Supplementary Material for manuscript

Crystallographic and theoretical study of osme bonds in nitrido-osmium(VI) complexes

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Cartesian Coordinates

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Os	0.0000000	0.0000000	-3.7754260
Cl	-0.0000000	-2.2452362	-4.3533015
Cl	2.2349415	0.0000000	-4.3803476
Cl	-0.0000000	2.2452362	-4.3533015
Cl	-2.2349415	0.0000000	-4.3803476
N	0.0000000	0.0000000	-2.1581439
N	0.0000000	0.0000000	1.3727567
C	0.0000000	-1.2310377	0.5264419
C	1.2148022	0.0000000	2.2285074
C	0.0000000	1.2310377	0.5264419
C	-1.2148022	0.0000000	2.2285074
H	-0.8811042	-1.2280703	-0.1105126
H	0.0000000	-2.0966657	1.1875079
H	2.0940015	0.0000000	1.5869358
H	1.2115095	-0.8922871	2.8528439
H	0.8811042	1.2280703	-0.1105126
H	0.0000000	2.0966657	1.1875079
H	-2.0940015	0.0000000	1.5869358
H	-1.2115095	0.8922871	2.8528439
H	-1.2115095	-0.8922871	2.8528439
H	0.8811042	-1.2280703	-0.1105126
H	1.2115095	0.8922871	2.8528439
H	-0.8811042	1.2280703	-0.1105126

2

Os	0.0000000	0.0000000	-2.9252262
Cl	0.0000000	-2.3071800	-3.3416070
Cl	2.3039392	0.0000000	-3.3517208
Cl	0.0000000	2.3071800	-3.3416070
Cl	-2.3039392	0.0000000	-3.3517208
N	0.0000000	0.0000000	-1.3093211
N	0.0000000	0.0000000	2.1896681
C	0.0000000	-1.2336676	1.3463086
C	1.2145830	0.0000000	3.0448437
C	0.0000000	1.2336676	1.3463086
C	-1.2145830	0.0000000	3.0448437
H	-0.8804114	-1.2328447	0.7086714
H	0.0000000	-2.0960328	2.0119192
H	2.0933326	0.0000000	2.4026393
H	1.2115159	-0.8924476	3.6690031
H	0.8804114	1.2328447	0.7086714
H	0.0000000	2.0960328	2.0119192
H	-2.0933326	0.0000000	2.4026393
H	-1.2115159	0.8924476	3.6690031
H	-1.2115159	-0.8924476	3.6690031
H	0.8804114	-1.2328447	0.7086714
H	1.2115159	0.8924476	3.6690031
H	-0.8804114	1.2328447	0.7086714
N	0.0000000	0.0000000	-5.4477537
C	0.0000000	0.0000000	-6.5877245
H	0.0000000	0.0000000	-7.6551066

3

Os	-0.0000000	0.0000000	-3.2320606
Cl	0.0000000	-2.2945716	-3.6924565
Cl	2.2919952	0.0000000	-3.7010879
Cl	0.0000000	2.2945716	-3.6924565
Cl	-2.2919952	0.0000000	-3.7010879

N	-0.0000000	0.0000000	-1.6147389
N	0.0000000	0.0000000	1.9038056
C	-0.0000000	-1.2325373	1.0594753
C	1.2160689	0.0000000	2.7575080
C	-0.0000000	1.2325373	1.0594753
C	-1.2160689	0.0000000	2.7575080
H	-0.8811132	-1.2311397	0.4227978
H	-0.0000000	-2.0963538	1.7230603
H	2.0935435	0.0000000	2.1134310
H	1.2148752	-0.8926496	3.3812981
H	0.8811132	1.2311397	0.4227978
H	0.0000000	2.0963538	1.7230603
H	-2.0935435	0.0000000	2.1134310
H	-1.2148752	0.8926496	3.3812981
H	-1.2148752	-0.8926496	3.3812981
H	0.8811132	-1.2311397	0.4227978
H	1.2148752	0.8926496	3.3812981
H	-0.8811132	1.2311397	0.4227978
C	0.0000000	0.0000000	-5.8358180
O	-0.0000000	0.0000000	-6.9574322

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Os	0.0000000	0.0000000	-1.2312646
Cl	0.0000000	-2.3022429	-1.6580740
Cl	2.3490873	-0.0000000	-1.4797496
Cl	0.0000000	2.3022429	-1.6580740
Cl	-2.3490873	0.0000000	-1.4797496
N	0.0000000	0.0000000	0.3877369
N	0.0000000	0.0000000	3.8918478
C	0.0000000	-1.2336716	3.0485353
C	1.2139402	-0.0000000	4.7478820
C	0.0000000	1.2336716	3.0485353
C	-1.2139402	0.0000000	4.7478820
H	-0.8804813	-1.2330012	2.4109023
H	0.0000000	-2.0958885	3.7143029

H	2.0935199	0.0000000	4.1068132
H	1.2099312	-0.8923301	5.3722072
H	0.8804813	1.2330012	2.4109023
H	0.0000000	2.0958885	3.7143029
H	-2.0935199	0.0000000	4.1068132
H	-1.2099312	0.8923301	5.3722072
H	-1.2099312	-0.8923301	5.3722072
H	0.8804813	-1.2330012	2.4109023
H	1.2099312	0.8923301	5.3722072
H	-0.8804813	1.2330012	2.4109023
N	0.0000000	0.0000000	-3.7862092
C	-1.1416310	0.0000000	-4.4730517
C	1.1416310	-0.0000000	-4.4730517
C	-1.1879228	-0.0000000	-5.8567546
H	-2.0464824	0.0000000	-3.8793602
C	1.1879228	0.0000000	-5.8567546
H	2.0464824	0.0000000	-3.8793602
C	0.0000000	0.0000000	-6.5667892
H	-2.1474433	-0.0000000	-6.3588928
H	2.1474433	0.0000000	-6.3588928
H	0.0000000	0.0000000	-7.6510611

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Os	0.0000000	0.0000000	-3.4188900
Cl	0.0000000	-2.4065342	-3.4978711
Cl	2.4038490	0.0000000	-3.5123532
Cl	0.0000000	2.4065342	-3.4978711
Cl	-2.4038490	-0.0000000	-3.5123532
N	0.0000000	0.0000000	-1.7903523
N	0.0000000	0.0000000	1.4598032
C	0.0000000	-1.2572163	0.6408271
C	1.2139870	-0.0000000	2.3107899
C	0.0000000	1.2572163	0.6408271
C	-1.2139870	0.0000000	2.3107899
H	-0.8750910	-1.2761482	-0.0030785

H	0.0000000	-2.0914208	1.3444088
H	2.0878783	0.0000000	1.6618435
H	1.2153140	-0.8932777	2.9344289
H	0.8750910	1.2761482	-0.0030785
H	0.0000000	2.0914208	1.3444088
H	-2.0878783	0.0000000	1.6618435
H	-1.2153140	0.8932777	2.9344289
H	-1.2153140	-0.8932777	2.9344289
H	0.8750910	-1.2761482	-0.0030785
H	1.2153140	0.8932777	2.9344289
H	-0.8750910	1.2761482	-0.0030785
Cl	0.0000000	0.0000000	-5.8712528

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Os	0.0000000	0.0000000	-2.8794703
Cl	-0.0000000	-2.3860359	-3.0424170
Cl	2.3824934	0.0000000	-3.0581748
Cl	-0.0000000	2.3860359	-3.0424170
Cl	-2.3824934	-0.0000000	-3.0581748
N	0.0000000	0.0000000	-1.2578001
N	0.0000000	0.0000000	2.0386126
C	0.0000000	-1.2517162	1.2139266
C	1.2138491	0.0000000	2.8905372
C	0.0000000	1.2517162	1.2139266
C	-1.2138491	0.0000000	2.8905372
H	-0.8758744	-1.2653949	0.5709008
H	0.0000000	-2.0927208	1.9084385
H	2.0888362	0.0000000	2.2431948
H	1.2141138	-0.8931344	3.5142666
H	0.8758744	1.2653949	0.5709008
H	0.0000000	2.0927208	1.9084385
H	-2.0888362	0.0000000	2.2431948
H	-1.2141138	0.8931344	3.5142666
H	-1.2141138	-0.8931344	3.5142666
H	0.8758744	-1.2653949	0.5709008

H	1.2141138	0.8931344	3.5142666
H	-0.8758744	1.2653949	0.5709008
C	0.0000000	0.0000000	-6.2038605
O	0.0000000	0.0000000	-4.9747475
N	0.0000000	0.0000000	-7.3744139