Electronic Supplementary Information For

Design and Synthesis of Phenylene-Bridged Isoxazole and Tetrazole-1-ol Based Energetic Materials of Low Sensitivity

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Table S1. Calculated Total Energy (E_0), Zero-point Energy (ZPE), values of Thermal Correction (H_T) and Enthalpy of Formation ($\Delta H_f^{\circ}(g)$) of the compounds using B3LYP/6-31+ $G^{**}/MP2/6$ -311+ $+G^{**}$ level of theory (Isodesmic)¹

		/		
Compounds	Eo	ZPE	$H_{ m T}$	$\Delta H_{f}^{\circ}(g)$
	[Hartree/Particle]	[Hartree/Particle]	[Hartree/Particle]	kJ/mol
CH ₄	-40.3796224	0.044793	0.003812	-74.60 ^a
CH ₃ ONO ₂	-319.509055	0.054251	0.005933	-137.28
CH ₃ N ₃	-203.607680	0.050250	0.00543	296.54
	-231.5842377	0.100451	0.005346	82.90 ^b
N ₃ N-OH	-371.870596	0.076242	0.008229	301.80 ^b
	-371.8748474	0.077582	0.007588	280.72 ^b
	-371.3480753	0.065401	0.006759	108.09 ^b
	-363.0455559	0.140777	0.009666	-41.26 ^b

[a] Data are from Ref. [D. R. Lide ed., CRC Handbook of Chemistry and Physics, 88th Edition (Internet Version **2008**), CRC Press/Taylor and Francis, Boca Raton, FL.] ^bObtained at G2 level. ^cCalculated according to the isodesmic equations as shown in Figure 1.

The gas phase enthalpies of formation $\Delta H_f^{\circ}(g)$ were predicted using isodesmic equations as shown in Figure 1. Subsequently, their solid phase enthalpy of formation ΔH_f° (s) were calculated by using equations 6-7.²⁻⁴



Figure 1: Isodesmic reactions for the title compounds 4, 5, 6-9, 12, and 14.

$\Delta H_f^{\circ}(g)_{\text{Compound 4}}$	$= \Delta H_{\rm f}^{\rm o}(g)_{\rm Benzene}$	$+ 2\Delta H_{\rm f}^{\circ}(g)_{\rm MAzoxime}$	- $2\Delta H_{f}^{\circ}(g)_{Methane}$		(1)
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$$\Delta H_{f}^{\circ}(g)_{\text{Compound 5}} = \Delta H_{f}^{\circ}(g)_{\text{Benzene}} + 2\Delta H_{f}^{\circ}(g)_{\text{MTetz-ol}} - 2\Delta H_{f}^{\circ}(g)_{\text{Methane}}$$
(2)

$$\Delta H_{f}^{\circ}(g)_{\text{Compound 6-9}} = \Delta H_{f}^{\circ}(g)_{\text{Benzene}} + 2\Delta H_{f}^{\circ}(g)_{\text{MTetz-o-anion}} - 2\Delta H_{f}^{\circ}(g)_{\text{Methane}}$$
(3)

$$\Delta H_{f}^{\circ}(g)_{\text{Compound 12}} = \Delta H_{f}^{\circ}(g)_{\text{Benzene}} + 2\Delta H_{f}^{\circ}(g)_{\text{TMISO}} + 4\Delta H_{f}^{\circ}(g)_{\text{Methylazide}} - 6\Delta H_{f}^{\circ}(g)_{\text{Methane}}$$
(4)

$$\Delta H_{f}^{\circ}(g)_{\text{Compound14}} = \Delta H_{f}^{\circ}(g)_{\text{Benzene}} + 2\Delta H_{f}^{\circ}(g)_{\text{TMISO}} + 4\Delta H_{f}^{\circ}(g)_{\text{Methylnitrate}} - 6\Delta H_{f}^{\circ}(g)_{\text{Methane}}$$
(5)

$$\Delta H_{f}^{\circ}(s) = \Delta H_{f}^{\circ}(g) - \Delta H_{sub}$$
(6)

Where $\Delta H_f^{\circ}(s)$ is the solid phase enthalpy of formation, $\Delta H_f^{\circ}(g)$ is the gas phase enthalpy of formation and ΔH_{sub} is the enthalpy of sublimation.

The enthalpy of sublimation was calculated based on Trouton's rule according to equation 2.³ $\Delta H_{sub} = T \times 188 / Jmol^{-1} K^{-1}$ (7)

Where, T, represents either the melting point or the decomposition temperature when no melting occurs before decomposition.

For salts, the solid-state enthalpy of formation is obtained using a Born-Haber energy cycle.⁴

Table S2. The standard enthalpies of combustion $\Delta H_{f(combust)}$ for the title compounds were calculated by following equation

$\Delta H_{f(comb})$	oust) =	= $\Sigma \Delta H_{f \text{ (products)}}$ - $\Sigma \Delta H_{f \text{ (reactants)}}$				(8)
RDX	=	$C_{3}H_{6}N_{6}O_{6}\left(s\right) \ \ + \ \ 1.5 \ O_{2}\left(g\right)$	\longrightarrow	$3CO_2(g) + 3H_2O(g)$	+	$3N_{2}\left(g ight)$
TNT	=	$C_7H_5N_3O_6(s) + 5.25O_2(g)$		$7CO_2(g) + 2.5H_2O(g)$	+	1.5N ₂ (g)
HNS	=	$C_{14}H_6N_6O_{12}(s)\ +\ 9.5\ O_2(g)$	\longrightarrow	$14CO_2(g) + 3H_2O(g)$	+	3N ₂ (g)
4	=	$C_{8}H_{6}N_{8}O_{2}\left(s\right) \ + \ 8.5 \ O_{2}\left(g\right)$	\longrightarrow	$8CO_{2}(g) + 3H_{2}O(g)$	+ 4	4N ₂ (g)
5	=	$C_{8}H_{6}N_{8}O_{2}\left(s\right) \ + \ 8.5 \ O_{2}\left(g\right)$	\longrightarrow	$8CO_{2}(g) + 3H_{2}O(g)$	+ 4	4N ₂ (g)
6	=	$C_8H_{12}N_{10}O_4(s) + 9 O_2(g)$	\longrightarrow	$8CO_2(g) + 6H_2O(g)$	+ 5	5N ₂ (g)
7	=	$C_8 H_{12} N_{10} O_2 \ (s) \ + \ 10 \ O_2 \ (g)$	\longrightarrow	$8CO_2(g) + 6H_2O(g)$	+	5N ₂ (g)
8	=	$C_8 H_{14} N_{12} O_2 \ (s) + \ 10.5 \ O_2 \ (g)$	\longrightarrow	$8CO_{2}(g) + 7H_{2}O(g)$	+ 6	5N ₂ (g)
9	=	$C_{8}H_{4}K_{2}N_{8}O_{2}\left(s\right) \ + \ 8 \ O_{2}\left(g\right)$	\longrightarrow	$8CO_2(g) + 2H_2O(g)$	+ 4	$N_2(g)$
12	=	$C_{16}H_{12}N_6O_{14}(s) \ \ + \ \ 12 \ O_2(g)$	\longrightarrow	$16CO_2(g) + 6H_2O(g)$	+	3N ₂ (g)
14	=	$C_{16}H_{12}N_{14}O_2(s) + 18 O_2(g)$	\longrightarrow	$16CO_2(g) + 6H_2O(g)$	+ ′	7N ₂ (g)

The standard enthalpy of formation for CO₂ ($\Delta H_{f (CO2)} = -393.51 \text{ kJmol}^{-1}$); H₂O ($\Delta H_{f (H2O)} = -243.015 \text{ kJmol}^{-1}$).

Table S3. Computed electrostatic potential (ESP) of RDX and TNT



Computed electrostatic potential (ESP) maps of (a) TNT, (b) RDX. Color ranges in kcal/mol: Red, more positive; Blue, more negative and Greyer, in between positive and negative.

 Table S4: Crystal data and structure refinement⁵⁻¹¹ for compound 12

	1 2
$O_2 NO$	
O2NO NO	
	TTT I
ONO ₂	
	CCDC = 2206847
Compound	12
CCDC Number	2206847
Formula	$C_{16}H_{12}N_6O_{14}$
D_{calc} / g cm ⁻³	1.697
m/mm^{-1}	1.345
Formula Weight	512.32
Color	vellow
Shape	plate-shaped
Size/mm ³	$0.23 \times 0.13 \times 0.02$
	100.00(10)
Crystal System	monoclinic
Space Group	
	Γ2]/C 7 59025/14)
u/A	1.30033(14) 12.1240(2)
	13.1249(3)
	10.13126(18)
	90
<i>b</i> /	95.9409(16)
g/	90
V/A ³	1002.56(3)
Z	2
Z'	0.5
Wavelength/Å	1.54184
Radiation type	Cu Ka
$Q_{min}/^{\circ}$	5.535
$Q_{max}/^{\circ}$	76.070
Measured Refl's.	11142
Indep't Refl's	2018
Refl's I $\geq 2 s(I)$	1831
R _{int}	0.0332
Parameters	194
Restraints	6
Largest Peak	0.333
Deepest Hole	-0.231
GooF	1.064
wR_2 (all data)	0.0955
wR_2	0.0924
R_1 (all data)	0.0382
R,	0.0302
11	0.0071

Atom	X	У	Z	U_{eq}
01	6021.0(12)	5989.9(7)	1888.0(10)	22.9(2)
O2	4463.9(13)	2686.9(7)	1297.4(9)	24.0(2)
03	7398.2(14)	2808.1(8)	1853.2(10)	30.1(3)
O4	6302.2(17)	1703.8(8)	397.8(11)	38.0(3)
05	8004(3)	5287.2(19)	4485(2)	24.7(6)
O5B	8900(2)	5639.4(14)	3696.8(19)	25.7(6)
06	9180(3)	6595.9(17)	3430(2)	31.3(6)
O6B	6917(3)	5450.7(16)	5165(2)	34.3(6)
O7	8970(70)	6660(30)	5540(30)	33.6(5)
O7B	8930(60)	6620(30)	5450(30)	33.6(5)
N1	4327.1(15)	6097.4(9)	1196.0(11)	21.9(3)
N2	6212.2(17)	2384.0(9)	1185.4(11)	26.0(3)
N3	8786(4)	6268(2)	4462(3)	25.3(7)
N3B	8172(4)	5923(2)	4869(3)	25.5(6)
C1	3554.1(17)	5205.7(10)	1271.6(12)	19.5(3)
C2	4697.2(17)	4487.7(10)	2007.7(13)	20.1(3)
C3	6192.4(18)	5031.3(10)	2364.1(13)	21.4(3)
C4	4296.5(18)	3415.2(10)	2372.1(13)	22.1(3)
C5	7933(2)	4773.7(11)	3116.1(15)	28.2(3)
C6	1724.6(17)	5086.4(10)	636.6(12)	19.7(3)
C7	603.2(18)	5936.9(10)	508.8(13)	21.3(3)
C8	-1101.8(18)	5850.7(10)	-122.0(13)	20.9(3)

Table S5: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **12**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} .

Table S6: Anisotropic Displacement Parameters (×10⁴) for **12**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
01	22.5(5)	16.9(5)	28.4(5)	-1.5(4)	-2.0(4)	0.0(3)
O2	29.8(5)	17.1(5)	24.1(5)	-0.5(4)	-1.4(4)	1.5(4)
03	29.5(5)	26.4(5)	33.9(6)	-3.5(4)	1.3(4)	2.1(4)
O4	59.1(8)	24.6(6)	28.8(6)	-7.7(4)	-2.6(5)	14.7(5)
05	29.1(12)	19.6(13)	24.8(11)	-0.5(9)	-0.9(9)	-4.6(9)
O5B	23.2(10)	26.2(11)	27.4(10)	-6.6(8)	2.0(7)	-4.2(7)
06	30.5(12)	30.2(13)	33.2(12)	4.8(9)	2.7(9)	-6.6(9)
O6B	44.5(13)	28.6(11)	31.4(11)	-3.4(8)	12.1(9)	-6.5(9)
O7	36.6(19)	25(2)	36(2)	-9.4(12)	-9(2)	0.4(12)
O7B	36.6(19)	25(2)	36(2)	-9.4(12)	-9(2)	0.4(12)
N1	20.7(6)	19.2(6)	25.2(6)	-0.3(4)	-0.9(4)	2.0(4)
N2	36.1(7)	18.8(6)	23.0(6)	1.9(4)	2.0(5)	5.9(5)
N3	20.6(14)	24.8(16)	29.5(16)	-0.9(13)	-2.3(11)	0.0(11)
N3B	28.0(14)	21.4(16)	25.7(14)	-2.1(12)	-4.0(11)	4.4(11)
C1	23.1(7)	16.8(6)	19.0(6)	-1.3(5)	3.4(5)	2.0(5)
C2	22.4(6)	18.3(7)	19.4(6)	-1.7(5)	1.2(5)	2.5(5)
C3	26.0(7)	16.3(6)	21.2(6)	-2.0(5)	-0.1(5)	2.4(5)
C4	27.2(7)	18.4(7)	20.3(6)	0.5(5)	1.3(5)	1.1(5)
C5	28.3(7)	21.1(7)	32.9(8)	-4.7(6)	-8.5(6)	2.2(5)
C6	22.0(6)	18.8(6)	18.1(6)	1.8(5)	2.3(5)	1.0(5)
C7	25.4(7)	15.6(6)	22.8(6)	-0.1(5)	2.1(5)	0.4(5)
C8	23.5(6)	17.1(6)	21.9(6)	1.7(5)	1.8(5)	3.5(5)

Atom	Atom	Atom	Angle/°
C3	01	N1	108.74(10)
N2	O2	C4	113.67(10)
N3	O5	C5	111.01(19)
N3B	O5B	C5	108.9(2)
C1	N1	01	105.75(10)
03	N2	O2	118.77(11)
O4	N2	O2	112.55(12)
O4	N2	O3	128.68(13)
O6	N3	O5	118.9(2)
06	N3	O7	128.3(18)
O7	N3	O5	112.8(18)
O6B	N3B	O5B	117.6(3)
O7B	N3B	O5B	114.0(17)
O7B	N3B	O6B	128.4(17)
N1	C1	C2	111.46(12)
N1	C1	C6	118.27(11)
C2	C1	C6	130.26(12)
C1	C2	C4	128.27(12)
C3	C2	C1	103.64(12)
C3	C2	C4	127.98(12)
01	C3	C2	110.40(12)
01	C3	C5	116.18(12)
C2	C3	C5	133.39(13)
O2	C4	C2	113.32(10)
O5B	C5	C3	114.49(13)
C3	C5	O5	107.92(13)
C7	C6	C1	119.32(12)
C81	C6	C1	121.44(12)
C81	C6	C7	119.21(12)
C8	C7	C6	120.36(13)
C7	C8	C61	120.42(12)

 Table S7: Bond Angles in for compound 12.

 Table S8: Bond Lengths in Å for compound 12.

Atom	Atom	Length/Å	
01	N1	1.4050(14)	
01	C3	1.3488(16)	
O2	N2	1.3994(16)	
O2	C4	1.4642(16)	
O3	N2	1.2042(16)	
O4	N2	1.2039(16)	
O5	N3	1.419(4)	
O5	C5	1.538(3)	
O5B	N3B	1.410(3)	
O5B	C5	1.444(2)	

Atom	Atom	Length/Å	
<u>O6</u>	N3	1.197(4)	
O6B	N3B	1.200(4)	
O7	N3	1.199(16)	
O7B	N3B	1.199(15)	
N1	C1	1.3146(18)	
C1	C2	1.4357(18)	
C1	C6	1.4755(18)	
C2	C3	1.3562(19)	
C2	C4	1.4945(18)	
C3	C5	1.4923(19)	
C6	C7	1.4010(19)	
C6	$C8^1$	1.3987(19)	
C7	C8	1.3860(19)	

Table S9:	Torsion	Angles in	° for com	pound 1	2
I unic D/.	10151011	1 mgres m		pound 1	-

Atom	Atom	Atom	Atom	Angle/°
01	N1	C1	C2	0.03(14)
01	N1	C1	C6	179.43(10)
01	C3	C5	O5	74.45(17)
01	C3	C5	O5B	24.18(19)
N1	O1	C3	C2	0.78(14)
N1	O1	C3	C5	179.16(11)
N1	C1	C2	C3	0.42(15)
N1	C1	C2	C4	176.88(12)
N1	C1	C6	C7	-28.19(18)
N1	C1	C6	$C8^1$	149.78(12)
N2	O2	C4	C2	81.13(13)
N3	O5	C5	C3	-91.6(2)
N3B	O5B	C5	C3	78.8(2)
C1	C2	C3	01	-0.72(14)
C1	C2	C3	C5	-178.72(15)
C1	C2	C4	O2	81.32(16)
C1	C6	C7	C8	177.92(11)
C2	C1	C6	C7	151.07(13)
C2	C1	C6	$C8^1$	-30.9(2)
C2	C3	C5	O5	-107.64(18)
C2	C3	C5	O5B	-157.91(16)
C3	O1	N1	C1	-0.48(13)
C3	C2	C4	O2	-103.05(15)
C4	O2	N2	O3	-7.62(16)
C4	O2	N2	O4	172.26(11)
C4	C2	C3	01	-177.19(12)
C4	C2	C3	C5	4.8(2)
C5	O5	N3	O6	4.3(3)
C5	O5	N3	O7	-175(3)
C5	O5B	N3B	O6B	-1.8(3)
C5	O5B	N3B	O7B	178(3)
C6	C1	C2	C3	-178.88(13)

Atom	Atom	Atom	Atom	Angle/°	
C6	C1	C2	C4	-2.4(2)	
C6	C7	C8	$C6^1$	0.1(2)	
$C8^1$	C6	C7	C8	-0.1(2)	

Table S10: Hydrogen Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **compound 12**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} .

Atom	х	У	Z	U_{eq}	
H4A	5114.13	3212.6	3153.54	26	
H4B	3072.68	3383.79	2629.07	26	
H5AA	8917.03	5023.07	2632.16	34	
H5AB	8050.15	4026	3220.12	34	
H5BC	7723.38	4289.38	3832.7	34	
H5BD	8678.22	4423.49	2509.64	34	
H7	1013.81	6576.32	856.54	26	
H8	-1852.36	6431.75	-205.52	25	

 Table S11: Atomic Occupancies for all atoms that are not fully occupied in compound 12.

Atom	Occupancy
05	0.475(3)
O5B	0.525(3)
O6	0.475(3)
O6B	0.525(3)
07	0.475(3)
O7B	0.525(3)
N3	0.475(3)
N3B	0.525(3)
H5AA	0.475(3)
H5AB	0.475(3)
H5BC	0.525(3)
H5BD	0.525(3)



Figure S2. FTIR-Spectrum of Compound 2





Current I NAME EXPNO PROCNO F2 - Acqu Date_ Time INSTRUM PROBHD PUL PROC	Data Paran Di uisition 1 202 5 mm QNP	neters 2PT135 94 1 220727 16.45 spect 1H/13	ers					— 126.80									HO ^{-N}			≷ _N _OI	Н
PULPROG TD SOLVENT NS DS SWH FIDRES AQ RG DW DE TE CNST2 D1 d2 d12 DELTA	1999 0.0 0.82 140.00 2.000 0.003 0.000 0.000	Pt135 32768 DMSO 8 60.080 609133 208384 3390.4 25.050 6.00 300.0 000000 300.0 000000 357143 022000 000891	Hz Hz sec usec usec K sec sec sec sec									ΛL	1S-SOHAN	1−326R−I	DEPT135				2		
NUC1 P1 p2 PL1 SF01	CHANNEL : 75.4 CHANNEL :	E1 ==== 13C 7.00 14.00 -5.00 760505 E2 ====	usec usec dB MHz																		
CPDPRG[2 NUC2	Wá	altz16 1H	n ann ai bhe an an an	ta allan ta anto da cata						. Note marched a come to			encolorie at his carac	1 mm - 1 m 10 1 mm		1	a de su a tanta at an an		st a construct a familiar	Bits, to Lible a Basel	100-11-11-11-11-11-11-11-11-11-11-11-11-
P3 p4 PCPD2 PL2 PL12 SF02	300.13	6:10 12.20 100.00 -6.00 18.54 312005	usec usec dB dB MHz		માં પ્રાપ્ય નાં પ્રાપ્ય પ્રાપ્ય જેવા છે.	anna ann an Iol	and the state of the second second	analisi i	а т у турки (,			<u>, , , , , , , , , , , , , , , , , , , </u>	and a start of the s	ul er her let der fijk	1-11-0-0-0-0-0-0-0-0-0-0-0-0-0-0-0-0-0-	2 - 44- 4 - 4 - 4 - 4 - 4 - 4 - 4 - 4 -			
F2 - Prod SI SF WDW SSB LB GB PC	cessing pa 75.40	aramete 32768 677765 EM 0 1.00 0 1.40	ers MHz Hz																		
210) 200	190	180	170	160	150	140	130	120	110	100	90	80	70	60	50	40	30	20	10	ppm

Figure S5. ¹³C-DEPT135 NMR Spectrum of Compound 2



Figure S6. DSC of compound 2 at 5 °C min⁻¹



Figure S7. FTIR-Spectrum of Compound 3







Figure S10. FTIR-Spectrum of Compound 4



Current NAME EXPNO PROCNO	Data	Para	ameter 130 34	5 C L L					-132.04	- 125.72	JMS	-SOHAN-	-336-130				/ 40.06 39.79	39.51 39.23	- 38.68 38.68		
F2 - Acc Date_ Time INSTRUM PROBHD PULPROG TD SOLVENT NS DS SWH FIDRES AQ RG DW DE TE D1 d11 d12 ======= NUC1 P1 P1	quisi 5 m = CHA	tion 20 m QNH 199 0.2 0.2 1.00 0.03 0.00 NNEL	Param 22080 21.4 spec 21.4 spec 21.4 spec 21.4 spec 21.4 spec 21.4 spec 21.4 spec 21.4 spec 20.08 20.0	eters 5 5 5 5 5 5 5 5 5 5 5 5 5												ŀ	10 ^{-N}	N ₃ 4	N ₃	N ^{_OH}	
SF01 CPDPRG[2 NUC2 PCPD2 PL2 PL12 PL13 SF02 F2 - Prc SI SF WDW SSB LB GB PC	CHA	75.4 NNEL 300.1 ing <u>p</u> 75.4	176050. f2 ==: valtz1 100.0 120.00 17.0	5 MHz 6 1 0 USEC 0 dB 0 dB 0 dB 0 dB 5 MHz Cers 3 0 MHz 4 0 0 Hz 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1	160.4 w 144.5 11 /2 14.1	1 db .m. 3.1 , 20m.unu	ist da, and da, ad	usileer for a star	and the state of t	a he antition in the s	من المنابعة	د. د بالا المراجع الم	1 1 101 11 1 1 1 1 1 1	Alter siles si da		ak di nada jik din	e. son fabile des vers			п, шайила, ", сы	. ed. un vola v. A. mod J. i
ראייזאיקאייאאי 211	райдай 0 2		190	180	170	160	اسراپاریانیانیستین 150	140	130	120	110	100	90	80	70	60	50	үлт чүр 40	30	יאאיין אווי איאין אוויי 20	ppm
							F	igure	S12. ¹	³ C NM	R Spec	trum o	of Com	pound 4	4						



Figure S13. DSC of compound 4 at 5 °C min⁻¹



Figure S14. TGA of compound **4** at 5 °C min⁻¹



Figure S15. FTIR-Spectrum of Compound 5



Figure S16. ¹H NMR Spectrum of Compound 5

Current NAME EXPNO PROCNO	Data Parameters 13C 350 1	- 145.22	~ 128.29 ~ 125.26	JMS-SOHAN-341-13C	40.32 39.77 39.21 38.65 38.65	
F2 - Acc Date_ Time INSTRUM PROBHD PULPROG TD SOLVENT NS DS SWH FIDRES AQ RG QW DE	quisition Parameters 20220817 13.30 spect 5 mm QNP 1H/13 zgpg 32768 DMSO 343 0 19960.080 Hz 0.609133 Hz 0.8208384 sec 20642.5 25.050 usec 6.00 usec			HONNN		
TE D1 d11 d12	300.0 K 1.00000000 sec 0.03000000 sec 0.00002000 sec			N <mark>NN</mark> 5 N-NOH		
======= NUC1 P1 PL1 SF01	= CHANNEL f1 ======= 13C 4.00 usec -5.00 dB 75.4760505 MHz					
CPDPRG[2 NUC2 PCPD2 PL2 PL12 PL13 SF02	CHANNEL f2 ====== waltz16 1H 100.00 usec 120.00 dB 17.00 dB 17.00 dB 300.1312005 MHz					
F2 - Prc SI SF WDW SSB LB GB PC	ocessing parameters 32768 75.4677700 MHz EM 0 1.00 Hz 0 1.40	at with the program to the providence of the program of the the state of the state		na y të un dët interpreta mjeri në përijan kë përijan të kandëre të un të mënderi të në përijanë të d		and works from the state of the
210	0 200 190 180 17(0 160 150 140 Figure S	130 120 17. ¹³ C NMR S	110 100 90 80 70 Spectrum of Compound 5	60 50 40 30 20	ppm

Current NAME	Data Par	ameters DEPT135						28.29													
EXPNO PROCNO		102																			
F2 - Acq Date_ Time PROBHD PULPROG TD SOLVENT NS DS SWH FIDRES AQ RG DW DE TE CNST2 D1 d2 d12	uisition 2 5 mm QN 19 0 0. 140. 2.0 0.0 0.0	Parame 0220817 13.42 spect P 1H/13 dept135 32768 960.080 .609133 8208384 18390.4 25.050 6.00 0300.0 000000 0000000 0357143	Hz Hz sec usec usec K sec sec sec										JMS-	SOHAN-3	HO HO	T135					
DELTA ======= NUC1 P1 p2 PL1 SF01	0.0 = CHANNEL 75.	0000891 f1 === 13C 7.00 14.00 -5.00 4760505	sec usec usec dB MHz										N(<mark>,</mark> N	-N OH	5						
NUC2 P3 P4 PCPD2 PL2 PL2 PL12 SF02	BART TOP MANY	100.00 18.54 1312005	usec usec usec dB dB MHz	Ling (sandhananda 11) (sall karl Maran ya sanay ya gasang Maran ya sanay ya gasang	n jan laikan kunda Marina (kunda kunda ku	lind, i ki dan ti anger Mangan ngan ngan ngan ngan ngan ngan nga	na All Linkalan (Ang Ang)an Ing ng pang na mpang pangan Ing ng pang ng na mpang pangan	in and a start a start and	Norad Population	a parta da	la dia kaominina dia kaomin Ny faritr'ora dia kaominina d	det hoge til stød stød so fo en er og som er som e		ili in analam inali pina Mala ny positra panya	allan bara da di di di da kana di sana Kana di pipa da manda di sana di pipa da manda di pipa da manda di pipa da manda di pipa di di di di di di di d Kana di pipa da di	tin bar, variadi k kali a landar Mara ng		anna lákakinaka ana lita		da la subsecta da sub Nano nga kangan ta vi ta Nano nga kangan ta vi ta	in de dense in de de Nyser op in gelegen
F2 - Pro SI SF WDW SSB LB GB PC	ocessing 75.	paramet 32768 4677703 EM 0 1.00 0 1.40	ers MHz Hz																		
 21(0 200	190	180	170	160	150	140	130	120	110	100			.		50	40	30	20	 10	ppm

Figure S18. ¹³C-DEPT135 NMR Spectrum of Compound 5



Figure S19. DSC of compound **5** at 5 °C min⁻¹



File: C:...\TGA\Sohan\SOHAN-341 at 5°C.001

Sample: SOHAN-341 at 5°C

Figure S20. TGA of compound 5 at 5 °C min⁻¹



Figure S21. FTIR-Spectrum of Compound 6



Figure S22. ¹H NMR Spectrum of Compound 6



Current NAME EXPNO PROCNO	Data Parameters DEPT135 105 1			- 125.79						
F2 - Acq Date_ Time INSTRUM PROBHD FULPROG TD SOLVENT NS DS SWH FIDRES AQ DW DE RG DW DE TE CNST2 D1 d2 d12 DELTA	uisition Paramet 20220820 11.52 spect 5 mm QNP 1H/13 dept135 32768 DMSO 6 19960.080 0.609133 0.8208384 18390.4 25.050 6.00 300.0 140.000000 0.00357143 0.0000200 0.0000891	Hz Hz Hz sec usec k sec sec sec sec				JMS-SOHAN-3	49-DEPT135	N_N_N_0- +NH ₃ OH	- ⁺ NH ₃ OH N-N N N 6	
NUC1 P1	- CHANNEL f1 13C 7.00 000000000000000000000000000000000	usec usec	is a shiran a fa ka a na milan ika Liyak ka sha miladan i ni miladiki na shiran ka miladiki na Arifiya may ka shiran suy ka sana yariya ka shiran ka sana ka miladiki na shiran ka sa	ilin, dada da gana kuning sa	ville for et al sing a station of all first boost a Theorem in the spectrum in part of the station	ulandihuhimla bahahari ula baka Partikang mapaping minang pang	as, un forde a chantair an can an dùthair Martair an Airtean	daa adadaha kadaa Dahaddii waxa waxay barya barya gabaa ahara	an <mark>da ya sa kutu ya kutu ya kutu ya kutu ya kutu kutu kutu kutu kutu kutu kutu kut</mark>	di na sulis Protografia
CPDPRG[2 NUC2 P3 P4 PCPD2 PL2 PL12 SF02	CHANNEL f2 ==== waltz16 1H 6.10 12.20 100.00 -6.00 18.54 300.1312005	usec usec usec dB dB MHz								
F2 - Pro SI SF WDW SSB LB GB PC	cessing paramete 32768 75.4677790 EM 0 1.00 0 1.40	ers MHz Hz								

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

Figure S24. ¹³C-DEPT135 NMR Spectrum of Compound 6

15N{1H]	}_5861	Soha	n 349	64	36 36	33				7.38			
Current I NAME EXPNO PROCNO	Data Paran New :	meters folder 5861 1		-12	-15. -59.	-89							
F2 - Acqu Date Time PROBHD PULPROG TD SOLVENT NS DS SWH FIDRES AQ RG DW DE TE D1 D11 TD0 ======= SF01	10.000 CHANNEL 50.6	Paramete 220921 17.00 spect 30 BB/ zgig 16248 DMSO 5918 0 22.223 H 137015 H 339712 S 27.83 14.400 H 303.2 H 000000 S 000000 S 000000 S 10240 f1 =====	Hz Hz Hz Sec Isec Sec Sec							1	N-N-O- *NH3OH	- ⁺ NH ₃ OH 0 N-N N N 6	
NUC1 P1 PLW1	155.00	15N 12.00 ι 000000 ι	isec N										
SF02 NUC2 CPDPRG[2 PCPD2 PLW2 PLW12	CHANNEL : 500.1 wa 26.00 0.27	f2 ==== 920008 M 1H altz16 80.00 M 000000 M 649999 M	Hz 19 19 19 19 19 19 19 19 19 19 19 19 19										
F2 - Proc SI WDW SSB LB GB PC	cessing pa 50.70	arameter 32768 031345 M EM 0 3.00 H 0 0.20	rs MHz Hz			I							
		dili malandan dan dan Perpendian dan dan dan dan dan dan dan dan dan d		teority (1919), data da Teority (1919), data di			an an filmin Ìreacht Irla (19) Mainte Cantol a mar agus a		lindersen er de le	indates dia 1. and all formationed a an average of the later of the states of the stat			
- <u> </u>	150	100	50 Fim	0 1re S25 ¹⁵	- 50 N NMR Sr	-10	0 -150	-200	-250 dc (at 50 70	-300 MH ₇)	-350	-400	ppm
			rigi	110 023.	ra ramir oh		Compound		u ₀ (at 50.70	will'iz)			



Figure S26. DSC of compound 6 at 5 °C min⁻¹


Figure S27. TGA of compound **6** at 5 °C min⁻¹



Figure S28. FTIR-Spectrum of Compound 7



Figure S29. ¹H NMR Spectrum of Compound 7





Figure S31. DSC of compound 7 at 5 °C min⁻¹



Sample: SOHAN-348 at 5°C

File: C:...\TGA\Sohan\SOHAN-348 at 5°C.001 Operator: SOHAN Run Date: 22-Aug-2022 14:50 Instrument: TGA Q50 V20.13 Build 39



Figure S32. TGA of compound 7 at 5 °C min⁻¹



Figure S33. FTIR-Spectrum of Compound 8



Current	Data Para	ameters).63	5.63 5.48			35	23	95 67		
EXPNO		360				140	<u>15</u>			<u> </u>	ວ ດີ ດີ ດີ	ක් ක්		
PROCNO		1					$\overline{\langle}$							
F2 - Acq	quisition	Parame	ters			I	Y							
Date_	20	0220826												
TIME		18.58 spect												
PROBHD	5 mm QNI	P 1H/13											_ ⁺ NH₂NH	2
PULPROG		zgpg										(ריין. ר	2
TD		32768 DMSO					i.	JMS-SOHAN-352-	-13C				N-N	
NS		277											Î ÎN	
DS		0											N	
SWH	199	960.080	Hz											
FIDRES	0.	.609133	Hz									N /		
AQ RG	0.0	20642 5	sec								N			
DW	-	25.050	usec									N-N	8	
DE		6.00	usec									0	•	
TE	1 0/	300.0	K									⁺ NH ₂ NH ₂		
DI d11	1.00	30000000	Sec									11131112		
d12	0.00	002000	sec											
	- CHANNEL	f1 ====												
NUC1		13C												
P1		4.00	usec											
SF01	75.4	4760505	dB MHz											
	- CHANNEL	f2 ====												
CPDPRG[2	2 1	waltz16												
NUC2		1H												
PCPD2		120.00	usec dp											
PT-12		17.00	dB											
PL13		17.00	dB											
SFO2	300.1	1312005	MHz			1								
F2 - Pro	cessing p	paramet	ers											
SI		32768												
SF	75.4	4677747	MHz								8			
SSB		EM 0									P .			
LB		0.50	Hz								п			
GB		0				L.				1	II	L L	1 J to I have 1	
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	220	200)	180	160	140	120	100	80	60	40	20	0	ppm
		_50	-		Fiom	re S35 ⁻¹³ C	NMR Spe	ctrum of Con	nound 8			_•	~	220
					<u>-</u> <u>-</u> <u>-</u> <u>-</u> -		1 min ope							

Current NAME EXPNO PROCNO	Data Parameters DEPT135 108 1						175 AB	04.07												
FROCINO F2 - Acq Date_ Time INSTRUM PROBHD PULPROG TD SOLVENT NS SWH FIDRES AQ RG DW DE TE CNST2 D1 d2 d12 DELTA	uisition Paramet 20220826 19.09 spect 5 mm QNP 1H/13 dept135 32768 DMSO 27 16 19960.080 0.609133 0.8208384 18390.4 25.050 6.00 300.0 140.000000 2.0000000 0.00357143 0.00002000 0.00002000	Hz Hz sec usec K sec sec sec sec								J	MS-SOHA	N-352-D	EPT135		N	-N +NHaN		⁺ NH₃NH N-N N N	H ₂	
======= NUC1 P1 p2 PL1 SF01	CHANNEL f1 13C 7.00 14.00 -5.00 75.4760505	usec usec dB MHz																		
CPDPRG[2 NUC2 P3 P4 P12 PL2 PL12	CHANNEL f2 ==== waltz16 1H 6.10 war war war war war war - 6.00 18.54	usec Laffinition dB dB	verdetalla desteta a tara da general deste a parte deste			i fan leithing fan de sta	n gubios sus legal		ling for the state of the state of the	a ta lan saka marang sa Jajah ka Kalifat Papatang sa Pang		i dan sekaran yang sekaran sekaran Kanan kang sekaran sekaran sekaran sekaran sekaran sekaran sekaran sekaran s	en di unital en di la di se di Tipoter di unital di seguna di seguna di seguna di seguna di seguna di seguna di	indentificities. Den mit de la dem 19 aug 20 auguste en la dem par par p	in the survey of	an la ser ann an		Aller Martin Martin Martin Martin Martin Martin Martin	n de geste kalder och för en förstande för ger och	
SFO2 F2 - Pro SI SF WDW SSB LB GB PC	300.1312005 cessing paramete 32768 75.4677747 EM 0 1.00 0 1.40	MHz ers MHz Hz																		
 21(0 200 190	180		160	150	140	130	120	110	100		 80	.	60	50	40	30	20	 10	ppm

210 200 190 180 170 160 150 140 130 120 110 100

Figure S36. ¹³C-DEPT135 NMR Spectrum of Compound 8





Figure S38. DSC of compound 8 at 5 °C min⁻¹



Figure S39. TGA of compound 8 at 5 °C min⁻¹



Figure S40. FTIR-Spectrum of Compound 9



Current NAME EXPNO PROCNO	Data Parameters 13C 361 1			∕_ 126.73 ∕_ 124.79	40.34 39.51 38.96 38.68
F2 - Acc Date_ Time INSTRUM PROBHD PULPROG TD SOLVENT NS DS SWH FIDRES AQ RG	quisition Paramete 20220826 19.15 spect 5 mm QNP 1H/13 zgpg 32768 DMSO 3413 0 19960.080 F 0.609133 F 0.8208384 s 20642.5	ers Hz Hz Sec			JMS-SOHAN-353-13C
DW DE TE D1 d11 d12	25.050 t 6.00 t 300.0 f 1.00000000 s 0.03000000 s 0.00002000 s	ISEC ISEC SEC SEC SEC			N N 0- K ⁺
======= NUC1 P1 PL1 SF01	= CHANNEL f1 ====== 13C 4.00 t -5.00 c 75.4760505 M	-=== 1sec 1B MHz			
CPDPRG[2 NUC2 PCPD2 PL2 PL12 PL13 SF02	= CHANNEL f2 ===== 2 waltz16 1H 100.00 t 120.00 c 17.00 c 300.1312005 N	ISEC IB IB IB IHZ			
F2 - Pro SI SF WDW SSB LB GB PC	ocessing parameter 32768 75.4677840 M EM 0 0.50 F 0 1740	cs MHz Hz			
	220 200	180	160 140 Figure S42	0 120 2. ¹³ C NMR	100 80 60 40 20 0 ppm Spectrum of Compound 9



Figure S43. DSC of compound 9 at 5 °C min⁻¹



Figure S44. TGA of compound 9 at 5 °C min⁻¹



Figure S45. FTIR-Spectrum of Compound 11



Figure S46. ¹H NMR Spectrum of Compound 11



S57

Current I NAME EXPNO PROCNO F2 - Acqu Date_	Data Parameters DEPT135 99 1 uisition Parameters 20220808				53.27 51.44	
TIME INSTRUM PROBHD PULPROG TD SOLVENT NS DS SWH FIDRES AQ RG DW	23.24 spect 5 mm QNP 1H/13 dept135 32768 DMSO 9 16 19960.080 Hz 0.609133 Hz 0.8208384 sec 18390.4 25.050 usec		JMS-SOHAN-338-D	IPT135		
DE TE CNST2 D1 d2 d12 DELTA ======= NUC1	6.00 usec 300.0 K 140.000000 2.0000000 sec 0.00357143 sec 0.00002000 sec 0.0000891 sec CHANNEL f1 ======== 13C					
PI p2 Billing balance weippingen	7.00 used 14.00 used Mumphine States Tail Angle Angle Mumphine Strates Tail Angle Angle Angle Angle Ang	Αν οβατιλοποιη με ματοποληληλική ηλοπόλητη δολλοβουνική το δου Αγγορία από θα με παραλληθία τη μουτολογία το υ Αναλληλοποιηματική τη παραγογραφική του ματοποίο το το προγραφικό τη του το προγραφικό το το προγραφικό το του	ן איז אין איז	i New Markes and all behavior and a first standing of the same birth south of the same behavior by the same be I where and poster and a same standard and the same birth stands and same stand and same same same same same sa	n dag talah dag at pang baran dan pang baran dag baran dan pang baran dan pang baran dan pang baran dan pang ba Barang pang barang pang barang bar	la silandina sasing barang saka pala dahara ang sa sila di kuratika sadi a pali palang para na mang palipang pang mang pang sa sang pang barang pang sa sang pang sa sang pang sa sang
====== CPDPRG[2 NUC2 P3 P4 PCPD2 PL2 PL12 SF02	CHANNEL f2 ======= waltz16 1H 6.10 used 12.20 used 100.00 used -6.00 dB 18.54 dB 300.1312005 MHz		НО	N~O		
F2 - Prod SI SF WDW SSB LB GB PC	cessing parameters 32768 75.4677817 MHz EM 0 1.00 Hz 0 1.40		0 _{-N} 11	ОН		
210) 200 190 18	30 170 160 150 140 1 3	30 120 110 100	90 80 70 60	0 50 40	30 20 10 ppm

Figure S48. ¹³C-DEPT135 NMR Spectrum of Compound **11**



Figure S49. DSC of compound 11 at 5 °C min⁻¹



Figure S50. TGA of compound 11 at 5 °C min⁻¹



Figure S51. FTIR-Spectrum of Compound 12



Figure S52. ¹H NMR Spectrum of Compound 12



15N{1H	}_5894	Sohai	n 343	58	3.15 1.97								
Current NAME EXPNO PROCNO	Data Para New	meters folder 5894 1			× 44								
F2 - Acq Date_ Time INSTRUM PROBHD PULPROG TD SOLVENT NS DS SWH FIDRES AQ RG DW DE TE D1 D1 TD0	uisition 20 5 mm PAB 407 2. 0.1 10.00 0.03	Paramete 220926 18.07 spect BO BB/ zgig 16248 DMSO 5626 0 60.871 H 993088 27.83 12.267 8.00 303.2 H 000000 s 000000 s 000000 s	Hz Hz Sec Isec Isec Sec Sec						0 ₂ 0 ₂ NO				
SF01 NUC1 P1 PLW1	CHANNEL 50.6 155.00	f1 ===== 963210 M 15N 12.00 N 000000 M	ISEC									L	
SF02 NUC2 CPDPRG[2 PCPD2 PLW2 PLW12	CHANNEL 500.1 w 26.00 0.27	f2 ==== 920008 M 1H altz16 80.00 W 649999 W	antes MHz 1800 V										
F2 - Pro SI SF WDW SSB LB GB PC PC	cessing p 50.7	arameter 32768 031345 M EM 0 1.00 H 0 0.20	rs 4Hz Hz	ւր անուն ասկարերու է ու նե	harnadh a latu, a na la ata	talin law of statistica to ca	1.1	. or the no-stillant death of starts	allala a statica com	n Küllənində ir oda ı	d of, to build and to be to	na dali una sadilannadat da si	kellert have alle date as
	ajne hydrydd far yn	n provinski po na sinje po po Transferancija (1991) na slovenski po	n King King King King King King King Kin	na prednje po na prima da na prednje po na prima da		lla <mark>pris (</mark> angélésengeses) Kanani (strant na sasati	territe and encoded as	n ann a pragair na baileann Ann Albhan a bailean A	n inde a de la contraction de la contra La contraction de la c	Ngalateration (d	^{na} ng ng manang ng ma Tang ng manang ng manang ng mga ng	n shi na sa sa ka ha sa	line of the trees
	150	100	50	0	-50	-100	-150	-200	-250	-300	-350	-400	ppm
			Figure S	54. ¹⁵ N NN	AR Spectru	m of Comp	ound 12 in	DMSO-d ₆ (at 50.70 M	Hz)			



Figure S55. DSC of compound 12 at 5 °C min⁻¹



Figure S56. TGA of compound 12 at 5 °C min⁻¹



Figure S57. FTIR-Spectrum of Compound 13



Figure S58. ¹H NMR Spectrum of Compound 13



Current Data Parameters NAME DEPT135		28. CI.		3.85
PROCNO 101		÷		ကိုကို
F2 - Acquisition Parameters Date_ 20220817 Time 12.46 INSTRUM spect PROBHD 5 mm QNP 1H/13 PULPROG dept135 TD 32768 SOLVENT DMSO			CI	$\backslash/$
NS 163 DS 16 SWH 19960.080 Hz FIDRES 0.609133 Hz AQ 0.8208384 sec RG 18390.4 DW 25.050 usec DE 6.00 usec		JMS-SOHAN-344-DI	PEPT135	
TE 300.0 K CNST2 140.000000 D1 2.0000000 sec d2 0.00357143 sec d12 0.00002000 sec DELTA 0.00000891 sec				
	anya Namada daha taka taka da sa Kanangsang dalam da sina da kada da da sa taka di sa kana di sa kana di sa ka Grayon pengangan angga mangga mpangnan pengangan manganan na menana menang tang tang tang pang pang	All Marcharda, falle sid all a descarabilite la del caratterità più real anno alla si the art atterioristi Marchard anno serve se anno serve per a representa del garanterita del caratterità si transferante se porteri se	al, ad inal i dhahaanii la haling ar dan ar yah adah yulaana shi dhahail Myanayay 1995 ya	telika nata 1919-1919 - Angela Karlandara, a Ukan periodikan dan periodikan dan periodikan dan periodikan dari 1919 - Angela Karlandara, angela karlandara dari karlandara dari karlandara dari karlandara dari karlandara dari
CHANNEL f2 f2 CPDPRG[2 waltz16 NUC2 1H P3 6.10 usec p4 12.20 usec PCPD2 100.00 usec PL2 -6.00 dB FL12 18.54 dB SFO2 300.1312005 MHz				
F2 - Processing parameters SI 32768 SF 75.4677853 MHz WDW EM SSB 0 LB 1.00 Hz GB 0 PC 1.40				
220 210 200 190 1	80 170 160 150 140 13 Figure S60. ¹³ C-DEF	30 120 110 100 90 8 PT135 NMR Spectrum of Compou	60 70 60 50 4 und 13	0 30 20 10 ppm



Figure S61. FTIR-Spectrum of Compound 14



Figure S62. ¹H NMR Spectrum of Compound 14
Current Data Parameters NAME 13C EXPNO 357 PROCNO 1	- 166.81 - 161.28 ^ 129.56	- 128.65 - 111.15 - 111.15	42.92 41.65 40.34 39.51 38.95 38.95 38.95 38.95
F2 - Acquisition Parameters Date20220824 Time12.27 INSTRUMspect PROBHD_5 mm_QNP_1H/13 PULPROGZgpg TD22769		/ JMS-SOHAN-345-13C	
ID 32768 SOLVENT DMSO NS 412 DS 0 SWH 19960.080 Hz FIDRES 0.609133 Hz AQ 0.8208384 sec		N_3	
RG 20042.5 DW 25.050 usec DE 6.00 usec TE 300.0 K D1 1.00000000 sec d11 0.03000000 sec d12 0.00002000 sec			∠N ₃
===== CHANNEL f2 ====== E CPDPRG[2 waltz16 NUC2 1H PCPD2 100.00 usec PL2 120.00 dB PL12 17.00 dB PL13 17.00 dB SF02 300.1312005 MHz			
F2 - Processing parameters SI 32768 SF 75.4677853 MDW EM SSB 0 LB 0.50 GB 0 PC 1.40			
210 200 190 180 17	70 160 150 140 130 Figure S63. ¹³ C	0 120 110 100 90 80 70 6 NMR Spectrum of Compound 14	.0 50 40 30 20 ppm

S73

Current Data Parameters NAME DEPT135 EXPNO 107 PROCNO 1 E2 - Acquisition Parameter	28 5 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	69.02 7 	42.91
P2 - Acquisition Parameter Date20220824 Time 12.41 INSTRUM spect PROBHD 5 mm QNP 1H/13 PULPROG dept135 TD 32768 SOLVENT DMSO NS 86 DS 16 SWH 19960.080 H FIDRES 0.609133 H AQ 0.8208384 s RG 18390.4 DW 25.050 t DE 6.00 t TE 300.0 F CNST2 140.0000000 s d12 0.0002000 s d12 0.00002000 s DELTA 0.000000891 s ====== CHANNEL f1 P1 7.00 t P2 14.00 t H1 13C P1 7.00 t P2 14.00 t	iz iz iz isec isec sec sec sec sec sec sec	JMS-SOHAN-345-DEPT135 N_3	t f
CHANNEL f2 CPDPRG[2 waltz16 NUC2 1H P3 6.10 u p4 12.20 u PCPD2 100.00 u PL2 -6.00 c PL12 18.54 c SFO2 300.1312005 k	ISEC ISEC ISEC IB IB IHZ		
F2 - Processing parameter SI 32768 SF 75.4677851 M WDW EM SSB 0 LB 1.00 F GB 0 PC 1.40	rs MHz Hz		
210 200 190	180 170 160 150 140 13 Figure S64. ¹³ C-DE	0 120 110 100 90 80 70 60 5 PT135 NMR Spectrum of Compound 14) 40 30 20 10 ppm

S74



S75



Figure S66. DSC of compound 14 at 5 °C min⁻¹



Figure S67. TGA of compound 14 at 5 °C min⁻¹

Table S12. Cartesian coordinates (in Å) for the optimized structure of compound 4 obtained using the B3LYP/6-311++G(d,p) level of theory



optimized structure

Center Number	Atomic Symbol		Coordinates (A	Angstroms)
	-	Х	Y	Z
1	С	1.719694	3.543572 -(0.265989
2	С	3.093502	3.299594 -	0.186882
3	С	3.995430	4.352361 -	0.060970
4	С	3.545175	5.674430 -0	0.011194
5	С	2.163550	5.919163 -	0.090135
6	С	1.267406	4.873097 -0	0.215286
7	Н	3.459905	2.282452 -	0.224399
8	Н	5.055446	4.144887 -	0.001218
9	Н	1.803747	6.938652 -	0.051728
10	Н	0.206005	5.073278 -	0.275367
11	С	4.501516	6.799017	0.121988
12	С	0.755662	2.425841 -().401359
13	Ν	5.842076	6.391216	0.187347
14	Ν	6.800185	7.169294	0.301698
15	Ν	7.803309	7.675461	0.402485
16	Ν	1.362589	1.161461 -	0.429865
17	Ν	0.741208	0.094811 -	0.542144
18	Ν	0.394876	-0.974965 -	0.632989
19	Ν	4.031562	7.996691	0.163168
20	Ν	-0.497936	2.708238 -	0.477161
21	0	5.036581	8.960175	0.289485
22	Н	4.548300	9.790057	0.306718
23	0	-1.295044	1.566544 -	0.601177
24	Н	-2.188585	1.922802 -	0.646742

 $E_0 = -896.756502$ Hartree/particle; ZPE = 0.157956 Hartree/particle. Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S13. Cartesian coordinates (in Å) for the optimized structure of compound **4A** obtained using the B3LYP/6-311++G(d,p) level of theory

HO N -N ₂ N_3 -N ₂ I -N	HO-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N	он 🤷	optimized	d structure	- 6 19
Center Number	Atomic Symbol	Y	Coordinates V	s (Angstroms)	7
1	0	1.7(1241	1	0.020056	L
1	C	1./61341	3.499892	-0.038856	
2	C	3.141568	3.20/010	-0.060069	
3	C	4.024944	4.330804	-0.016846	
4	C C	3.344879	5.055255	0.040139	
5	C C	2.159/12	5.8/9250	0.005575	
0 7		1.273030	4.813447	0.023940	
/ 0	П	5.011203	<i>L.L.</i> 31032	-0.109033	
0 0	п	3.091460	4.130107	-0.032092	
9	п	0.206405	0.094230	0.034357	
10	II C	1 / 80/86	6 706057	0.004337	
11	C C	0.835/139	2 393127	-0.072419	
12	N	5 836307	6 413795	0.050901	
13	N	6 784356	7 213856	0.077932	
15	N	7 780194	7 742157	0.089978	
15	N	0.699296	1.151112	-0.153522	
17	N	3.997103	7.984013	0.161102	
18	N	-0.551965	2.164738	-0.059610	
19	0	4.983668	8.968910	0.196925	
20	Ĥ	4.481315	9.789359	0.247955	
21	0	-1.035011	2.432808	-1.387280	
22	Н	-1.902625	2.008835	-1.385235	

 $E_0 = -787.214664$ Hartree/particle; ZPE = 0.146786 Hartree/particle.

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S14. Cartesian coordinates (in Å) for the optimized structure of compound **5** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms)		
		Х	Y	Ζ
1	С	1.262547	4.405405 -0.547907	,
2	С	2.385756	3.582238 -0.398174	
3	С	3.587806	4.109076 0.060529	
4	С	3.689234	5.468631 0.381189	
5	С	2.562072	6.293799 0.229181	
6	С	1.365896	5.769545 -0.226916	i
7	Н	2.330875	2.530077 -0.638841	
8	Н	4.442019	3.455457 0.165964	
9	Н	2.641763	7.344808 0.474793	
10	Н	0.497190	6.404739 -0.341556	i
11	С	4.923851	6.082732 0.864221	
12	С	-0.028710	3.912623 -1.021825	i
13	Ν	6.988424	6.394798 1.593025	
14	Ν	6.373128	7.537160 1.530780	1
15	Ν	5.115635	7.383548 1.083648	
16	Ν	-1.149762	4.627764 -1.119015	
17	Ν	-2.106157	3.817513 -1.601407	,
18	Ν	-1.643899	2.620355 -1.803921	
19	Ν	-0.357121	2.675212 -1.452643	5
20	Ν	6.093874	5.490097 1.188074	
21	0	6.424622	4.163134 1.119559	1
22	Н	7.215238	4.090929 1.679418	
23	0	0.435473	1.561308 -1.530985	
24	Н	-0.071356	0.955451 -2.096675	

 $E_0 = -896.758882$ Hartree/particle; ZPE = 0.160846 Hartree/particle. Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S15. Cartesian coordinates (in Å) for the optimized structure of compound **5A** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms)		
		Х	Y	Z
1	С	1.240868	4.425749 -0.524535	
2	С	2.295552	3.593036 -0.119649	
3	С	3.492937	4.151683 0.342708	
4	С	3.567141	5.522514 0.376643	
5	С	2.569696	6.391967 0.000948	
6	С	1.379993	5.822839 -0.457801	
7	Н	2.189796	2.517164 -0.155025	
8	Н	4.311437	3.516118 0.660477	
9	Н	2.684832	7.468507 0.052043	
10	Н	0.553211	6.451017 -0.766409	
11	С	-0.037805	3.899608 -1.003829	
12	Ν	-1.161128	4.594956 -1.149094	
13	Ν	-2.097672	3.750727 -1.631851	
14	Ν	-1.622159	2.556297 -1.777388	
15	Ν	-0.336456	2.641149 -1.404391	
16	О	0.467851	1.534032 -1.396521	
17	Н	0.332588	1.119476 -2.263010	

 $E_0 = -563.806523$ Hartree/particle; ZPE = 0.117484 Hartree/particle.

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S16. Cartesian coordinates (in Å) for the optimized structure of compound 5B of	btained
using the B3LYP/6-311++ $G(d,p)$ level of theory	



optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms)		
		Х	Y	Z
1	С	-0.018166	3.874794	-1.367008
2	Ν	-0.950452	4.632538	-1.805932
3	Ν	-2.028407	3.770184	-2.021024
4	Ν	-1.722465	2.555702	-1.700268
5	Ν	-0.437162	2.601093	-1.302496
6	0	0.210800	1.528291	-0.769410
7	Н	0.369430	0.921107	-1.508677

 $E_0 = -332.757968$ Hartree/particle; ZPE = 0.036750 Hartree/particle. Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S14. Cartesian coordinates (in Å) for the optimized structure of compound **5**C obtained using the B3LYP/6-311++G(d,p) level of theory



optimized structure

Center Number	Atomic Symbol	(Coordinates	(Angstroms)	
		Х	Y		Ζ
1	С	1.201957	4.365221	-0.571996	
2	С	2.226602	3.468572	-0.239403	
3	С	3.447823	3.942087	0.226732	
4	С	3.667724	5.315209	0.368924	
5	С	2.642891	6.211866	0.038541	

6	С	1.423924	5.744061	-0.425310
7	Н	2.076340	2.402755	-0.337828
8	Н	4.232982	3.243033	0.482585
9	Н	2.808623	7.277240	0.141092
10	Н	0.632359	6.435399	-0.683855
11	С	4.970501	5.835861	0.883071
12	С	-0.104386	3.934386	-1.065743
13	Ν	5.064921	7.010813	1.407190
14	Ν	-1.142508	4.729391	-1.326663
15	Ν	-2.146122	3.953101	-1.768512
16	Ν	-1.794343	2.703064	-1.788220
17	Ν	-0.529031	2.686449	-1.360849
18	Ν	6.034046	4.969365	0.755642
19	0	7.167561	5.517470	1.275153
20	Н	7.838438	4.838214	1.124199
21	0	0.151607	1.503741	-1.244292
22	Н	-0.361992	0.885676	-1.789987

 $E_0 = -787.209997$ Hartree/particle; ZPE = 0.147372 Hartree/particle. Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S17. Cartesian coordinates (in Å) for the optimized structure of compound 12 obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms)		
	_	Х	Y	Ζ
1	С	1.826055	4.118684 -0.465678	
2	С	2.989533	3.337694 -0.481338	
3	С	4.222433	3.906135 -0.186997	
4	С	4.319926	5.267005 0.130300	
5	С	3.156663	6.048358 0.144352	
6	С	1.923849	5.479880 -0.150273	
7	Н	2.927645	2.276245 -0.687645	
8	Н	5.116608	3.295531 -0.189877	
9	Н	3.218788	7.109847 0.349803	
10	Н	1.030011	6.090940 -0.149621	
11	С	5.638648	5.857312 0.425281	
12	С	0.506878	3.528051 -0.756514	

13	Ν	-0.549310	3.933635	-0.086259
14	Ν	6.696459	5.455619	-0.243957
15	С	-1.201972	2.402628	-1.567711
16	С	-2.233522	1.572988	-2.245273
17	Н	-1.828733	0.608152	-2.553472
18	Н	-3.086688	1.414593	-1.585251
19	С	0.144777	2.536840	-1.732915
20	С	5.998672	6.839314	1.412529
21	С	5.141430	7.508627	2.427087
22	Н	4.359885	6.843062	2.797709
23	Н	5.726904	7.868876	3.273386
24	С	7.347051	6.972448	1.253854
25	С	8.378350	7.800267	1.932932
26	Н	8.110041	7.993286	2.972749
27	Н	9.349797	7.306219	1.895004
28	0	-1.630109	3.226262	-0.598986
29	0	7.776222	6.157580	0.277837
30	0	-2.642222	2.330471	-3.415973
31	0	4.516619	8.647212	1.762834
32	0	8.430198	9.052016	1.200259
33	Ν	3.696996	9.442235	2.627006
34	0	3.657991	9.127487	3.791688
35	0	3.152930	10.336465	2.048201
36	Ν	9.415410	9.966929	1.702116
37	0	10.053800	9.610536	2.662455
38	0	9.456726	10.982632	1.075299
39	Ν	-3.701599	1.709097	-4.161402
40	0	-4.020170	2.348193	-5.119132
41	0	-4.119533	0.657518	-3.744192
42	С	0.993483	1.860570	-2.750565
43	Н	1.783705	2.517237	-3.117437
44	Н	0.405012	1.512729	-3.599482
45	0	1.600289	0.710146	-2.084817
46	Ν	2.439875	-0.077576	-2.937240
47	0	2.951780	-0.991397	-2.358077
48	0	2.524145	0.260628	-4.092007

 $E_0 = -1998.131739$ Hartree/particle; ZPE = 0.316338 Hartree/particle. Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S18. Cartesian coordinates (in Å) for the optimized structure of compound **12A** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms)
		X Y Z
1	С	1.735682 4.217984 -0.417912
2	С	2.894456 3.439957 -0.543627
3	С	4.143671 3.991258 -0.287683
4	С	4.263279 5.331611 0.101159
5	С	3.104824 6.110161 0.226043
6	С	1.855820 5.558745 -0.030706
7	Н	2.817986 2.392297 -0.807258
8	Н	5.034267 3.381856 -0.376785
9	Н	3.180930 7.158155 0.488486
10	Н	0.965172 6.168185 0.056837
11	С	5.598152 5.903989 0.355612
12	С	0.399717 3.643722 -0.666176
13	Ν	-0.607037 3.998997 0.098076
14	Ν	6.615676 5.545811 -0.395713
15	С	-1.353430 2.570057 -1.451620
16	С	-2.461412 1.774950 -2.085333
17	Н	-2.807659 0.985456 -1.385083
18	Н	-3.366117 2.404559 -2.196392
19	С	-0.018840 2.722100 -1.691362
20	С	6.016036 6.822458 1.380716
21	С	5.218714 7.424814 2.482136
22	Н	4.455273 6.737328 2.850343
23	Н	5.850910 7.728442 3.317003
24	С	7.353808 6.965859 1.155668
25	С	8.423639 7.749242 1.827392
26	Н	8.204564 7.891356 2.886757
27	Н	9.387358 7.250231 1.720062
28	0	-1.721131 3.318726 -0.401200
29	0	7.725468 6.214209 0.108151
30	0	-2.180135 1.178463 -3.269063
31	0	4.563970 8.605430 1.928747
32	0	8.455726 9.036482 1.157241
33	Ν	3.792343 9.340258 2.884202
34	0	3.813335 8.950256 4.026457
35	0	3.220255 10.269857 2.394498
36	Ν	9.475282 9.914132 1.655306
37	0	10.154919 9.503206 2.564308
38	0	9.499787 10.959897 1.078750
39	С	0.791285 2.121782 -2.786471
40	Н	1.581154 2.796714 -3.119291
41	Н	0.169808 1.834817 -3.630774
42	0	1.408831 0.918746 -2.222732
43	Ν	2.186601 0.174006 -3.157621
44	0	2.684230 -0.801057 -2.669147
45	0	2.252529 0.597078 -4.285855

 $E_0 = -1792.955713$ Hartree/particle; ZPE = 0.299583 Hartree/particle. Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S19. Cartesian coordinates (in Å) for the optimized structure of compound 14 obtainedusing the B3LYP/6-311++G(d,p) level of theory

N35

N_{3} N_{3} N_{3} N_{3} I_{2} $C_{16}H_{12}N_{14}O_{2}$ $MW = 432.37$	N_3		optimized s	structure	
Center Number	Atomic Symbol	X	Coordinates Y	(Angstroms)	Z
1	С	1.765621	4.329901	-0.442053	
2	С	2.907838	3.517601	-0.461767	
3	С	4.153665	4.047849	-0.154124	
4	С	4.289719	5.401251	0.181468	
5	С	3.147643	6.213434	0.200982	
6	С	1.901712	5.682778	-0.106520	
7	Н	2.815514	2.461253	-0.685186	
8	Н	5.032075	3.415059	-0.163021	
9	Н	3.239763	7.269859	0.423172	
10	Н	1.023350	6.315681	-0.098619	
11	С	5.624089	5.949635	0.487129	
12	С	0.432597	3.778434	-0.746717	
13	Ν	-0.619273	4.231642	-0.100689	
14	Ν	6.676982	5.475847	-0.141785	
15	С	-1.289147	2.691737	-1.570386	
16	С	-2.352293	1.850577	-2.198082	
17	Н	-2.287123	0.825374	-1.812736	
18	Н	-3.326014	2.261068	-1.912103	
19	С	0.062364	2.780304	-1.712720	
20	С	6.001166	6.953906	1.445814	
21	С	5.142195	7.712558	2.401862	
22	Н	4.341889	7.066481	2.778884	
23	Н	5.738723	8.039439	3.259864	
24	C	7.355958	7.023522	1.317762	
25	C	8.414140	7.854849	1.966507	
26	H	8.070577	8.192540	2.942754	
27	Н	9.313545	7.247403	2.110767	
28	0	-1.711544	3.547384	-0.624056	
29	0	7.774440	6.151538	0.382192	
30	C	0.924139	2.046640	-2.686507	
31	H	1.755195	2.684700	-3.004467	
32	H	0.334541	1./85069	-5.568280	
33	N	4.543705	8.899461	1./26809	
34	N	3.976584	9.695037	2.4/18/5	
35	Ν	3.437737	10.499368	3.068443	

36	Ν	8.727785 9.094989 1.215783
37	Ν	9.402729 8.947197 0.192036
38	Ν	10.018913 8.958789 -0.758161
39	Ν	1.465427 0.807195 -2.050531
40	Ν	2.060969 0.046335 -2.815490
41	Ν	2.621649 -0.730965 -3.422150
42	Ν	-2.183913 1.856890 -3.668981
43	Ν	-2.969731 1.138097 -4.290346
44	Ν	-3.633428 0.521832 -4.971190

 $E_0 = -1533.563301$ Hartree/particle; ZPE = 0.303009 Hartree/particle. Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S20. Cartesian coordinates (in Å) for the optimized structure of compound **14** obtained using the B3LYP/6-311++G(d,p) level of theory

N_{3} N_{4} N_{3} N_{3	$\sim \frac{N_3}{-N_2} \frac{N_3}{O-N}$	$- \underbrace{N_{0}}_{12A} \underbrace{N_{0}}_{N_{3}} =$	opti	mized structure	
Center Number	Atomic Symbol	X	Coordinates Y	(Angstroms)	Z
1	С	1.980601	4.161155	-0.647610	
2	С	3.079640	3.321163	-0.421886	
3	С	4.302162	3.847134	-0.027906	
4	С	4.457684	5.228260	0.150824	
5	С	3.359730	6.069109	-0.074336	
6	С	2.136171	5.540508	-0.466202	
7	Н	2.970314	2.247611	-0.519744	
8	Н	5.145219	3.192747	0.153611	
9	Н	3.472440	7.142081	0.024763	
10	Н	1.292368	6.194876	-0.644813	
11	С	5.768888	5.770872	0.552415	
12	С	0.669024	3.612928	-1.041532	
13	Ν	-0.423175	4.120338	-0.519364	
14	Ν	6.866175	5.178244	0.136194	
15	С	-1.003694	2.484648	-1.932479	
16	С	-1.999740	1.635575	-2.655254	
17	Н	-1.452808	1.004201	-3.351711	
18	Н	-2.519948	0.989040	-1.938323	
19	С	0.365484	2.550204	-1.965010	
20	С	6.070473	6.889079	1.405772	
21	С	5.137661	7.794901	2.141583	
22	Н	4.265979	7.229149	2.488110	
23	Н	5.642461	8.217705	3.013574	
24	С	7.432517	6.898216	1.441961	

25	С	8.452385	7.752197	2.138206
26	Н	8.588341	7.413720	3.166987
27	Н	9.412395	7.633591	1.624796
28	Ο	-1.481665	3.403895	-1.084707
29	О	7.922086	5.893568	0.695212
30	С	1.285673	1.794793	-2.813881
31	Н	2.295509	2.212687	-2.884365
32	Н	1.687188	0.376667	-4.004378
33	Ν	4.687254	8.899357	1.244851
34	Ν	4.061656	9.801744	1.805734
35	Ν	3.484335	10.689247	2.211137
36	Ν	8.058467	9.170280	2.247124
37	Ν	8.103573	9.819558	1.195292
38	Ν	8.108681	10.527447	0.312925
39	Ν	0.923284	0.741890	-3.435966
40	Ν	-2.961785	2.433552	-3.446476
41	Ν	-3.932675	2.885446	-2.833718
42	Ν	-4.874719	3.346275	-2.404751

 $E_0 = -1424.100658$ Hartree/particle; ZPE = 0.293828 Hartree/particle. Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S21. Cartesian coordinates (in Å) for the optimized structure of compound **TNT** obtained using the B3LYP/6-311++G(d,p) level of theory



U	p	u	 	2	e	u	3	u	ľ	1	C	U	u	I	e

Center Number	Atomic Symbol	Coordinates (Angstroms)			
		Х	Y		Ζ
1	С	1.597261	4.608254	-0.850586	
2	С	2.657772	3.781366	-0.520382	
3	С	3.551130	4.220788	0.445588	
4	С	3.437258	5.444490	1.129105	
5	С	2.329845	6.217375	0.737487	
6	С	1.406789	5.826941	-0.221553	
7	Н	2.783498	2.820556	-0.999509	
8	Н	0.561655	6.454127	-0.468170	
9	С	4.373170	5.854860	2.235370	

10	Н	5.209381 6.429721 1.831596
11	Н	3.865132 6.482326 2.964868
12	Н	4.786447 4.984463 2.740763
13	Ν	4.682632 3.301131 0.729155
14	0	5.787103 3.800233 0.881851
15	0	4.429510 2.106955 0.762326
16	Ν	2.083680 7.547550 1.350937
17	0	0.923199 7.835382 1.599371
18	0	3.052508 8.267559 1.538711
19	Ν	0.637246 4.174154 -1.893531
20	0	-0.285036 4.931852 -2.152145
21	0	0.837781 3.090177 -2.419191

 $E_0 = -885.154386$ Hartree/particle; ZPE = 0.134371 Hartree/particle.

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S22. Cartesian coordinates (in Å) for the optimized structure of compound **TNT-A** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol		Coordinates	(Angstroms)	
		Х	Y		Z
1	С	1.591948	4.601005	-0.833609	
2	С	2.651918	3.762255	-0.475255	
3	С	3.475031	4.257161	0.498263	
4	С	3.404740	5.468670	1.158326	
5	С	2.309046	6.254927	0.738237	
6	С	1.404086	5.835931	-0.232521	
7	Н	2.782896	2.798284	-0.950078	
8	Н	0.569865	6.463293	-0.510171	
9	С	4.413441	5.826863	2.218565	
10	Н	5.086213	6.608208	1.859756	
11	Н	3.931608	6.214226	3.117486	
12	Н	4.997731	4.943298	2.474969	

13	Ν	2.058124 7.595392 1.326884
14	Ο	0.908768 8.009485 1.311081
15	Ο	3.018951 8.201511 1.780986
16	Ν	0.640651 4.157094 -1.880540
17	0	-0.269412 4.917460 -2.174936
18	Ο	0.833111 3.056879 -2.378711

 $E_0 = -679.935543$ Hartree/particle; ZPE = 0.119143 Hartree/particle.

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S23. Cartesian coordinates (in Å) for the optimized structure of compound **RDX** obtained using the B3LYP/6-311++G(d,p) level of theory



optimized structure

		-			
Center Number	Atomic Symbol		Coordinates	(Angstroms)	
		Х	Y		Ζ
1	С	1.816365	-0.180319	0.408278	
2	С	-0.138655	0.573606	1.753153	
3	С	1.642655	2.196997	1.126967	
4	Н	2.423146	-0.515542	1.265272	
5	Н	2.233384	2.081240	2.050319	
6	Н	0.287267	0.308304	2.734482	
7	Н	2.055562	-0.778842	-0.461929	
8	Н	-1.217239	0.483652	1.789297	
9	Н	1.764945	3.201517	0.741427	
10	Ν	2.055917	1.229800	0.114034	
11	Ν	3.255253	1.519777	-0.555184	
12	0	3.636600	2.676666	-0.513734	
13	0	3.787506	0.595563	-1.145094	
14	Ν	0.389907	-0.288735	0.700205	
15	Ν	0.226962	1.935438	1.372693	
16	Ν	-0.151688	-1.581794	0.637646	
17	0	0.485893	-2.410137	0.010757	
18	0	-1.226661	-1.749848	1.187054	
19	Ν	-0.480820	2.961172	2.018260	

20	0	-1.543401	2.652274	2.529283
21	0	0.015144	4.073872	1.979381

 $E_0 = -897.516473$ Hartree/particle; ZPE = 0.141466 Hartree/particle.

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S24. Cartesian coordinates (in Å) for the optimized structure of compound **RDX-A** obtained using the B3LYP/6-311++G(d,p) level of theory



optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms)				
	-	Х	Y		Z	
1	С	1.729397	-0.135230	0.242168		
2	С	-0.066072	0.531506	1.851363		
3	6	1.586271	2.223979	1.032743		
4	Н	2.363649	-0.921563	0.678771		
5	Н	2.148909	2.657285	1.873329		
6	Н	0.492004	0.257247	2.760821		
7	Н	1.751433	-0.300874	-0.842540		
8	Н	-1.128030	0.407489	2.029541		
9	Н	1.546393	3.006872	0.264488		
10	Ν	2.330636	1.125004	0.518705		
11	Ν	0.339334	-0.278807	0.714634		
12	Ν	0.208514	1.902285	1.452293		
13	Ν	-0.218467	-1.545026	0.605552		
14	0	0.340579	-2.307974	-0.171027		
15	0	-1.222981	-1.778803	1.260573		
16	Ν	-0.480986	2.906993	2.116230		
17	0	-1.475949	2.586889	2.749105		
18	0	-0.036682	4.038882	1.977731		

 $E_0 = -692.338611$ Hartree/particle; ZPE = 0.124580 Hartree/particle.

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

References

- M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. L. Caricato, X., H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, 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, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Revision D.01 ed., Gaussian, Inc., Wallingford, CT, 2003.
- 2. P. W. Atkins, Physical Chemistry, Oxford University Press, Oxford, 1982.
- M. S. Westwell, M. S. Searle, D. J. Wales, D. H. Williams, J. Am. Chem. Soc., 1995, 117, 5013–5015
- H. Gao, C. Ye, C. M. Piekarski, J. M. Shreeve, J. Phys. Chem. C, 2007, 111, 10718-10731.
- 5. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, J. *Appl. Cryst.* 2009, **42**, 339-341.
- 6. G. M. Sheldrick, Acta Cryst., 2008, A64, 112-122.
- 7. S. Parsons, Acta Cryst., 2003, D59, 1995-2003.
- 8. CrysAlisPro (ROD), Rigaku Oxford Diffraction, Poland.
- 9. CrysAlisPro Software System, Rigaku Oxford Diffraction, 2020.
- 10. G. M. Sheldrick, Acta Cryst., 2015, C71, 3-8.
- 11. G. M. Sheldrick, Acta Cryst., 2015, A71, 3-8.