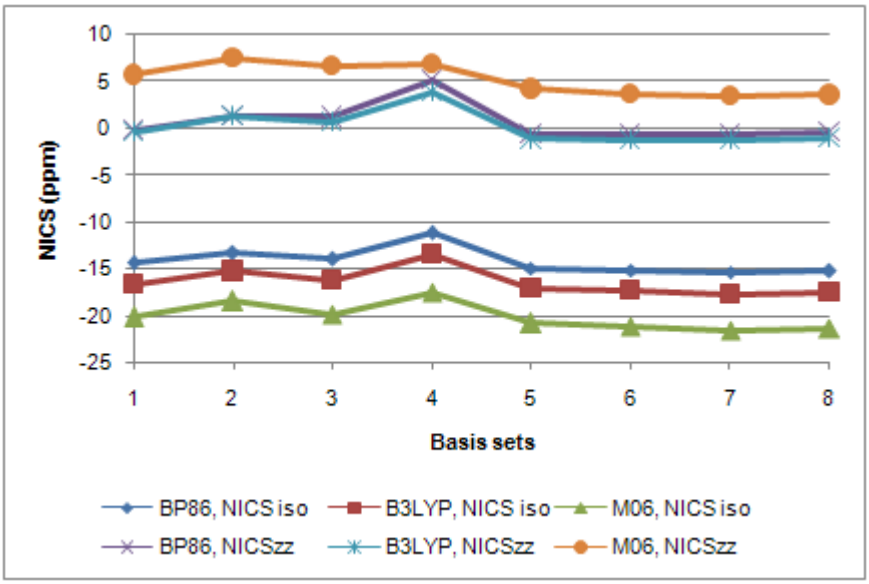

Figure S-52B

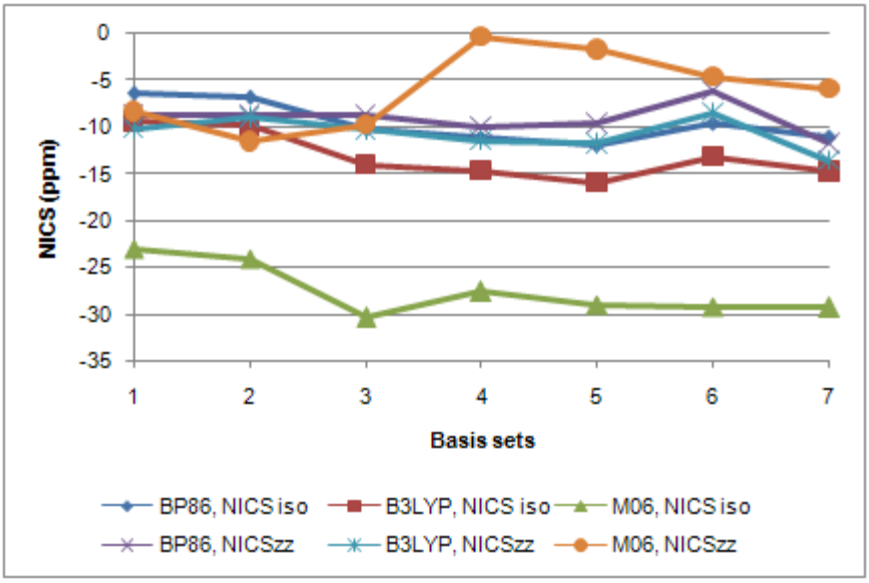

Figure S-53A

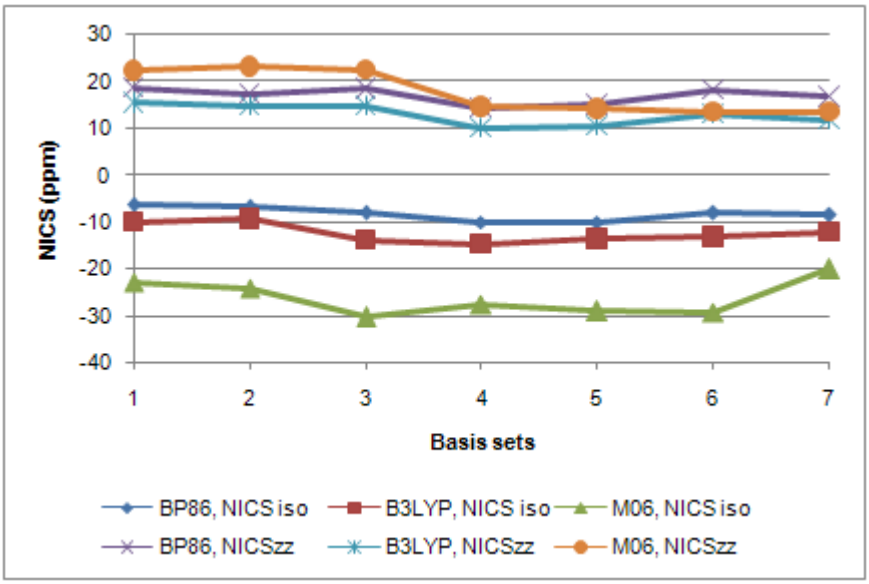

Figure S-53B

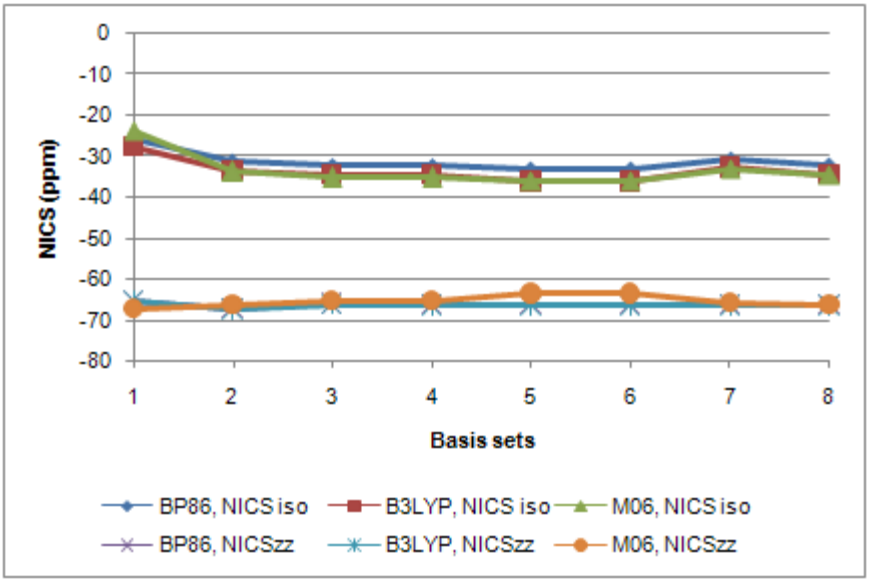

Figure S-54A

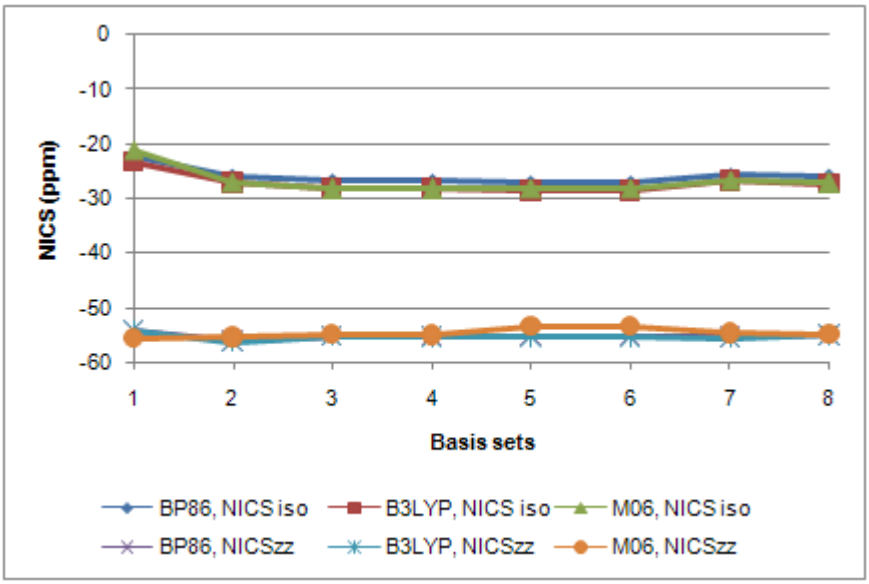

Figure S-54B

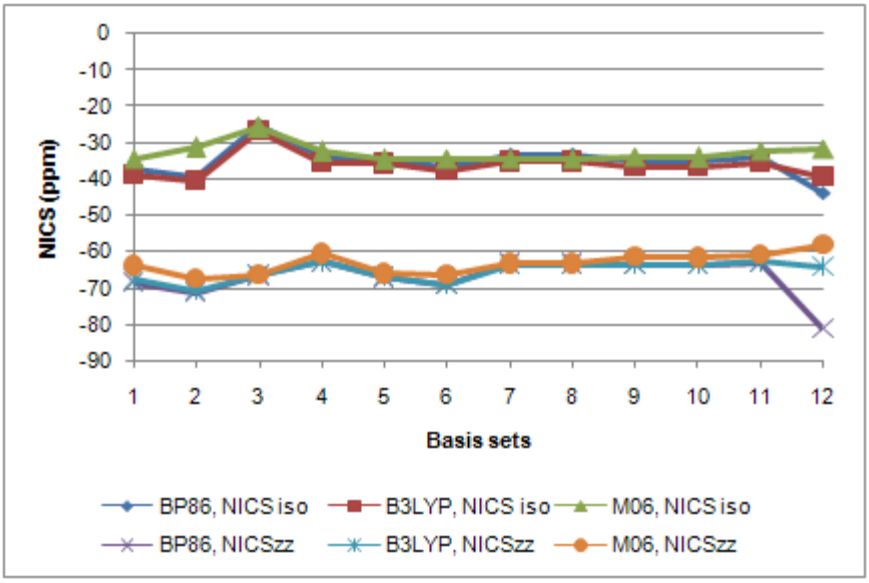

Figure S-55A

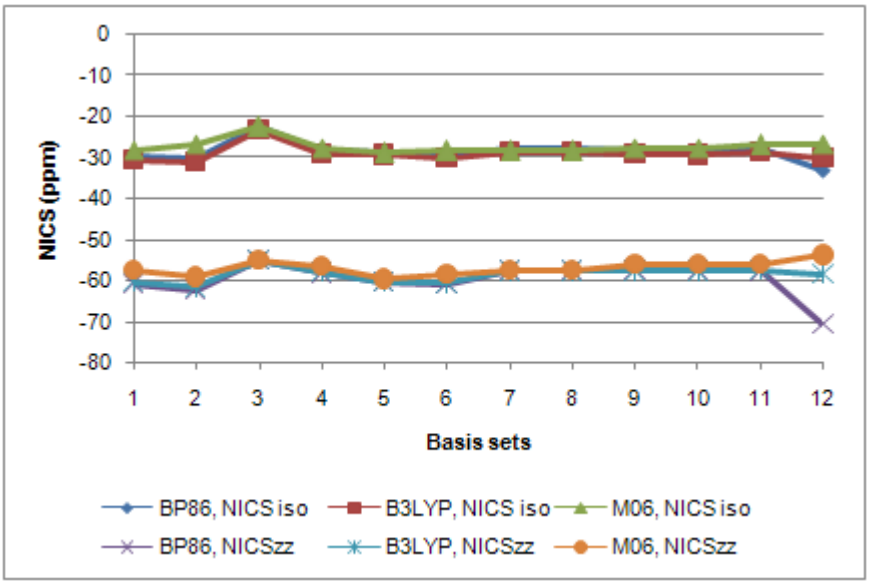

Figure S-55B

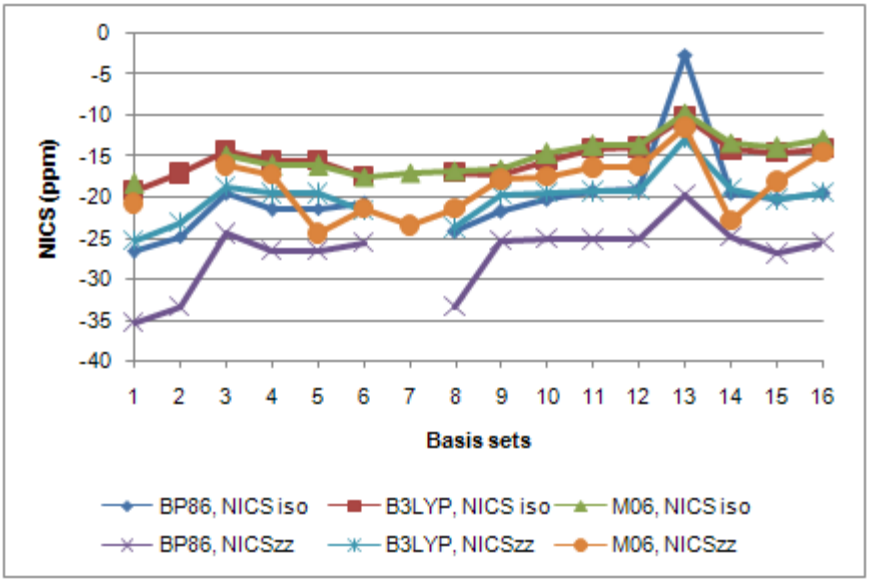

Figure S-56A

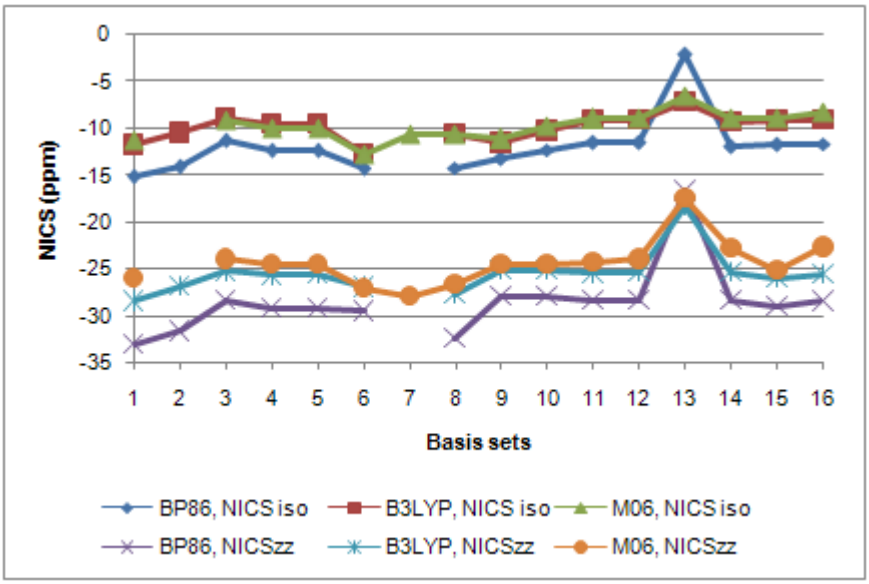

Figure S-56B

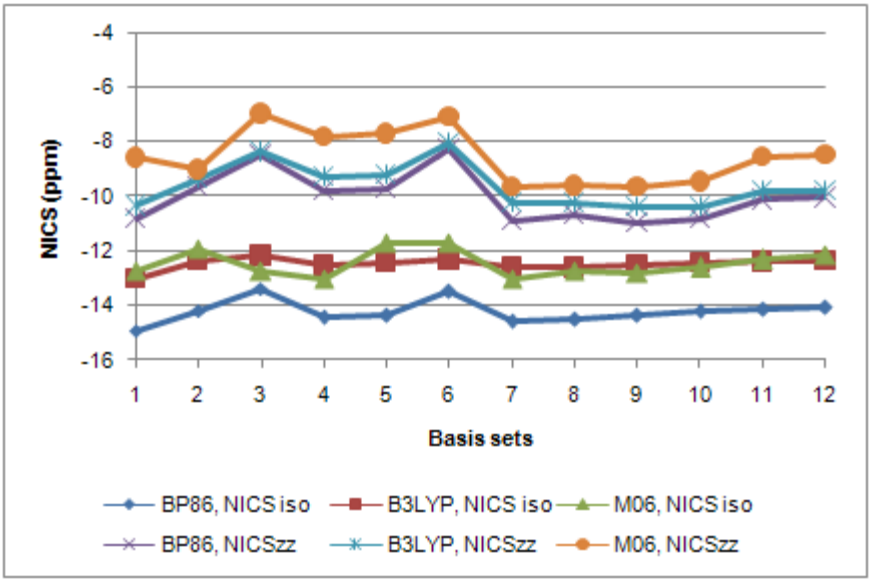

Figure S-57A

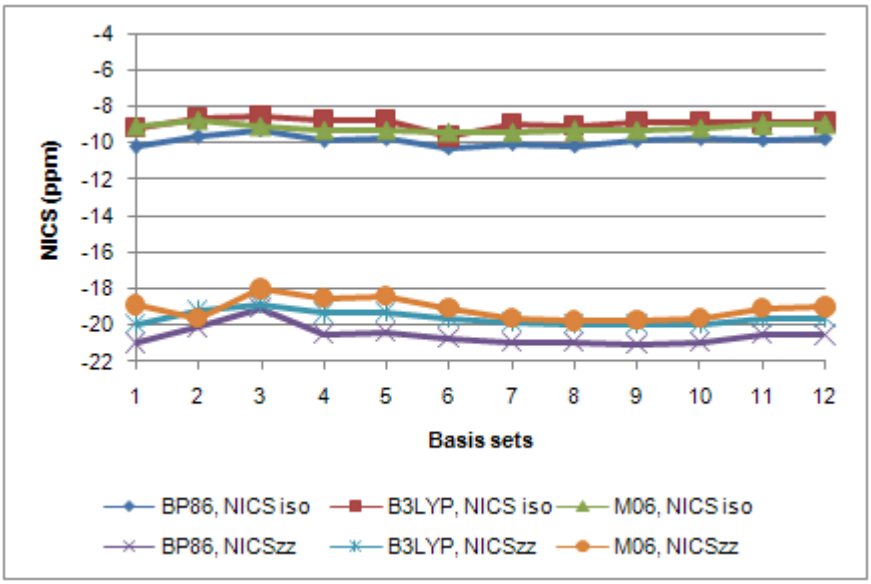

Figure S-57B

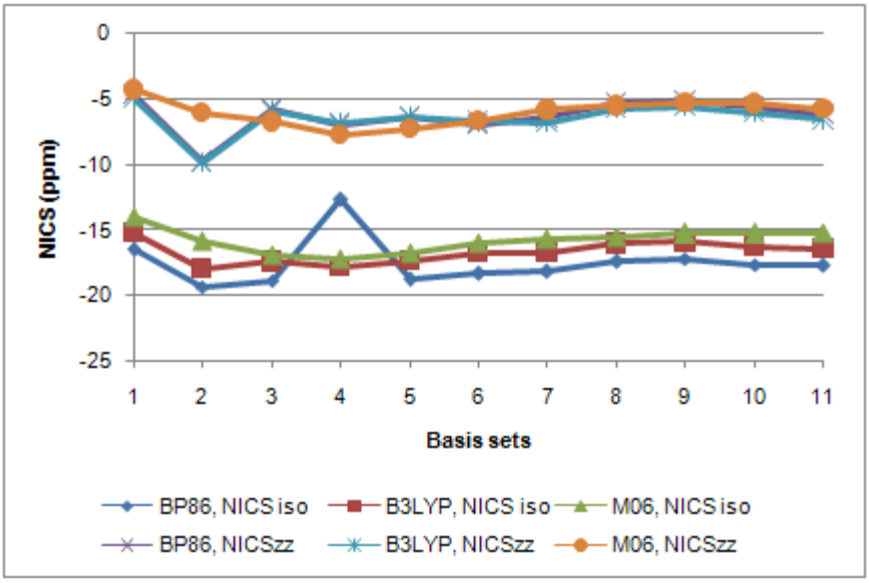

Figure S-58A

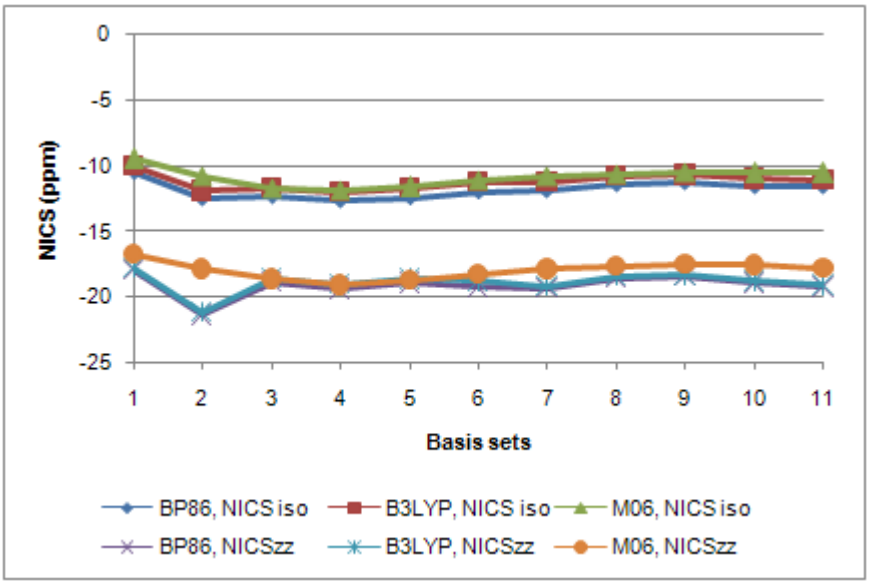

Figure S-58B

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