Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

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

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