Supporting Information

Oxy-bridged Bis(1*H*-tetrazol-5-yl)furazan and its Energetic Salts Paired with Nitrogen-Rich Cations: Highly Thermally Stable Energetic Materials with Low Sensitivity

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X-ray crystallography: Crystals of **6**, **7**, **8** and **13** were removed from the flask and covered with a layer of hydrocarbon oil. A suitable crystal was then selected, attached to a glass fiber, and placed in the low-temperature nitrogen stream. Data for 6, 7, 8 and 13 were collected at 153(2) K using a Rigaku Saturn724 CCD (AFC10/Saturn724+ for 7) diffractometer equipped with a graphite-monochromatized MoKα radiation (λ = 0.71073 Å) using omega scans. Data collection and reduction were performed and the unit cell was initially refined by using CrystalClear -SM Expert 2.0 r2i software. The reflection data were also corrected for Lp factors. The structure was solved by direct methods and refined by the least squares method on F2 using the SHELXTL-97 system of programs.ii Structure were solved in the space group C2/c for 6, C2/n for 7, Pī for 8 and P2(1) for 13 by analysis of systematic absences. In this all-light-atom structure the value of the Flack parameter did not allow the direction of polar axis to be determined and Friedel reflections were then merged for the final refinement. Band angles and dihedral angles of the data collection and refinement are given in Table S1, S2, S3, S4.

Table S1. Band angles and dihedral angles for the structure of **6**.

N1—O1—N2	111.34 (11)	C4—N9—H9B	120.9 (12)
C1—O2—C1^{i}	120.00 (16)	H9A—N9—H9B	119.3 (16)
C1—N1—O1	104.11 (12)	N1—C1—O2	124.95 (13)
C2—N2—O1	105.66 (12)	N1—C1—C2	111.13 (12)
C3—N3—N4	103.90 (11)	O2—C1—C2	123.85 (13)
N5—N4—N3	109.56 (12)	N2—C2—C1	107.76 (13)
N4—N5—N6	109.90 (12)	N2—C2—C3	121.05 (13)
C3—N6—N5	103.75 (12)	C1—C2—C3	131.17 (12)
C4—N7—H7A	118.4 (10)	N6—C3—N3	112.89 (12)
C4—N7—H7B	120.4 (11)	N6—C3—C2	125.30 (13)
H7A—N7—H7B	121.0 (15)	N3—C3—C2	121.80 (12)
C4—N8—H8A	120.4 (11)	N9—C4—N7	120.80 (14)
C4—N8—H8B	116.9 (15)	N9—C4—N8	119.70 (15)
H8A—N8—H8B	118.2 (18)	N7—C4—N8	119.47 (15)
C4—N9—H9A	119.5 (11)	N2—O1—N1—C1	−0.20 (16)
N1—O1—N2—C2	0.33 (16)	O2—C1—C2—N2	−176.83 (12)
C3—N3—N4—N5	−0.15 (16)	N1—C1—C2—C3	−178.45 (14)
N3—N4—N5—N6	0.26 (17)	O2—C1—C2—C3	4.5 (2)
N4—N5—N6—C3	−0.26 (16)	N5—N6—C3—N3	0.17 (16)
O1—N1—C1—O2	177.00 (12)	N5—N6—C3—C2	178.87 (13)
O1—N1—C1—C2	0.00 (16)	N4—N3—C3—N6	−0.02 (16)
C1^{i}—O2—C1—N1	21.06 (11)	N4—N3—C3—C2	−178.77 (13)
C1^{i}—O2—C1—C2	−162.30 (16)	N2—C2—C3—N6	−178.62 (14)
O1—N2—C2—C1	−0.32 (15)	C1—C2—C3—N6	−0.1 (2)
N2—C2—C3—N3	0.0 (2)	O1—N2—C2—C3	178.51 (12)

N1—C1—C2—N2	0.21 (17)	C1—C2—C3—N3	178.48 (14)

Table S2. Band angles and dihedral angles for the structure of **7**.

N2—O1—N1	110.78 (10)	N10—N9—H9	117.2 (12)
C1^{i}—O2—C1	119.32 (15)	N9—N10—H10A	106.4 (14)
C1—N1—O1	104.43 (10)	N9—N10—H10B	112.6 (14)
C2—N2—O1	106.68 (11)	H10A—N10—H10B	111.8 (19)
C3—N3—N4	104.39 (11)	N1—C1—O2	125.05 (12)
N5—N4—N3	109.44 (11)	N1—C1—C2	111.06 (12)
N4—N5—N6	109.80 (11)	O2—C1—C2	123.80 (12)
C3—N6—N5	103.86 (11)	N2—C2—C1	107.04 (12)
C4—N7—H7A	118.6 (11)	N2—C2—C3	121.24 (12)
C4—N7—H7B	119.4 (10)	C1—C2—C3	131.70 (12)
H7A—N7—H7B	121.2 (15)	N3—C3—N6	112.51 (12)
C4—N8—H8A	117.0 (11)	N3—C3—C2	122.98 (12)
C4—N8—H8B	118.4 (12)	N6—C3—C2	124.48 (12)
H8A—N8—H8B	124.1 (16)	N7—C4—N8	121.58 (13)
C4—N9—N10	117.56 (12)	N7—C4—N9	120.38 (13)
C4—N9—H9	121.0 (12)	N8—C4—N9	118.04 (13)
N2—O1—N1—C1	0.69 (14)	N1—C1—C2—C3	−177.47 (13)
N1—O1—N2—C2	−0.08 (15)	O2—C1—C2—C3	5.7 (2)
C3—N3—N4—N5	0.53 (15)	N4—N3—C3—N6	−0.53 (15)
N3—N4—N5—N6	−0.36 (16)	N4—N3—C3—C2	−178.43 (12)
N4—N5—N6—C3	0.03 (15)	N5—N6—C3—N3	0.32 (15)
O1—N1—C1—O2	175.79 (11)	N5—N6—C3—C2	178.18 (12)
O1—N1—C1—C2	−1.01 (14)	N2—C2—C3—N3	5.7 (2)
C1^{i}—O2—C1—N1	18.16 (10)	C1—C2—C3—N3	−176.02 (14)
C1^{i}—O2—C1—C2	−165.44 (14)	N2—C2—C3—N6	−171.96 (13)
O1—N2—C2—C1	−0.52 (15)	C1—C2—C3—N6	6.3 (2)
O1—N2—C2—C3	178.15 (11)	N10—N9—C4—N7	−9.9 (2)
N1—C1—C2—N2	1.01 (16)	N10—N9—C4—N8	170.69 (15)
O2—C1—C2—N2	−175.83 (11)		

Table S3. Band angles and dihedral angles for the structure of **8**.

N1—O1—N2	111.02 (9)	N20—N19—H19	121.9 (11)
C1—O2—C4	119.29 (10)	N19—N20—H20A	106.6 (11)
N7—O3—N8	111.37 (10)	N19—N20—H20B	106.4 (12)
C1—N1—O1	104.51 (11)	H20A—N20—H20B	108.7 (16)
C2—N2—O1	106.10 (11)	C8—N21—N22	116.72 (12)
C3—N3—N4	104.05 (11)	C8—N21—H21	121.5 (11)
N5—N4—N3	109.91 (10)	N22—N21—H21	121.7 (11)
N4—N5—N6	109.58 (10)	N21—N22—H22A	112.5 (10)

C3—N6—N5	103.74 (10)	N21—N22—H22B	108.0 (11)
C4—N7—O3	104.12 (12)	H22A—N22—H22B	106.0 (15)
C5—N8—O3	105.83 (12)	N1—C1—O2	124.95 (12)
C6—N9—N10	104.08 (12)	N1—C1—C2	111.01 (12)
N11—N10—N9	110.01 (12)	O2—C1—C2	124.00 (11)
N10—N11—N12	109.02 (12)	N2—C2—C1	107.36 (11)
C6—N12—N11	104.24 (11)	N2—C2—C3	121.54 (12)
C7—N13—H13A	120.6 (11)	C1—C2—C3	131.10 (12)
C7—N13—H13B	120.3 (11)	N6—C3—N3	112.72 (11)
H13A—N13—H13B	118.8 (15)	N6—C3—C2	124.26 (12)
C7—N14—N15	118.90 (12)	N3—C3—C2	123.01 (11)
C7—N14—H14	117.3 (11)	N7—C4—O2	124.90 (13)
N15—N14—H14	123.4 (11)	N7—C4—C5	111.41 (12)
N14—N15—H15A	108.2 (11)	O2—C4—C5	123.56 (12)
N14—N15—H15B	109.4 (11)	N8—C5—C4	107.27 (13)
H15A—N15—H15B	107.2 (14)	N8—C5—C6	122.38 (13)
C7—N16—N17	116.65 (11)	C4—C5—C6	130.32 (12)
C7—N16—H16	119.1 (11)	N12—C6—N9	112.64 (13)
N17—N16—H16	115.5 (11)	N12—C6—C5	124.69 (12)
N16—N17—H17A	107.4 (11)	N9—C6—C5	122.64 (13)
N1—O1—N2	111.02 (9)	N20—N19—H19	121.9 (11)
N16—N17—H17B	106.4 (13)	N14—C7—N13	121.37 (13)
H17A—N17—H17B	109.4 (17)	N14—C7—N16	119.27 (12)
C8—N18—H18A	116.7 (12)	N13—C7—N16	119.36 (12)
C8—N18—H18B	119.3 (11)	N18—C8—N21	120.54 (13)
H18A—N18—H18B	124.0 (16)	N18—C8—N19	119.69 (13)
C8—N19—N20	117.57 (12)	N21—C8—N19	119.77 (12)
C8—N19—H19	117.5 (11)	C1—C2—C3—N3	173.32 (13)
N2—O1—N1—C1	−0.22 (15)	O3—N7—C4—O2	−175.65 (12)
N1—O1—N2—C2	0.09 (15)	O3—N7—C4—C5	0.30 (16)
C3—N3—N4—N5	−0.39 (14)	C1—O2—C4—N7	−30.3 (2)
N3—N4—N5—N6	0.11 (15)	C1—O2—C4—C5	154.19 (13)
N4—N5—N6—C3	0.22 (14)	O3—N8—C5—C4	0.67 (14)
N8—O3—N7—C4	0.12 (16)	O3—N8—C5—C6	−177.67 (12)
N7—O3—N8—C5	−0.52 (15)	N7—C4—C5—N8	−0.65 (17)
C6—N9—N10—N11	−0.42 (16)	O2—C4—C5—N8	175.37 (12)
N9—N10—N11—N12	0.45 (16)	N7—C4—C5—C6	177.51 (13)
N10—N11—N12—C6	−0.27 (15)	O2—C4—C5—C6	−6.5 (2)
O1—N1—C1—O2	−177.52 (12)	N11—N12—C6—N9	0.00 (15)
O1—N1—C1—C2	0.26 (15)	N11—N12—C6—C5	−178.22 (12)
C4—O2—C1—N1	−12.4 (2)	N10—N9—C6—N12	0.25 (16)

C4—O2—C1—C2	170.08 (12)	N10—N9—C6—C5	178.52 (12)
O1—N2—C2—C1	0.07 (14)	N8—C5—C6—N12	174.24 (13)
O1—N2—C2—C3	179.21 (11)	C4—C5—C6—N12	−3.7 (2)
N1—C1—C2—N2	−0.22 (16)	N8—C5—C6—N9	−3.8 (2)
O2—C1—C2—N2	177.59 (12)	C4—C5—C6—N9	178.27 (14)
N1—C1—C2—C3	−179.25 (13)	N15—N14—C7—N13	6.21 (19)
O2—C1—C2—C3	−1.4 (2)	N15—N14—C7—N16	−173.40 (12)
N5—N6—C3—N3	−0.49 (14)	N17—N16—C7—N14	−7.01 (18)
N5—N6—C3—C2	178.60 (12)	N17—N16—C7—N13	173.37 (13)
N4—N3—C3—N6	0.55 (15)	N22—N21—C8—N18	−4.3 (2)
N4—N3—C3—C2	−178.55 (12)	N22—N21—C8—N19	176.24 (12)
N2—C2—C3—N6	175.40 (13)	N20—N19—C8—N18	−175.46 (13)
C1—C2—C3—N6	−5.7 (2)	N20—N19—C8—N21	3.95 (19)
N2—C2—C3—N3	−5.6 (2)		

Table S4. Band angles and dihedral angles for the structure of **13**.

N2—O1—N1	111.86 (16)	C13—N27—H27	111 (2)
C1—O2—C4	125.63 (18)	N28—N27—H27	121 (2)
N8—O3—N7	111.72 (15)	N27—N28—H28A	113.5 (17)
N14—O4—N13	111.89 (16)	N27—N28—H28B	112 (2)
C7—O5—C10	125.73 (19)	H28A—N28—H28B	102 (2)
N19—O6—N20	111.49 (16)	N27—N28—H28C	103.8 (15)
H8A—O8—H8B	110.7	H28A—N28—H28C	116 (2)
H9A—O9—H9B	105.3	H28B—N28—H28C	110 (2)
H10A—O10—H10B	106.2	N1—C1—O2	129.8 (2)
H11A—O11—H11B	109.6	N1—C1—C2	111.93 (19)
C1—N1—O1	103.02 (18)	O2—C1—C2	118.29 (19)
C2—N2—O1	105.29 (18)	N2—C2—C1	107.90 (19)
C3—N3—N4	105.41 (19)	N2—C2—C3	124.6 (2)
N5—N4—N3	110.55 (18)	C1—C2—C3	127.38 (19)
N4—N5—N6	106.92 (19)	N3—C3—N6	109.5 (2)
C3—N6—N5	107.66 (19)	N3—C3—C2	125.70 (19)
C3—N6—H6	135 (2)	N6—C3—C2	124.83 (19)
N5—N6—H6	118 (2)	N7—C4—O2	128.6 (2)
C4—N7—O3	103.11 (17)	N7—C4—C5	111.9 (2)
C5—N8—O3	105.33 (17)	O2—C4—C5	119.52 (19)
C6—N9—N10	103.88 (18)	N8—C5—C4	107.91 (19)
N11—N10—N9	110.22 (18)	N8—C5—C6	124.98 (19)
N10—N11—N12	109.04 (18)	C4—C5—C6	127.1 (2)
C6—N12—N11	104.61 (17)	N9—C6—N12	112.25 (19)
C7—N13—O4	103.00 (18)	N9—C6—C5	124.22 (19)
C8—N14—O4	105.28 (18)	N12—C6—C5	123.53 (19)

C9—N15—N16	105.29 (18)	N13—C7—O5	129.5 (2)
N17—N16—N15	110.53 (18)	N13—C7—C8	111.9 (2)
N16—N17—N18	107.06 (19)	O5—C7—C8	118.57 (19)
C9—N18—N17	108.00 (19)	N14—C8—C7	107.9 (2)
C9—N18—H18	133 (2)	N14—C8—C9	124.7 (2)
N17—N18—H18	119 (2)	C7—C8—C9	127.36 (19)
C10—N19—O6	103.26 (18)	N15—C9—N18	109.1 (2)
C11—N20—O6	105.83 (17)	N15—C9—C8	126.4 (2)
C12—N21—N22	103.97 (19)	N18—C9—C8	124.49 (19)
N23—N22—N21	109.88 (18)	N19—C10—O5	128.3 (2)
N22—N23—N24	109.38 (19)	N19—C10—C11	112.2 (2)
C12—N24—N23	104.73 (17)	O5—C10—C11	119.5 (2)
C13—N25—N26	116.21 (18)	N20—C11—C10	107.2 (2)
C13—N25—H25	117.5 (18)	N20—C11—C12	126.0 (2)
N26—N25—H25	114.9 (18)	C10—C11—C12	126.7 (2)
N25—N26—H26B	107.3 (16)	N21—C12—N24	112.0 (2)
N25—N26—H26C	109.7 (18)	N21—C12—C11	125.3 (2)
H26B—N26—H26C	114 (3)	N24—C12—C11	122.61 (19)
N25—N26—H286	110.9 (16)	O7—C13—N25	125.15 (19)
H26B—N26—H286	106 (2)	O7—C13—N27	123.6 (2)
H26C—N26—H286	110 (3)	N25—C13—N27	111.24 (19)
C13—N27—N28	114.57 (18)		
N2—O1—N1—C1	−0.5 (3)	N10—N9—C6—N12	0.2 (3)
N1—O1—N2—C2	0.2 (2)	N10—N9—C6—C5	−179.7 (2)
C3—N3—N4—N5	0.2 (3)	N11—N12—C6—N9	−0.3 (2)
N3—N4—N5—N6	−0.2 (3)	N11—N12—C6—C5	179.6 (2)
N4—N5—N6—C3	0.2 (3)	N8—C5—C6—N9	3.9 (4)
N8—O3—N7—C4	−0.5 (2)	C4—C5—C6—N9	−178.5 (2)
N7—O3—N8—C5	1.0 (2)	N8—C5—C6—N12	−175.9 (2)
C6—N9—N10—N11	0.1 (3)	C4—C5—C6—N12	1.7 (3)
N9—N10—N11—N12	−0.3 (3)	O4—N13—C7—O5	−178.5 (2)
N10—N11—N12—C6	0.3 (2)	O4—N13—C7—C8	0.6 (3)
N14—O4—N13—C7	−0.4 (3)	C10—O5—C7—N13	−2.7 (4)
N13—O4—N14—C8	0.0 (3)	C10—O5—C7—C8	178.2 (2)
C9—N15—N16—N17	−0.4 (3)	O4—N14—C8—C7	0.4 (2)
N15—N16—N17—N18	0.2 (3)	O4—N14—C8—C9	−178.1 (2)
N16—N17—N18—C9	0.1 (3)	N13—C7—C8—N14	−0.7 (3)
N20—O6—N19—C10	−0.1 (2)	O5—C7—C8—N14	178.5 (2)
N19—O6—N20—C11	0.2 (3)	N13—C7—C8—C9	177.7 (2)
C12—N21—N22—N23	−0.1 (3)	O5—C7—C8—C9	−3.1 (4)
N21—N22—N23—N24	0.3 (3)	N16—N15—C9—N18	0.4 (2)

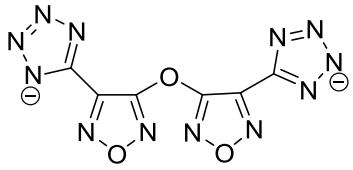
N22—N23—N24—C12	−0.5 (2)	N16—N15—C9—C8	−178.0 (2)
O1—N1—C1—O2	−178.6 (2)	N17—N18—C9—N15	−0.3 (3)
O1—N1—C1—C2	0.6 (3)	N17—N18—C9—C8	178.1 (2)
C4—O2—C1—N1	−8.2 (4)	N14—C8—C9—N15	2.8 (4)
C4—O2—C1—C2	172.7 (2)	C7—C8—C9—N15	−175.4 (2)
O1—N2—C2—C1	0.2 (2)	N14—C8—C9—N18	−175.4 (2)
O1—N2—C2—C3	−177.0 (2)	C7—C8—C9—N18	6.4 (4)
N1—C1—C2—N2	−0.5 (3)	O6—N19—C10—O5	179.7 (2)
O2—C1—C2—N2	178.8 (2)	O6—N19—C10—C11	−0.1 (3)
N1—C1—C2—C3	176.5 (2)	C7—O5—C10—N19	0.5 (4)
O2—C1—C2—C3	−4.2 (3)	C7—O5—C10—C11	−179.7 (2)
N4—N3—C3—N6	0.0 (3)	O6—N20—C11—C10	−0.2 (2)
N4—N3—C3—C2	178.8 (2)	O6—N20—C11—C12	178.0 (2)
N5—N6—C3—N3	−0.1 (3)	N19—C10—C11—N20	0.2 (3)
N5—N6—C3—C2	−178.9 (2)	O5—C10—C11—N20	−179.6 (2)
N2—C2—C3—N3	−0.1 (4)	N19—C10—C11—C12	−178.0 (2)
C1—C2—C3—N3	−176.7 (2)	O5—C10—C11—C12	2.2 (3)
N2—C2—C3—N6	178.6 (2)	N22—N21—C12—N24	−0.2 (3)
C1—C2—C3—N6	2.0 (4)	N22—N21—C12—C11	−179.9 (2)
O3—N7—C4—O2	179.1 (2)	N23—N24—C12—N21	0.4 (3)
O3—N7—C4—C5	−0.2 (2)	N23—N24—C12—C11	−179.9 (2)
C1—O2—C4—N7	7.7 (4)	N20—C11—C12—N21	0.9 (4)
C1—O2—C4—C5	−173.0 (2)	C10—C11—C12—N21	178.8 (2)
O3—N8—C5—C4	−1.1 (2)	N20—C11—C12—N24	−178.7 (2)
O3—N8—C5—C6	176.9 (2)	C10—C11—C12—N24	−0.8 (3)
N7—C4—C5—N8	0.9 (3)	N26—N25—C13—O7	10.5 (3)
O2—C4—C5—N8	−178.5 (2)	N26—N25—C13—N27	−169.87 (18)
N7—C4—C5—C6	−177.0 (2)	N28—N27—C13—O7	10.5 (3)
O2—C4—C5—C6	3.5 (3)	N28—N27—C13—N25	−169.18 (19)

Theoretical study: Calculations were carried out by using the Gaussian 03 (Revision E.01) suite of programs.[3] The geometric optimization of the structures and frequency analyses were carried out by using the B3LYP functional with the 6-31+G** basis set,[4] and single-point energies were calculated at the MP2(full)/6-311++G** level. All of the

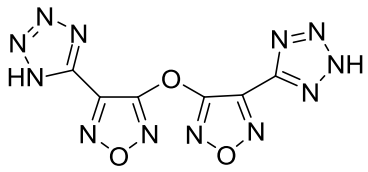
optimized structures were characterized to be true local energy minima on the potential-energy surface without imaginary frequencies.

Geometry coordinates

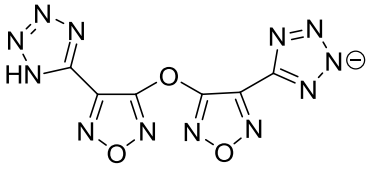
The optimized structure of the following structure



O	-0.017060	0.047786	-0.917485
C	0.867989	-0.684018	-0.065399
O	2.228299	-2.525490	-0.805419
C	-1.015214	0.696201	-0.124928
O	-2.275324	2.611434	-0.855061
C	2.301622	-0.193907	-0.215986
C	-2.411381	0.233021	-0.517831
C	-3.221907	-0.371290	0.643829
C	3.368669	0.177364	0.830517
N	-0.996685	2.202638	-0.361171
N	-3.152672	1.487384	-0.967900
N	0.891647	-2.159013	-0.451840
N	3.105491	-1.402171	-0.684379
N	-3.837213	-1.700819	0.230673
N	-5.344821	-1.597242	0.412281
N	-5.655358	-0.220618	0.982269
N	-4.352748	0.563577	1.047903
N	4.602622	-0.698337	0.667554
N	5.807965	0.216067	0.503009
N	5.301807	1.649666	0.432221
N	3.797679	1.628287	0.66402



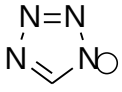
O	0.062517	-0.814768	-0.000512
C	-1.117815	-1.455077	-0.000269
O	-2.734189	-2.824539	-0.000007
C	1.283687	-1.401558	-0.000151
O	2.945118	-2.693222	0.000352
C	-2.349307	-0.726251	-0.000051
C	2.471578	-0.605762	0.000088
C	2.582395	0.844592	-0.000004
C	-2.538657	0.710596	0.000037
N	1.565162	-2.669965	0.000000
N	3.488510	-1.434643	0.000416
N	-1.353483	-2.736686	-0.000247
N	-3.328491	-1.595316	0.000160
N	2.042210	2.962263	-0.000135
N	3.334784	2.844123	-0.000131
N	3.707698	1.543738	-0.000055
N	-3.491230	2.684853	0.000216
N	-2.208799	2.832836	0.000117
N	-1.579757	1.627500	0.000052
N	1.540879	1.714131	-0.000056
H	0.523605	1.577598	-0.000044
N	-3.722630	1.355105	0.000135
H	-4.666438	0.987814	0.000166



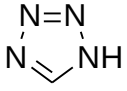
O	0.856869	-2.185187	1.602810
C	0.703132	-0.421695	0.416620
C	2.086720	-0.823059	0.440539
N	-0.031505	-1.259205	1.101838
N	2.149519	-1.916552	1.179632
O	0.194131	0.642304	-0.258321
C	-0.872178	1.335858	0.222397
C	-2.276614	1.057806	0.103753
O	-1.973086	2.970444	0.992969
N	-0.702577	2.515263	0.757609
N	-2.939025	2.076495	0.599636

C	3.205822	-0.178914	-0.202400
C	-2.945022	-0.126905	-0.415586
N	-4.059518	-0.198684	-1.128616
N	-4.266794	-1.522687	-1.336078
N	-3.333083	-2.247079	-0.776961
N	-2.493535	-1.375792	-0.202838
H	-1.646083	-1.625179	0.345470
N	3.064902	0.800706	-1.122561
N	4.307699	1.120330	-1.483020
N	5.171789	0.355567	-0.800435
N	4.505214	-0.470340	0.006498

O	-0.768830	-0.794977	-0.032344
C	-0.012025	1.097718	-0.106360
C	1.225138	0.292063	-0.015933
H	0.133000	2.443525	0.226355
H	2.530927	0.662188	0.101932
N	-1.279744	0.368556	0.061439
N	0.738035	-1.094925	0.033449

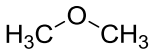


N	0.047529	-0.000055	0.053971
N	-0.024344	-0.000035	2.240111
N	1.334829	0.000026	0.466441
N	-0.757471	0.000217	1.104624
C	1.243960	0.000021	1.804416
H	2.103835	-0.000063	2.463370



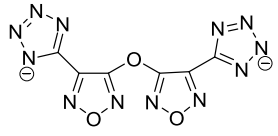
C	0.962584	0.523792	0.000018
N	0.693688	0.797291	0.000022
H	1.308118	1.599246	0.000030

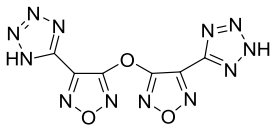
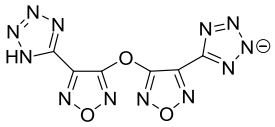
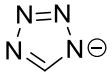
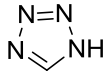
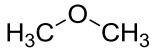
H	1.951727	0.955024	0.000018
N	0.179917	1.178933	0.000060
N	1.155301	0.225095	0.000083
N	0.649234	0.963670	0.000068



O	0.000000	0.587854	0.000003
C	1.178058	-0.195592	-0.000001
H	2.024917	0.494288	-0.000117
H	1.235972	-0.835995	0.894414
H	1.235862	-0.836155	-0.894309
C	-1.178058	-0.195592	0.000002
H	-1.235910	-0.836092	0.894351
H	-2.024917	0.494288	0.000005
H	-1.235924	-0.836058	-0.894372

Table S5. Ab Initio computional data (B3LYP/6-31+G(d,p)/MP2(full)/6-311++G**)

	E_0	ZPE	H_T	HOF ^{Exp}	HOF ^{Calcd}
	-1109.0365397	0.104157	0.015907	-	721.8

	-1110.1241291	0.131027	0.015939	-	858.6
	-1109.624703	0.117490	0.015844	-	674.7
	-261.5324597	0.045703	0.004418	196[a]	-
CH_4	-40.39849[2]	0.044791	0.003812	-74.6[b]	-
CH_3CH_3	-79.6068548	0.074609	0.00443	-84.68[c]	-
	-257.218829	0.033827	0.004225	-	170.0[c]
	-257.7256749	0.046855	0.00443	333.2[d]	-
	-154.6803049	0.079630	0.005285	-184.1[e]	-

[a] Struct Chem. **2011**, 22, 149-159 [b]Eur. J. Inorg. Chem. **2008**, 2560-2568; [c]Data calculated with the G2 method by using the Gaussian 03 program. [d] New J. Chem., **2008**, 32, 317-322 [e] NIST Chemistry WebBook

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(2) G. M. Sheldrick, SHELXTL-97, Structure Determination Software Suite. Bruker AXS, Madison WI, **2008**.

(3) Gaussian 03, Revision E.01, M. J.Frisch, G. W.Trucks, H. B.Schlegel, G. E.Scuseria, M. A.Robb, J. R.Cheeseman, J. A.Montgomery, J. T.Vreven, K. N.Kudin, J. C.Burant, J. M.Millam, S. S.Iyengar, J.Tomasi, V.Barone, B.Mennucci, M.Cossi, G.Scalmani, N.Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K .Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G .Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, Gaussian, Inc., Wallingford CT, **2004**.

(4) R. G. Parr, W. Yang, *Density Functional Theory of Atoms and Molecules*, Oxford University Press, New York, **1989**.

[i] CrystalClear: SM Expert 2.0 r2, An Integrated Program for the Collection and Processing of Area Detector Data, Rigaku Corporation, 2009.

[ii] G. M. Sheldrick, SHELXTL-97, Structure Determination Software Suite. Bruker AXS, Madison WI, 2008.