Supporting Information

The Electronic Structure of Diatomic Nickel Oxide

Nickolas A. Joyner, João Gabriel Farias Romeu, Brian Kent, and David A. Dixon*

The University of Alabama, Department of Chemistry and Biochemistry, Shelby Hall, Tuscaloosa

AL, 35487-0336, USA

Email: David A. Dixon dadixon@ua.edu

Ref. 60. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian 16, Revision A.03, Gaussian, Inc., Wallingford CT, **2016**.

Ref. 62. Werner, H.-J.; Knowles, P. J.; Manby, F. R.; Black, J. A.; Doll, K.; Heßelmann, A.; Kats, D.; Köhn, A.; Korona, T.; Kreplin, D. A.; Ma, Q.; Miller, T. F., III; Mitrushchenkov, A.; Peterson, K. A.; Polyak, I.; Rauhut, G.; Sibaev, M. The Molpro Quantum Chemistry Package. *J. Chem. Phys*. **2020**, *152*, 144107.

Ref. 63. Werner, H.-J.; Knowles, P. J.; Knizia, G.; Manby, F. R.; Schütz, M.; Celani, P.; Györffy, W.; Kats, D.; Korona, T.; Lindh, R.; Mitrushenkov, A.; Rauhut, G.; Shamasundar, K. R.; Adler, T. B.; Amos, R. D.; Bennie, S. J.; Bernhardsson, A.; Berning, A.; Cooper, D. L.; Deegan, M. J. O.; Dobbyn, A. J.; Eckert, F.; Goll, E.; Hampel, C.; Hesselmann, A.; Hetzer, G.; Hrenar, T.; Jansen, G.; Köppl, C.; Lee, S. J. R.; Liu, Y.; Lloyd, A. W.; Ma, Q.; Mata, R. A.; May, A. J.; McNicholas, S. J.; Meyer, W.; Miller , T. F., III; Mura, M. E.; Nicklass, A.; O'Neill, D. P.; Palmieri, P.; Peng, D.; Petrenko, T.; Pflüger, K.; Pitzer, R.; Reiher, M.; Shiozaki, T.; Stoll, H.; Stone, A. J.; Tarroni, R.; Thorsteinsson, T.; Wang, M.; Welborn, M. MOLPRO, version 2020.1, a package of ab initio programs, see https://www.molpro.net.

Table S1. Absolute energies (Hartrees) of Ni, O, and NiO at the icMRCI+Q/awn-DK, CCSD(T)/an-DK, CCSD(T)/awn-DK, and RKS-CCSD(T)/awn-DK levels.

Method	Basis set	State	Electronic Energy	R (Å) (opt)
CASSCF	awQ-DK	Triplet	-1594.020236	1.680
CASSCF	awQ-DK	Quintet	-1594.025192	1.780
icMRCI+Q	awT-DK	Triplet	-1594.617182	1.602
icMRCI+Q	awQ-DK	Triplet	-1594.649092	1.600
icMRCI+Q	awQ-DK	Quintet	-1594.642726	1.680
icMRCI+Q (BDE calc.)	awT-DK	Triplet	-1594.616654	1.602
icMRCI+Q (BDE calc.)	awT-DK	Triplet	-1594.468467	6.000[a]
icMRCI+Q (BDE calc.)	awQ-DK	Triplet	-1594.648711	1.600
icMRCI+Q (BDE calc.)	awQ-DK	Triplet	-1594.496842	6.000[a]
icMRCI+Q (BDE calc.)	CBS awn-DK	Triplet	-1594.667214	1.599
icMRCI+Q (BDE calc.)	CBS awn-DK	Triplet	-1594.513218	6.00 [a]
CCSD(T) NiO	aD-DK	Triplet	-1594.530630	1.636
CCSD(T) NiO	aT-DK	Triplet	-1594.648699	1.625
CCSD(T) NiO	aQ-DK	Triplet	-1594.693755	1.623
CCSD(T) NiO	awT-DK	Triplet	-1595.114970	1.625
CCSD(T) NiO	awQ-DK	Triplet	-1595.198462	1.624
CCSD(T) NiO	CBS awn-DK	Triplet	-1595.246651	1.624[b]
RKS-CCSD(T) NiO	awT-DK	Triplet	-1595.111563	1.615
RKS-CCSD(T) NiO	awQ-DK	Triplet	-1595.194258	1.614
RKS-CCSD(T) NiO	CBS awn-DK	Triplet	-1595.241987	1.614[b]
CCSD(T) NiO	awT-DK	Quintet	-1595.057724	1.685
CCSD(T) NiO	awQ-DK	Quintet	-1595.139342	1.684
CCSD(T) NiO	CBS awn-DK	Quintet	-1595.186449	1.683[b]
CCSD(T) O	aT-DK	Triplet	-75.04261954	
CCSD(T) O	aQ-DK	Triplet	-75.07747370	
CCSD(T) O	CBS an-DK	Triplet	-75.09759026	
CCSD(T) Ni	awT-DK	Triplet	-1519.924437	
CCSD(T) Ni	awQ-DK	Triplet	-1519.972133	
CCSD(T) Ni	CBS awn-DK	Triplet	-1519.999662	

[a] Separated atoms for BDE calculation. [b] Value obtained from extrapolated energies with subsequent curve refitting.

Table S2. Absolute energies (Hartrees) and bond distances (Å) of NiO at the DFT Level

Functional	Electronic Energy	R_e
B1B95	-244.776736	1.605
B1LYP	-244.672414	1.612
B3LYP	-244.819987	1.611
B3P86	-245.362026	1.601
B3PW91	-244.816634	1.605
B971	-244.711421	1.651
B972	-244.958305	1.608
B98	-244.749661	1.650
BP86	-244.932610	1.616
BMK	-244.050022	1.603
CAM-B3LYP	-244.670260	1.647
HSE06	-244.660065	1.602
HS06	-244.660416	1.602
HSE03	-244.948340	1.603
LC-ωPBE	-244.769096	1.590
M052X	-244.748685	1.621
M05	-244.844554	1.623
M062X	-244.757015	1.625
M06	-244.788893	1.599
M06HF	-244.709253	1.673
M08HX	-244.611761	1.632
M11	-244.705945	1.618
MN12SX	-243.221620	1.595
MN15	-244.890237	1.624
mPW1LYP	-244.672156	1.611
mPW1PBE	-244.739963	1.605
mPW1PW91	-244.791719	1.602
mPW3PBE	-244.774328	1.603
N12SX	-244.253231	1.645
O3LYP	-245.006141	1.616
PBE1PBE	-244.656418	1.602
PBEh1PBE	-244.661570	1.602
PBE	-244.755298	1.617
PBE0	-244.436199	1.600
PW91	-244.887901	1.617
SOGGA11X	-244.645748	1.663
SVWN5	-243.983381	1.586
τ-HCTH	-245.436178	1.621
TPSSh	-244.733401	1.611
ωB97	-244.813024	1.596
ωB97X	-244.708437	1.644
ωB97XD	-244.712788	1.652

X3LYP	-244.735765	1.610