Supplementary information for Kaltsoyannis and Plane

Table S1: B3LYP geometric data for NO_2, NO_3 and INO_3 (planar). Bond lengths *r* in Å, bond and dihedral angles ∠ in degrees. Atom numbers for INO_3 are given in Figure 1.

	r(O1–I1)	*r*(O1–N1)	*r*(N1–O2)	*r*(N1–O3)	∠I1O1N1	∠O1N1O2	∠O2N1O3
NO_2		1.192	1.192			134.5	
NO_3		1.232				120.0	
INO_3	2.023	1.452	1.198	1.195	117.8	118.0	131.5

Table S2: B3LYP geometric data for I_2O_3. Bond lengths *r* in Å, bond and dihedral angles ∠ in degrees. Atom numbers are given in Figure 2.

r(I1–O1)	*r*(O1–I2)	*r*(I2–O2)	*r*(I2–O3)	∠I1O1I2	∠O1I2O2	∠O1I2O3	∠O2I2O3	∠I1O1I2O2	∠I1O1I2O3
2.019	1.971	1.784	1.784	121.1	102.5	102.5	108.1	56.0	56.0

Table S3: B3LYP geometric data for I_2O_4. Bond lengths *r* in Å, bond and dihedral angles ∠ in degrees. Atom numbers are given in Figure 3.

r(O1–I1)	*r*(I1–O2)	*r*(O2–I2)	*r*(I2–O3)	*r*(I2–O4)	∠O1I1O2	∠I1O2I2	∠O2I2O3	∠O2I2O4	∠O3I2O4	∠O1I1O2I2	∠I1O2I2O3	∠I2O2I2O4
1.824	2.010	1.997	1.783	1.787	103.9	123.1	100.1	99.3	109.0	-93.1	-108.9	2.5

Table S4: B3LYP geometric data for I_2O_5. Bond lengths *r* in Å, bond and dihedral angles ∠ in degrees. Atom numbers are given in Figure 4.

Variable		Variable		Variable	
r(O1–I1)	1.779	∠O1I1O2	108.9	∠O1I1O3I2	173.5
r(I1–O2)	1.781	∠O1I1O3	96.2	∠O2I1O3I2	–76.0
r(I1–O3)	2.019	∠O2I1O3	99.5	∠I1O3I2O4	–120.4
r(O3–I2)	1.969	∠I1O3I2	123.7	∠I1O3I2O5	–9.4
r(I2–O4)	1.779	∠O3I2O4	100.6		
r(I2–O5)	1.790	∠O3I2O5	99.6		

Table S5: B3LYP geometric data for I_2, IO, OIO and three isomers of I_2O_2; IOIO, IOOI and OI(I)O. Bond lengths *r* in Å, bond and dihedral angles ∠ in degrees. Experimental data (in italics) for I_2 and IO from *Thermodynamic Properties of Individual Substances*, Hemisphere, New York, 1989, and for O_3 from N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, Pergamon Press, Oxford, 2nd edition, 1997.

	r(I–I)	*r*(I–O)	*r*(O–O)	*r*(O–I)	*r*(I–O)	∠OOO	∠IOI	∠OIO	∠IOO	∠OOI	∠OII	∠IOIO	∠IOOI	∠IIOO
I_2	2.708 *2.665*													
IO		1.892 *1.868*												
OIO				1.819				110.5						
IO_3		1.804						110.8						
O_3			1.255 *1.278*			118.3 *116.8*								
IOIO (chain)		2.029		1.994	1.828		122.0	105.9				73.7		
IOOI (chain)		2.065	1.384	2.065					113.6	113.6			86.3	
OI(I)O	2.823	1.793			1.793						102.8			108.5

Table S6: B3LYP vibrational wavenumbers and point groups for all target systems.

NO_2 (C_{2v})		**I_2O_5 (C_1)**		**IOOI (C_1)**		**INO (C_s)**	
A_1	766.2	A	36.2	A	64.3	A'	233.2
A_1	1385.6	A	48.1	A	224.5	A'	512.4
B_2	1688.0	A	59.9	A	328.6	A'	1873.0
		A	161.8	A	509.3		
NO_3 (D_{3h})		A	174.5	A	534.9	**ICN ($C_{\infty v}$)**	
E'	218.5	A	249.3	A	806.2	Π	327.1
A_2''	806.0	A	261.5			Σ	506.2
E'	1096.5	A	297.6	**OI(I)O (C_1)**		Σ	2277.3
A_1'	1126.0	A	313.5	A	138.6		
		A	459.4	A	146.3	**I_2 ($D_{\infty h}$)**	
INO_3 (C_s)		A	583.4	A	215.6	Σ_g	214.6
A''	97.7	A	866.1	A	285.9		
A'	181.0	A	881.3	A	847.6	**IO ($C_{\infty v}$)**	
A'	368.2	A	905.3	A	882.4	Σ	685.3
A'	579.8	A	911.2				
A'	729.4			**IOIO (C_1)**		**OIO (C_{2v})**	

A"	752.2	**I_2O_4 (C_1)**		A	64.3	A_1	264.4
A'	824.3	A	34.5	A	125.8	A_1	799.6
A'	1311.4	A	66.3	A	220.5	B_2	821.1
A'	1716.2	A	92.6	A	433.0		
		A	159.7	A	568.3	**IO_3 (C_1)**	
I_2O_3 (C_1)		A	239.2	A	804.0	A	258.7
A	43.4	A	255.5			A	259.1
A	88.2	A	305.2	**HI ($C_{\infty v}$)**		A	268.2
A	236.8	A	431.3	Σ	2318.7	A	765.0
A	254.6	A	530.8			A	765.2
A	297.5	A	811.2	**HOI (C_s)**		A	795.3
A	442.5	A	868.2	A'	587.4		
A	625.7	A	900.7	A'	1097.6	**O_3 (C_{2v})**	
A	872.7			A'	3791.3	A_1	746.0
A	901.2	**IOI (C_{2v})**				B_2	1189.4
		A_1	127.6			A_1	1248.9
		A_1	443.0				
		B_2	619.6				