Supplementary Online Materials for

Infrared Spectroscopy and Structure of $(NO)_n$ Clusters

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$(NO)_3$ – C_s point group

E(MRMP2(3,3)/QZ) = –389.260268 hartree

ATOM	CHARGE	X	Y	Z
N	7.0	0.7188301741	-0.4951749406	1.2351765960
N	7.0	0.7188301741	-0.4951749406	-1.2351765960
O	8.0	1.5643434342	0.2987672799	1.2262333113
O	8.0	1.5643434342	0.2987672799	-1.2262333113
N	7.0	-1.8465058291	0.5182442819	0.0000000000
O	8.0	-2.7695082775	-0.1856834902	0.0000000000

$(NO)_2$ ------- (NO) – C_s point group (super system of dimer + monomer separated by large distance)

E(MRMP2(3,3)/QZ) = –389.257857 hartree

ATOM	CHARGE	X	Y	Z
N	7.0	0.7179626927	-0.4954167329	1.2362267491
N	7.0	0.7179626927	-0.4954167329	-1.2362267491
O	8.0	1.5631350743	0.2990060339	1.2290505271
O	8.0	1.5631350743	0.2990060339	-1.2290505271
N	7.0	-101.8449298867	0.5190033591	0.0000000000
O	8.0	-102.7669325373	-0.1864364909	0.0000000000

$(NO)_4$ – C_i point group

E(MRMP2(4,4)/QZ) = –519.021552 hartree

ATOM	CHARGE	X	Y	Z
N	7.0	1.9304682211	-1.0355713953	0.4446020835
N	7.0	-1.9304682211	1.0355713953	-0.4446020835
O	8.0	2.7178271420	-0.6050845978	-0.2922488593
O	8.0	-2.7178271420	0.6050845978	0.2922488593
N	7.0	0.8551612587	1.0939111523	0.5659725214
N	7.0	-0.8551612587	-1.0939111523	-0.5659725214
O	8.0	1.6370830854	1.5406797688	-0.1672271168
O	8.0	-1.6370830854	-1.5406797688	0.1672271168

$(NO)_2$ ------- $(NO)_2$ – C_i point group (super system of dimer + dimer separated by large distance)

E(MRMP2(4,4)/QZ) = –519.017501 hartree

ATOM	CHARGE	X	Y	Z
N	7.0	33.9243180666	39.5474891508	21.5628022872
N	7.0	-33.9243180666	-39.5474891508	-21.5628022872
O	8.0	34.7056791307	39.9897865862	20.8262350000
O	8.0	-34.7056791307	-39.9897865862	-20.8262350000
N	7.0	32.7845896874	41.6472139769	21.6521112493
N	7.0	-32.7845896874	-41.6472139769	-21.6521112493
O	8.0	33.5549778356	42.1097325118	20.9164062340
O	8.0	-33.5549778356	-42.1097325118	-20.9164062340