On the nature of NO-bonding in *N*-oxide group

by

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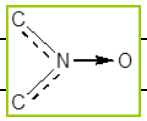
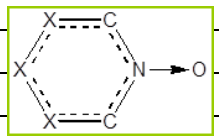
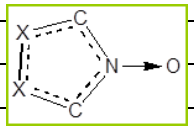
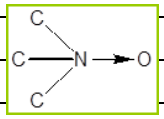
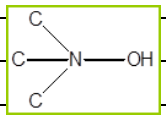
SUPPLEMENTARY INFORMATION

Table S.1. Statistic of d(NO) bond lengths [Å] on the base of CSD searches.

acyclic imine *N*-oxides (type **A**)	all data	room T data	low T data
minimum 	1.261	1.261	1.277
maximum	1.368	1.344	1.368
mean	**1.301**	**1.298**	**1.304**
median	1.296	1.295	1.298
mean SE	0.019	0.018	0.019
observations	76	42	34
aromatic imine *N*-oxides (type **B**)			
minimum 	1.275	1.275	1.277
maximum	1.371	1.371	1.358
mean	**1.318**	**1.318**	**1.314**
median	1.317	1.317	1.313
mean SE	0.017	0.017	0.016
observations	545	355	190
aromatic *N*-oxides (type **C**)			
minimum 	1.248	1.248	1.269
maximum	1.375	1.360	1.375
mean	**1.300**	**1.289**	**1.322**
median	1.284	1.280	1.344
mean SE	0.033	0.025	0.040
observations	39	29	10
aliphatic *N*-oxides (type **D**)			
minimum 	1.387	1.359	1.381
maximum	1.438	1.438	1.401
mean	**1.394**	**1.397**	**1.393**
median	1.395	1.400	1.393
mean SE	0.010	0.015	0.004
observations	48	19	29
hydroxyamines (single N-O bond; type **E**)			
minimum 	1.408	1.408	1.426
maximum	1.468	1.468	1.468
mean	**1.447**	**1.447**	**1.448**

median	1.450	1.450	1.450
mean SE	0.011	0.013	0.009
observations	86	51	35
nitrosoalkanes (double N=O bond; type **F**)			
minimum	1.213	1.213	1.234
maximum	1.326	1.301	1.326
mean	**1.272**	**1.261**	**1.276**
median	1.275	1.258	1.279
mean SE	0.022	0.022	0.021
observations	59	18	41

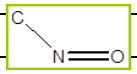


Table S 2. Geometric parameters of *N*-oxide halogen bonds obtained from CSD searches.

CSD refcode	d(NO) [Å]	d(O…X)[Å]	<(NO…X)[°]	<(O…XC)[°]	*N*-oxide type
N->O…Cl-C					
CECZUF	1.292	3.182	164.9	141.6	**B**
KACGEA	1.394	3.233	147.5	178.9	**D**
N->O…Br-C					
SILNIL	1.291	3.178	166.3	170.9	**A**
TAKBAJ	1.320	3.156	119.4	164.8	**A**
XIMVAR	1.324	3.029	127.9	158.2	**B**
YOFXEX	1.292	2.820	156.9	165.5	**B**
N->O…I-C					
COJJOB	1.307	2.823	149.5	173.9	**B**
EVIKOJ	1.335	2.848	116.1	169.4	**B**
EVIKOJ	1.328	3.264	114.8	175.7	**B**
OCOMUO	1.307	2.754	143.8	170.3	**B**
OCOMUO01	1.302	2.753	143.7	170.2	**B**
OCOMUO02	1.302	2.736	143.4	170.0	**B**
OCOMUO03	1.306	2.728	143.2	169.9	**B**
OCOMUO04	1.304	2.722	143.1	169.8	**B**
OCOMUO05	1.301	2.725	143.4	169.8	**B**
XIHCOG	1.291	2.988	104.1	162.9	**B**
IHUNAB	1.266	2.944	114.2	163.8	**C**
minimum	1.270	2.72	104.1	141.6	
maximum	1.340	3.26	166.3	175.7	
mean	**1.304**	**2.916**	**137.2**	**166.7**	
median	1.300	2.84	143.3	169.8	
mean SE	0.016	0.186	18.3	7.7	