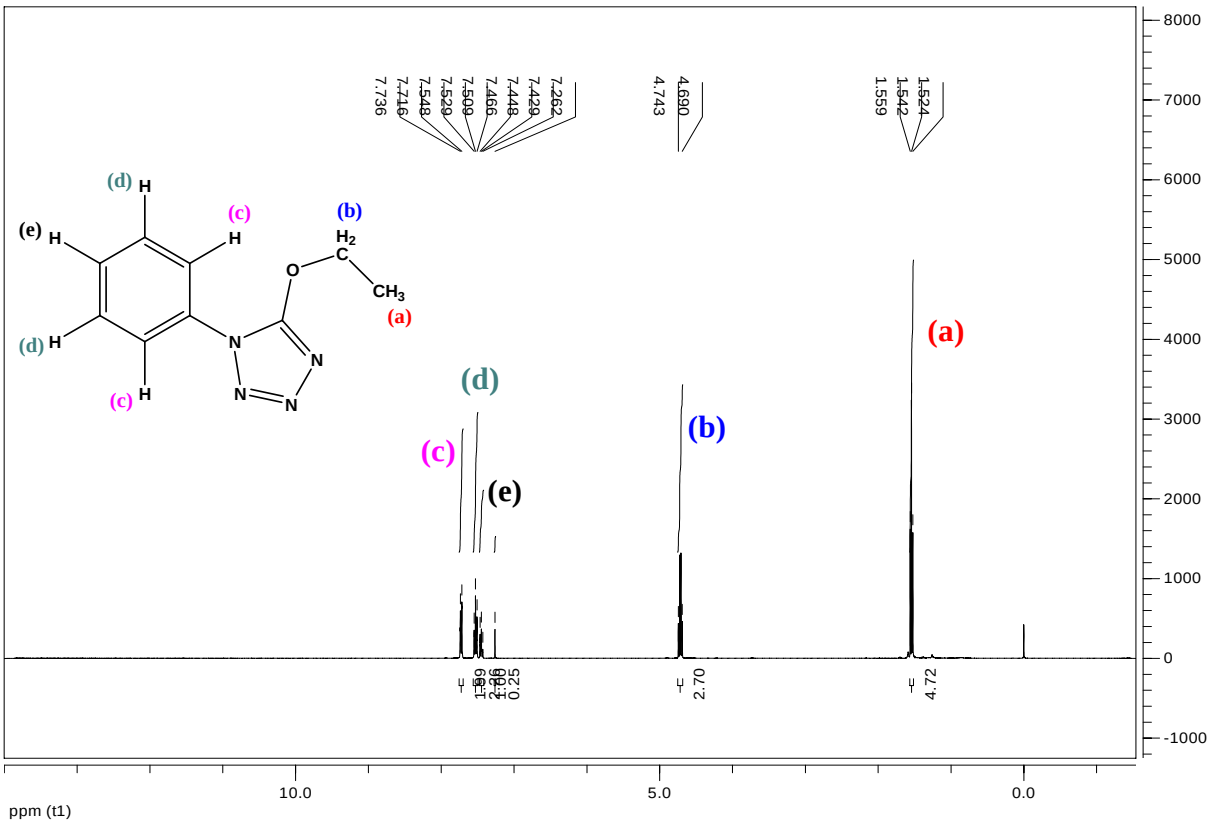
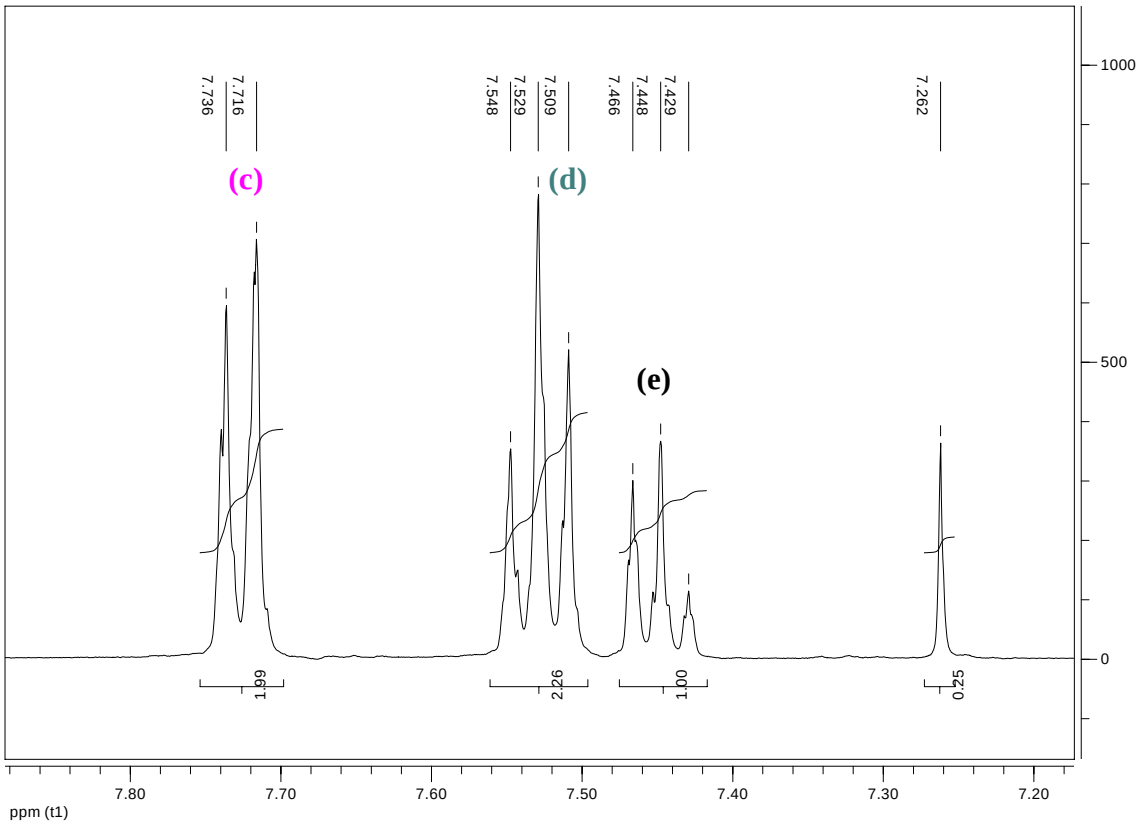
Appendix B

^{1}H-RMN Data for 5-Ethoxy-1-phenyl-*1H*-tetrazole (5EPT)

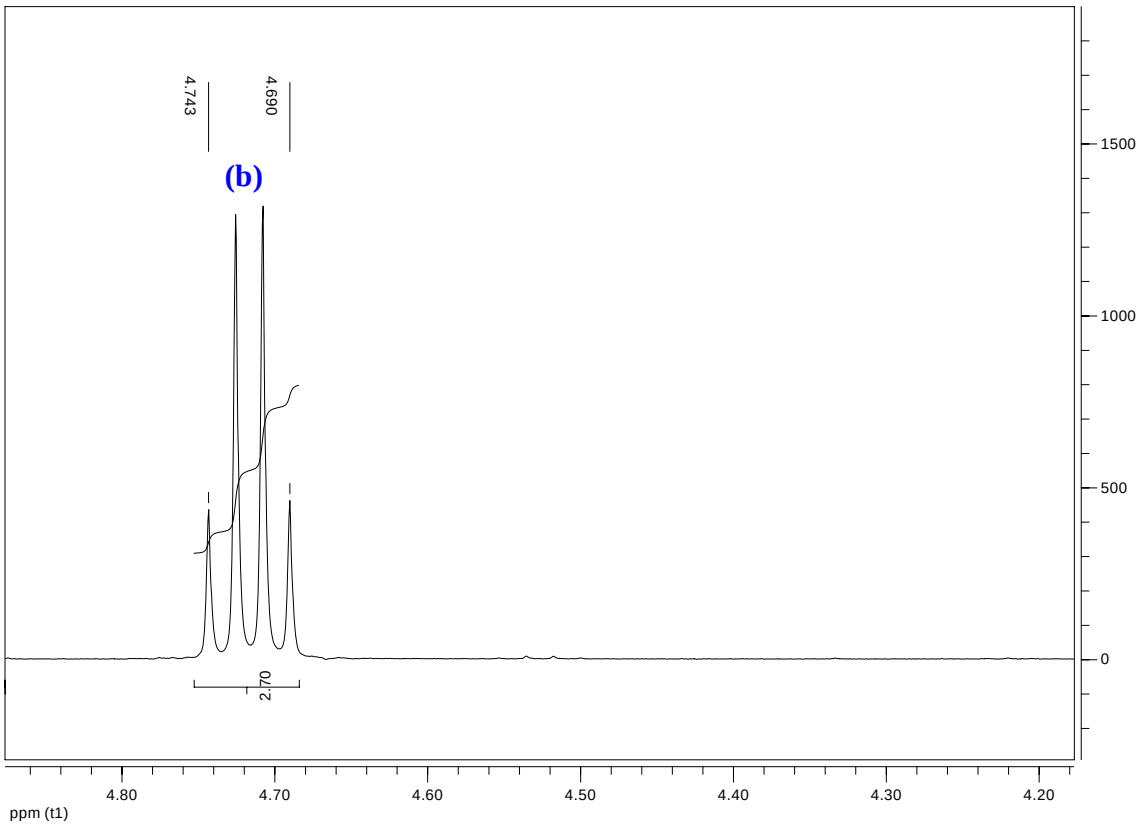
```
F2 - Acquisition Parameters
Date_           20060209
Time                5.59
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG               zg
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6218.905 Hz
FIDRES          0.189786 Hz
AQ             2.6345973 sec
RG                   181
DW                80.400 usec
DE                 6.00 usec
TE                302.7 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.40 usec
PL1                -3.00 dB
SFO1         400.1325018 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300083 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00
```



Expansion 7.18 ppm – 7.88 ppm



Expansion 4.18 ppm – 4.88 ppm



Expansion 1.02 ppm – 1.74 ppm

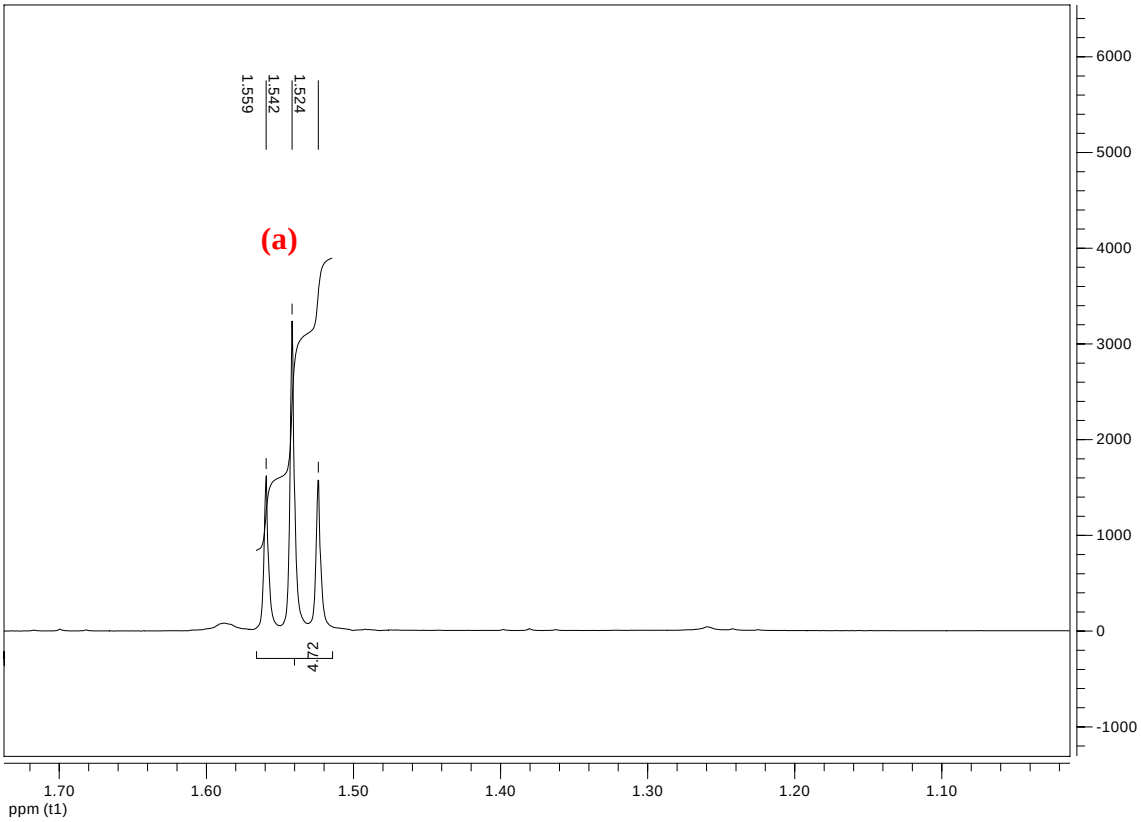


Table S1. Optimized [B3LYP/6-31G(d,p) and B3LYP/6-311++G(d,p)] geometries for 5-methoxy-1-phenyl-1*H*-tetrazole. See Figure 1 (Chapter 3 – Part I) for atom numbering.

Parameter	B3LYP/ 6-31G(d,p)	B3LYP/ 6-311++G(d,p)	Parameter	B3LYP/ 6-31G(d,p)	B3LYP/ 6-311++G(d,p)
Bond length/ pm			**Dihedral angles/ °**		
N_1-N_2	136.4	137.3	C_5-N_4-N_3-N_2	0.0	0.0
N_2=N_3	128.5	128.0	N_1-C_5-N_4-N_3	0.1	0.1
N_4-N_3	136.4	136.3	C_6-N_1-C_5-N_4	-178.2	-177.9
C_5-N_4	131.6	131.3	C_7-C_6-N_1-C_5	154.4	151.3
N_1-C_5	135.8	135.7	C_8-C_7-C_6-N_1	179.3	179.1
C_6-N_1	142.4	142.6	C_9-C_8-C_7-C_6	0.5	0.5
C_7-C_6	139.9	139.6	C_{10}-C_9-C_8-C_7	-0.4	-0.4
C_8-C_7	139.3	139.1	C_{11}-C_{10}-C_9-C_8	-0.2	-0.2
C_9-C_8	139.6	139.4	H_{12}-C_7-C_6-N_1	-0.2	-0.4
C_{10}-C_9	139.5	139.3	H_{13}-C_8-C_7-C_6	-179.8	-179.9
C_{11}-C_{10}	139.5	139.3	H_{14}-C_9-C_8-C_7	179.6	179.7
H_{12}-C_7	108.3	108.2	H_{15}-C_{10}-C_9-C_8	-179.7	-179.7
H_{13}-C_8	108.6	108.4	H_{16}-C_{11}-C_{10}-C_9	-179.4	-179.5
H_{14}-C_9	108.5	108.4	O_{17}-C_5-N_4-N_3	-179.4	-179.5
H_{15}-C_{10}	108.6	108.4	C_{18}-O_{17}-C_5-N_1	-177.8	-177.0
H_{16}-C_{11}	108.2	108.1	H_{19}-C_{18}- O_{17}-C_5	-61.0	-60.9
O_{17}-C_5	132.9	132.4	H_{20}-C_{18}- O_{17}-C_5	59.8	60.1
O_{17}-C_{18}	144.4	144.7	H_{21}-C_{18}- O_{17}-C_5	179.3	179.5
C_{18}-H_{19}	109.2	109.0			
C_{18}-H_{20}	109.2	109.0			
C_{18}-H_{21}	108.9	108.7			
Bond angles/ °					
N_4-N_3-N_2	111.7	111.7			
C_5-N_4-N_3	105.2	105.3			
N_1-C_5-N_4	109.9	109.8			
C_6-N_1-C_5	132.2	132.1			
C_7-C_6-N_1	118.5	118.7			
C_8-C_7-C_6	119.2	119.2			
C_9-C_8-C_7	120.5	120.5			
C_{10}-C_9-C_8	119.6	119.7			
C_{11}-C_{10}-C_9	120.6	120.6			
H_{12}-C_7-C_6	119.5	119.6			
H_{13}-C_8-C_7	119.3	119.3			
H_{14}-C_9-C_8	120.2	120.2			
H_{15}-C_{10}-C_9	120.2	120.2			
H_{16}-C_{11}-C_{10}	120.6	120.5			
O_{17}-C_5-N_1	122.4	122.4			
C_{18}-O_{17}-C_5	114.8	115.4			
H_{19}-C_{18}-O_{17}	110.3	110.1			
H_{20}-C_{18}-O_{17}	110.3	110.1			
H_{21}-C_{18}-O_{17}	105.2	105.0			

Table S2. Definition of internal coordinates used in the normal coordinate analysis of 5-methoxy-1-phenyl-1*H*-tetrazole.[a]

	Definition	Approximate description
S_1	$\nu(C_5\text{-}O_{17})$	νC-O
S_2	$\nu(O_{17}\text{-}C_{18})$	νO-C
S_3	$\nu(N_1\text{-}C_6)$	νN-C
S_4	$\nu(N_2\text{=}N_3)$	νN=N
S_5	$\nu(N_3\text{-}N_4)$	νN-N
S_6	$\nu(N_4\text{=}C_5)$	νN=C
S_7	$\nu(C_5\text{-}N_1)$	νC-N
S_8	$\nu(N_1\text{-}N_2)$	νN-N'
S_9	$\nu(C_6\text{-}C_7)+\nu(C_7\text{-}C_8)+\nu(C_8\text{-}C_9)+\nu(C_9\text{-}C_{10})+\nu(C_{10}\text{-}C_{11})+\nu(C_{11}\text{-}C_6)$	ν(C-C P-ring 1)
S_{10}	$-\nu(C_6\text{-}C_7)+2\nu(C_7\text{-}C_8)-\nu(C_8\text{-}C_9)-\nu(C_9\text{-}C_{10})+2\nu(C_{10}\text{-}C_{11})-\nu(C_{11}\text{-}C_6)$	ν(C-C P-ring 2)
S_{11}	$\nu(C_6\text{-}C_7)-\nu(C_7\text{-}C_8)+\nu(C_8\text{-}C_9)-\nu(C_9\text{-}C_{10})+\nu(C_{10}\text{-}C_{11})-\nu(C_{11}\text{-}C_6)$	ν(C-C P-ring 3)
S_{12}	$\nu(C_6\text{-}C_7)-\nu(C_8\text{-}C_9)+\nu(C_9\text{-}C_{10})-\nu(C_{11}\text{-}C_6)$	ν(C-C P-ring 4)
S_{13}	$\nu(C_6\text{-}C_7)-\nu(C_8\text{-}C_9)-\nu(C_9\text{-}C_{10})+\nu(C_{11}\text{-}C_6)$	ν(C-C P-ring 5)
S_{14}	$\nu(C_7\text{-}C_8)-\nu(C_{10}\text{-}C_{11})$	ν(C-C P-ring 6)
S_{15}	$\nu(C_7\text{-}H_{12})+\nu(C_8\text{-}H_{13})+\nu(C_9\text{-}H_{14})+\nu(C_{10}\text{-}H_{15})+\nu(C_{11}\text{-}H_{16})$	ν(C-H P-ring 1)
S_{16}	$\nu(C_7\text{-}H_{12})+\nu(C_8\text{-}H_{13})-\nu(C_{10}\text{-}H_{15})-\nu(C_{11}\text{-}H_{16})$	ν(C-H P-ring 2)
S_{17}	$\nu(C_7\text{-}H_{12})-2\nu(C_9\text{-}H_{14})+\nu(C_{11}\text{-}H_{16})$	ν(C-H P-ring 3)
S_{18}	$\nu(C_7\text{-}H_{12})-\nu(C_8\text{-}H_{13})+\nu(C_{10}\text{-}H_{15})-\nu(C_{11}\text{-}H_{16})$	ν(C-H P-ring 4)
S_{19}	$2\nu(C_7\text{-}H_{12})-3\nu(C_8\text{-}H_{13})+2\nu(C_9\text{-}H_{14})-3\nu(C_{10}\text{-}H_{15})+2\nu(C_{11}\text{-}H_{16})$	ν(C-H P-ring 5)
S_{20}	$\nu(C_{18}\text{-}H_{21})+\nu(C_{18}\text{-}H_{19})+\nu(C_{18}\text{-}H_{20})$	νCH_3 s
S_{21}	$2\nu(C_{18}\text{-}H_{21})-\nu(C_{18}\text{-}H_{19})-\nu(C_{18}\text{-}H_{20})$	νCH_3 as'
S_{22}	$\nu(C_{18}\text{-}H_{19})-\nu(C_{18}\text{-}H_{20})$	νCH_3 as''
S_{23}	$\delta(C_{18}O_{17}C_5)$	$\delta C\text{-}O\text{-}CH_3$
S_{24}	$\delta(O_{17}C_5N_4)-\delta(O_{17}C_5N_1)$	δCO
S_{25}	$\delta(H_{19}C_{18}H_{21})+\delta(H_{21}C_{18}H_{20})+\delta(H_{19}C_{18}H_{20})-\delta(H_{19}C_{18}O_{17})-\delta(H_{21}C_{18}O_{17})-\delta(H_{20}C_{18}O_{17})$	δCH_3 s
S_{26}	$2\delta(H_{19}C_{18}H_{20})-\delta(H_{21}C_{18}H_{20})-\delta(H_{19}C_{18}H_{21})$	δCH_3 as'
S_{27}	$\delta(H_{21}C_{18}H_{20})-\delta(H_{19}C_{18}H_{21})$	δCH_3 as''
S_{28}	$2\delta(H_{21}C_{18}O_{17})-\delta(H_{20}C_{18}O_{17})-\delta(H_{19}C_{18}O_{17})$	γCH_3'
S_{29}	$\delta(H_{20}C_{18}O_{17})-\delta(H_{19}C_{18}O_{17})$	γCH_3''
S_{30}	$\delta(N_4C_5N_1)-0.809\delta(N_3N_4C_5)-0.809\delta(C_5N_1N_2)+0.309\delta(N_2N_3N_4)+0.309\delta(N_1N_2N_3)$	δ(T-ring 1)
S_{31}	$-1.118\delta(N_3N_4C_5)+1.118\delta(C_5\ N_1N_2)+1.809\delta(N_2N_3N_4)-1.809\delta(N_1N_2N_3)$	δ(T-ring 2)
S_{32}	$\tau(C_{11}C_6N_1C_5)+\tau(C_7C_6N_1C_5)+\tau(C_{11}C_6N_1N_2)+\tau(C_7C_6N_1N_2)$	τC-N
S_{33}	C_5 out of plane $O_{17}N_4C_5N_1$	γCO
S_{34}	$\tau(N_4N_3N_2N_1)-0.809\tau(C_5N_4N_3N_2)-0.809\tau(N_3N_2N_1C_5)+0.309\tau(N_1C_5N_4N_3)+0.309\tau(N_2N_1C_5N_4)$	τ(T-ring 1)
S_{35}	$1.118\tau(C_5N_4N_3N_2)-1.118\tau(N_3N_2N_1C_5)-1.809\tau(N_1C_5N_4N_3)+1.809\tau(N_2N_1C_5N_4)$	τ(T-ring 2)
S_{36}	$\tau(H_{21}C_{18}O_{17}C_5)+\tau(H_{19}C_{18}O_{17}C_5)+\tau(H_{20}C_{18}O_{17}C_5)$	τCH_3
S_{37}	$\tau(C_{18}O_{17}C_5N_4)+\tau(C_{18}O_{17}C_5N_1)$	τC-O
S_{38}	N_4 out of plane $C_6N_2N_1C_5$	γCN
S_{39}	$\delta(C_6N_1N_2)-\delta(C_6N_1C_5)$	δNC
S_{40}	$\delta(C_{11}C_6C_7)-\delta(C_6C_7C_8)+\delta(C_7C_8C_9)-\delta(C_8C_9C_{10})+\delta(C_9C_{10}C_{11})-\delta(C_{10}C_{11}C_6)$	δ(P-ring 1)
S_{41}	$\delta(C_6C_7C_8)-\delta(C_7C_8C_9)+\delta(C_9C_{10}C_{11})-\delta(C_{10}C_{11}C_6)$	δ(P-ring 2)
S_{42}	$2\delta(C_{11}C_6C_7)-\delta(C_6C_7C_8)-\delta(C_7C_8C_9)+2\delta(C_8C_9C_{10})-\delta(C_9C_{10}C_{11})-\delta(C_{10}C_{11}C_6)$	δ(P-ring 3)
S_{43}	$\tau(C_{11}C_6C_7C_8)+\tau(C_{11}C_6C_7H_{12})+\tau(N_1C_6C_7C_8)+\tau(N_1C_6C_7H_{12})-\tau(C_6C_7C_8C_9)-\tau(C_6C_7C_8H_{13})$ $-\tau(H_{12}C_7C_8C_9)-\tau(H_{12}C_7C_8H_{13})+\tau(C_7C_8C_9C_{10})+\tau(C_7C_8C_9H_{14})+\tau(H_{13}C_8C_9C_{10})$ $+\tau(H_{13}C_8C_9H_{14})-\tau(C_8C_9C_{10}C_{11})-\tau(C_8C_9C_{10}H_{15})-\tau(H_{14}C_9C_{10}C_{11})-\tau(H_{14}C_9C_{10}H_{15})$ $+\tau(C_9C_{10}C_{11}C_6)+\tau(C_9C_{10}C_{11}H_{16})+\tau(H_{15}C_{10}C_{11}C_6)+\tau(H_{15}C_{10}C_{11}H_{16})-\tau(C_{10}C_{11}C_6C_7)$ $-\tau(C_{10}C_{11}C_6N_1)-\tau(H_{16}C_{11}C_6C_7)-\tau(H_{16}C_{11}C_6N_1)$	τ(P-ring 1)
S_{44}	$\tau(C_{11}C_6C_7C_8)+\tau(C_{11}C_6C_7H_{12})+\tau(N_1C_6C_7C_8)+\tau(N_1C_6C_7H_{12})-\tau(C_7C_8C_9C_{10})-\tau(C_7C_8C_9H_{14})$ $-\tau(H_{13}C_8C_9C_{10})-\tau(H_{13}C_8C_9H_{14})+\tau(C_8C_9C_{10}C_{11})+\tau(C_8C_9C_{10}H_{15})+\tau(H_{14}C_9C_{10}C_{11})$ $+\tau(H_{14}C_9C_{10}H_{15})-\tau(C_{10}C_{11}C_6C_7)-\tau(C_{10}C_{11}C_6N_1)-\tau(H_{16}C_{11}C_6C_7)-\tau(H_{16}C_{11}C_6N_1)$	τ(P-ring 2)

	$-\tau(C_{11}C_6C_7C_8)-\tau(C_{11}C_6C_7H_{12})-\tau(N_1C_6C_7C_8)-\tau(N_1C_6C_7H_{12})+2\tau(C_6C_7C_8C_9)+2\tau(C_6C_7C_8H_{13})$ $+2\tau(H_{12}C_7C_8C_9)+2\tau(H_{12}C_7C_8H_{13})-\tau(C_7C_8C_9C_{10})-\tau(C_7C_8C_9H_{14})-\tau(H_{13}C_8C_9C_{10})-\tau(H_{13}C_8C_9H_{14})$	
S_{45}	$-\tau(C_8C_9C_{10}C_{11})-\tau(C_8C_9C_{10}H_{15})-\tau(H_{14}C_9C_{10}C_{11})-\tau(H_{14}C_9C_{10}H_{15})+2\tau(C_9C_{10}C_{11}C_6)$ $+2\tau(C_9C_{10}C_{11}H_{16})+2\tau(H_{15}C_{10}C_{11}C_6)+2\tau(H_{15}C_{10}C_{11}H_{16})-\tau(C_{10}C_{11}C_6C_7)-\tau(C_{10}C_{11}C_6N_1)$ $-\tau(H_{16}C_{11}C_6C_7)-\tau(H_{16}C_{11}C_6N_1)$	τ(P-ring 3)
S_{46}	$\delta(C_7C_6N_1)-\delta(C_{11}C_6N_1)$	δCN
S_{47}	C_6 out of plane $N_1C_{11}C_6C_7$	γNC
S_{48}	$\delta(H_{12}C_7C_6)-\delta(H_{12}C_7C_8)+\delta(H_{13}C_8C_7)-\delta(H_{13}C_8C_9)+\delta(H_{14}C_9C_8)-\delta(H_{14}C_9C_{10})+\delta(H_{15}C_{10}C_9)$ $-\delta(H_{15}C_{10}C_{11})+\delta(H_{16}C_{11}C_{10})-\delta(H_{16}C_{11}C_6)$	δ(C-H P-ring 1)
S_{49}	$\delta(H_{12}C_7C_6)-\delta(H_{12}C_7C_8)+\delta(H_{13}C_8C_7)-\delta(H_{13}C_8C_9)-\delta(H_{15}C_{10}C_9)+\delta(H_{15}C_{10}C_{11})-\delta(H_{16}C_{11}C_{10})$ $+\delta(H_{16}C_{11}C_6)$	δ(C-H P-ring 2)
S_{50}	$\delta(H_{12}C_7C_6)-\delta(H_{12}C_7C_8)-2\delta(H_{14}C_9C_8)+2\delta(H_{14}C_9C_{10})+\delta(H_{16}C_{11}C_{10})-\delta(H_{16}C_{11}C_6)$	δ(C-H P-ring 3)
S_{51}	$\delta(H_{12}C_7C_6)-\delta(H_{12}C_7C_8)-\delta(H_{13}C_8C_7)+\delta(H_{13}C_8C_9)+\delta(H_{15}C_{10}C_9)-\delta(H_{15}C_{10}C_{11})-\delta(H_{16}C_{11}C_{10})$ $+\delta(H_{16}C_{11}C_6)$	δ(C-H P-ring 4)
S_{52}	$2\delta(H_{12}C_7C_6)-2\delta(H_{12}C_7C_8)-3\delta(H_{13}C_8C_7)+3\delta(H_{13}C_8C_9)+2\delta(H_{14}C_9C_8)-2\delta(H_{14}C_9C_{10})$ $-3\delta(H_{15}C_{10}C_9)+3\delta(H_{15}C_{10}C_{11})+2\delta(H_{16}C_{11}C_{10})-2\delta(H_{16}C_{11}C_6)$	δ(C-H P-ring 5)
S_{53}	$\gamma(H_{12}C_6C_7C_8)+\gamma(H_{13}C_7C_8C_9)+\gamma(H_{14}C_8C_9C_{10})+\gamma(H_{15}C_9C_{10}C_{11})+\gamma(H_{16}C_{10}C_{11}C_6)$	γ(C-H P-ring 1)
S_{54}	$\gamma(H_{12}C_6C_7C_8)+\gamma(H_{13}C_7C_8C_9)-\gamma(H_{15}C_9C_{10}C_{11})-\gamma(H_{16}C_{10}C_{11}C_6)$	γ(C-H P-ring 2)
S_{55}	$\gamma(H_{12}C_6C_7C_8)-2\gamma(H_{14}C_8C_9C_{10})+\gamma(H_{16}C_{10}C_{11}C_6)$	γ(C-H P-ring 3)
S_{56}	$\gamma(H_{12}C_6C_7C_8)-\gamma(H_{11}C_7C_8C_9)+\gamma(H_{15}C_9C_{10}C_{11})-\gamma(H_{16}C_{10}C_{11}C_6)$	γ(C-H P-ring 4)
S_{57}	$2\gamma(H_{12}C_6C_7C_8)-3\gamma(H_{13}C_7C_8C_9)+2\gamma(H_{14}C_8C_9C_{10})-3\gamma(H_{15}C_9C_{10}C_{11})+2\gamma(H_{16}C_{10}C_{11}C_6)$	γ(C-H P-ring 5)

[a] ν, bond stretching, δ, bending, γ rocking, τ torsion, s, symmetric, as, antisymmetric; P-ring, phenyl ring; T-ring, tetrazole ring. Normalizing factors (*N*) are not provided; they can be calculated as $N_j = \sqrt{\sum_i {}^{1}/_{c_i^2}}$, where *j* refer to the vibrational coordinate and c_i are the coefficients associated with each coordinate in which the vibrational coordinate expands.

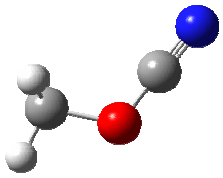
Table S3. DFT(B3LYP)/6-311++G(d,p) calculated frequencies and intensities, and normal coordinate analysis for 5-methoxy-1-phenyl-1*H*-tetrazole.[a]

Approximate Description	Calculated frequency	Intensity	PED[b]
ν(C-H P-ring 1)	3148.5	0.7	$S_{15}(32.8) + S_{16}(31.1) + S_{18}(15.4) + S_{17}(13.7) + S_{19}(6.7)$
ν(C-H P-ring 2)	3144.9	0.3	$S_{16}(36.5) + S_{15}(30.2) + S_{18}(16.7) + S_{17}(11.1) + S_{19}(5.1)$
ν(C-H P-ring 3)	3123.0	14.8	$S_{17}(52.2) + S_{15}(35.7) + S_{19}(11.5)$
ν(C-H P-ring 4)	3111.7	10.9	$S_{18}(67.7) + S_{16}(31.9)$
ν(C-H P-ring 5)	3101.5	0.0	$S_{19}(76.5) + S_{17}(22.7)$
νCH_3 as'	3096.5	9.3	$S_{21}(97.7)$
νCH_3 as''	3064.8	12.2	$S_{22}(100)$
νCH_3 s	2988.1	36.1	$S_{20}(97.8)$
ν(C-C P-ring 2)	1605.4	24.4	$S_{10}(65.2) + S_{51}(20.3) + S_{42}(9.7)$
ν(C-C P-ring 4)	1598.7	38.8	$S_{12}(64.5) + S_{50}(9.2) + S_{41}(7.9)$
νN=C	1562.4	259.5	$S_6(21.3) + S_1(35.5) + S_7(10.8) + S_{25}(9.4) + S_{30}(8.0) + S_{12}(5.5)$
δ(C-H ring 2)	1499.6	121.5	$S_{49}(48.6) + S_{13}(28.5) + S_3(11.0)$
δCH_3 as'	1466.8	19.4	$S_{26}(75.3) + S_{28}(10.1)$
δ(C-H P-ring 3)	1458.0	7.5	$S_{50}(29.9) + S_{14}(33.6) + S_{48}(9.9) + S_{52}(6.9) + S_{35}(6.7) + S_{46}(4.5)$
δCH_3 as''	1450.0	10.9	$S_{27}(92.6) + S_{29}(7.5)$
νC-N	1442.1	108.4	$S_7(24.9) + S_6(15.6) + S_{49}(9.3) + S_{26}(7.4) + S_{24}(6.9)$
δCH_3 s	1424.3	70.9	$S_{25}(77.7) + S_{26}(4.3)$
νN=N	1342.4	32.4	$S_4(67.9)$
δ(C-H P-ring 1)	1326.1	3.4	$S_{48}(56.6) + S_{14}(8.7) + S_4(8.3) + S_1(6.3)$
ν(C-C P-ring 3)	1299.7	5.8	$S_{11}(69.4) + S_4(12.2) + S_{48}(9.4)$
νN-C	1289.2	23.4	$S_3(25.4) + S_6(26.0) + S_{49}(7.4) + S_{30}(7.0)$
γCH_3'	1187.2	13.1	$S_{28}(75.9) + S_{26}(9.5)$
δ(C-H P-ring 4)	1177.2	1.2	$S_{51}(75.2) + S_9(23.4)$
δ(C-H P-ring 5)	1158.7	0.2	$S_{52}(67.6) + S_{50}(12.3) + S_{11}(12.2) + S_{12}(7.8)$
γCH_3''	1148.6	0.7	$S_{29}(92.1) + S_{27}(7.5)$
νN-N	1111.3	41.3	$S_5(27.2) + S_9(17.4) + S_7(8.6) + S_{50}(7.7) + S_1(6.7) + S_2(6.2)$
δ(T−ring 2)	1091.5	16.1	$S_{31}(21.0) + S_5(31.9) + S_{14}(19.1) + S_{50}(15.9) + S_{12}(3.2)$
ν(C-C P-ring 6)	1065.7	84.0	$S_{14}(23.6) + S_{31}(30.4) + S_{50}(10.4)$
ν(C-C P-ring 5)	1041.6	10.0	$S_{13}(41.6) + S_{49}(21.0) + S_8(18.3) + S_{30}(5.5)$
ν(C-C P-ring 1)	1015.6	18.5	$S_9(24.5) + S_{40}(25.6) + S_{13}(14.6) + S_{49}(5.7)$
νO-C	1001.5	42.1	$S_2(43.1) + S_{41}(19.6) + S_5(12.6) + S_9(10.4) + S_7(7.3)$
δ(P-ring 1)	994.8	0.3	$S_{40}(55.0) + S_9(43.0)$
γ(C-H P-ring 5)	979.3	0.1	$S_{57}(62.3) + S_{43}(28.6) + S_{44}(5.7) + S_{55}(5.2)$
τ(P-ring 3)	965.0	2.4	$S_{45}(41.5) + S_{56}(37.0) + S_{30}(6.5) + S_2(4.2)$
νN-N'	963.1	14.6	$S_8(16.0) + S_2(22.0) + S_{30}(18.2) + S_{31}(13.0) + S_{45}(9.9) + S_{56}(9.9) + S_7(5.7)$
γ(C-H P-ring 3)	909.5	4.4	$S_{55}(71.6) + S_{44}(11.0) + S_{57}(6.8)$
γ(C-H P-ring 2)	830.3	0.1	$S_{54}(99.8)$
γ(C-H P-ring 1)	753.4	57.8	$S_{53}(63.6) + S_{47}(20.9) + S_{55}(7.1)$
νC-O	736.2	4.1	$S_1(20.5) + S_{42}(13.7) + S_{24}(7.7) + S_{23}(7.2)$
τ(T−ring 2)	717.7	5.1	$S_{35}(46.5) + S_{33}(36.7) + S_{34}(14.0)$
τ(T−ring 1)	689.3	12.4	$S_{34}(44.4) + S_{43}(28.0) + S_{57}(12.7)$
τ(P-ring 1)	679.4	14.8	$S_{43}(20.8) + S_{34}(38.2) + S_{53}(14.0) + S_{47}(7.3)$
δ(T-ring 1)	670.4	17.9	$S_{30}(22.8) + S_{32}(40.9) + S_1(10.4) + S_3(5.3)$
δ(P-ring 2)	616.5	0.2	$S_{41}(85.4) + S_{12}(7.9)$
δNC	576.2	3.9	$S_{39}(15.6) + S_{24}(20.3) + S_{23}(12.4) + S_8(10.6) + S_2(6.1) + S_{46}(5.2)$
γNC	499.6	12.2	$S_{47}(43.1) + S_{44}(15.6) + S_{43}(6.8) + S_{38}(6.0) + S_{53}(5.5)$
γ(C-H P-ring 4)	405.5	0.2	$S_{56}(51.0) + S_{45}(47.3)$
γCO	378.6	3.3	$S_{33}(13.0) + S_{38}(7.8) + S_{35}(7.5) + S_{23}(6.9)$
δ(P-ring 3)	342.7	3.1	$S_{42}(21.7) + S_3(21.3) + S_{33}(9.5) + S_{35}(8.8) + S_8(7.5) + S_{30}(5.9) + S_{44}(5.8)$
$\delta C\text{-}O\text{-}CH_3$	313.0	4.1	$S_{23}(21.2) + S_{35}(13.6) + S_{33}(13.1) + S_7(8.5) + S_{46}(7.6) + S_{39}(6.7) + S_{42}(5.6)$
τ(P-ring 2)	268.5	2.6	$S_{44}(18.8) + S_{35}(14.3) + S_{23}(13.9) + S_{46}(11.9) + S_{39}(9.4) + S_{38}(6.8) + S_{33}(6.4)$
δCO	217.0	3.7	$S_{24}(30.1) + S_{23}(20.8) + S_{44}(16.3) + S_{46}(7.2) + S_{38}(6.5)$
τCH_3	153.3	0.2	$S_{36}(88.5) + S_{32}(7.1) + S_{34}(2.1)$
δCN	125.3	2.1	$S_{46}(13.5) + S_{37}(25.3) + S_{38}(26.5) + S_{39}(17.4) + S_{24}(5.3) + S_{32}(4.9)$
τC-O	109.9	2.4	$S_{37}(39.4) + S_{39}(24.1) + S_{46}(7.4) + S_{44}(7.4) + S_{24}(6.4)$
γCN	82.8	0.2	$S_{38}(42.4) + S_{37}(28.3) + S_{44}(8.1)$
τC-N	33.1	1.7	$S_{32}(92.8)$

[a] Frequencies in cm^{-1}, calculated intensities in km mol^{-1}. ν, bond stretching, δ, bending, γ rocking, τ torsion, s, symmetric, a, antisymmetric. See Table S2 for definition of internal coordinates.

[b] Only PED values greater than 10 % are given.

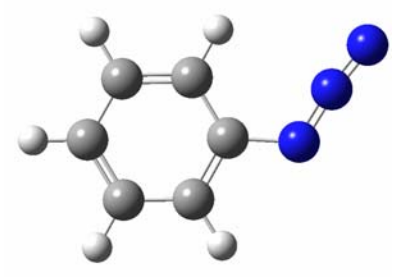
Table S4. Calculated IR spectrum of methylcyanate at the DFT(B3LYP)/6-311++G(d,p) level.

Symmetry	Frequency (cm^{-1})	Intensity (km mol^{-1})	
A'	3107.4	5.5	
A"	3069.1	13.4	
A'	2987.2	25.2	
A'	2300.9	208.6	
A'	1461.4	16.4	
A"	1455.1	12.2	
A'	1439.6	0.9	
A'	1200.1	62.1	
A"	1137.7	0.6	
A'	1110.9	104.2	
A'	864.1	39.3	
A'	600.4	3.8	
A"	512.9	9.2	
A'	223.9	7.8	
A"	134.9	<0.1	

Frequencies were scaled by 0.978. The compound belongs to the C_s symmetry point group. Sum of electronic and zero-point energies: -545988.9026 kJ mol^{-1}. Dipole moment: 4.72 Debye.

Table S5. Calculated IR bands of phenylazide at the DFT(B3LYP)/6-311++G(d,p) level.

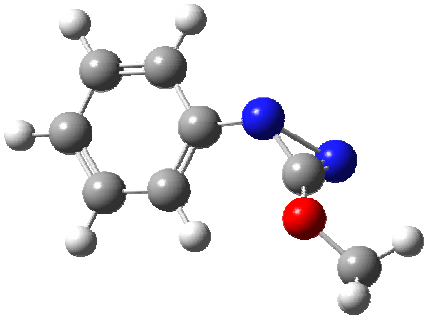
Symmetry	Frequency (cm^{-1})	Intensity (km mol^{-1})
A'	3128.8	4.8
A'	3122.0	13.4
A'	3111.9	11.1
A'	3103.8	2.2
A'	3096.4	2.4
A'	2191.4	843.5
A'	1600.5	59.2
A'	1585.3	6.4
A'	1487.7	86.3
A'	1450.9	1.1
A'	1336.4	151.2
A'	1325.0	29.8
A'	1296.8	18.2
A'	1174.6	2.4
A'	1156.3	0.1
A'	1128.9	18.3
A'	1080.2	9.7
A'	1022.0	4.4
A'	991.4	0.4
A"	961.2	0.1
A"	949.1	0.1
A"	887.7	5.2
A"	819.7	0.1
A'	805.5	5.3
A"	744.9	68.7
A"	675.2	23.2
A'	666.9	25.1
A'	616.7	0.1
A"	517.7	11.3
A"	488.7	4.9
A'	461.1	0.4
A"	407.1	0.0
A'	374.7	2.4
A"	227.2	<0.1
A'	138.1	0.6
A"	70.1	<0.1



Frequencies were scaled by 0.978. The compound belongs to the C_s symmetry point group. Sum of electronic and zero-point energies: -1039278.444 kJ mol^{-1}. Dipole moment: 1.95 Debye.

Table S6. Calculated IR bands of 3-methoxy-1-phenyl-1*H*-diazirene at the DFT(B3LYP)/6-311++G(d,p) level.

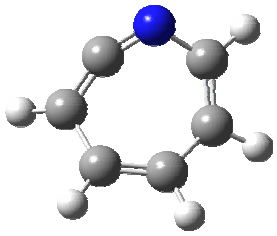
Frequency (cm^{-1})	Intensity (km mol^{-1})
3129.4	5.8
3122.1	10.9
3115.1	13.4
3105.5	6.6
3097.0	9.1
3096.4	0.7
3051.3	15.5
2979.2	28.7
1768.7	431.3
1593.9	1.2
1578.1	0.6
1479.2	9.9
1465.7	17.7
1454.8	14.1
1449.0	7.8
1436.1	2.6
1354.8	111.8
1321.4	4.9
1297.0	6.8
1194.3	72.5
1187.4	13.7
1159.4	18.3
1154.0	7.6
1144.3	0.6
1079.1	5.1
1028.5	133.4
1018.3	47.2
992.4	0.2
972.1	0.1
958.4	0.3
908.1	2.8
867.6	18.0
820.8	0.8
804.6	9.4
763.6	36.1
714.5	10.4
675.0	36.5
621.4	1.4
587.4	7.7
556.1	4.5
484.8	8.8
406.5	0.9
355.3	59.8
322.9	6.9
257.7	67.6
217.4	9.6
178.0	1.6
126.6	1.1
93.2	0.6
72.5	3.3
41.8	2.1



Frequencies were scaled by 0.978. The compound belongs to the C_1 symmetry point group. Sum of electronic and zero-point energies: -1297696.022 kJ mol^{-1}. Dipole moment: 3.00 Debye.

Table S7. Calculated IR bands of 1-aza-1,2,4,6-cycloheptatetraene at the DFT(B3LYP)/6-311++G(d,p) level.

Frequency (cm^{-1})	Intensity (km mol^{-1})
3138.2	1.1
3115.4	16.9
3089.8	14.6
3079.2	14.1
3063.3	5.5
1913.1	202.2
1578.8	2.8
1534.6	0.9
1397.2	0.5
1339.8	19.8
1301.5	3.0
1201.8	3.9
1183.6	1.6
1110.9	15.2
1008.1	2.1
979.7	25.6
951.4	3.0
945.7	4.5
894.1	1.7
850.6	4.7
823.2	2.6
754.3	62.3
685.0	45.5
663.8	28.2
595.5	10.9
517.1	7.3
450.0	1.2
376.7	14.3
310.0	0.5
296.2	9.3



Frequencies were scaled by 0.978. The compound belongs to the C_1 symmetry point group. Sum of electronic and zero-point energies: -751604.5681 kJ mol^{-1}. Dipole moment: 2.08 Debye.

Table S8. Optimized [B3LYP/6-311++G(d,p)] geometries for 5-ethoxy-1-phenyl-1*H*-tetrazole. See Figure 6 (Chapter 3 – Part I) for atom numbering.

Parameter	B3LYP/6-311++G(d,p)		
	T	G	G'
Bond length/ pm			
N_1-N_2	137.3	137.3	137.3
N_1-C_5	135.8	135.8	135.8
N_1-C_6	142.5	142.5	142.5
N_2=N_3	128.0	128.0	128.0
N_3-N_4	136.2	136.2	136.2
N_4=C_5	131.4	131.5	131.5
C_5-O_{17}	132.3	132.3	132.3
C_6-C_7	139.6	139.6	139.6
C_6-C_{11}	139.5	139.5	139.5
C_7-C_8	139.1	139.1	139.1
C_7-H_{12}	108.2	108.2	108.2
C_8-C_9	139.4	139.4	139.4
C_8-H_{13}	108.4	108.4	108.4
C_9-C_{10}	139.3	139.3	139.3
C_9-H_{14}	108.4	108.4	108.4
C_{10}-C_{11}	139.3	139.3	139.3
C_{10}-H_{15}	108.4	108.4	108.4
C_{11}-H_{16}	108.1	108.1	108.1
O_{17}-C_{18}	146.0	146.3	146.3
C_{18}-C_{19}	151.2	151.7	151.7
C_{18}-H_{20}	109.2	109.1	109.0
C_{18}-H_{21}	109.2	109.0	109.1
C_{19}-H_{22}	109.3	109.4	109.4
C_{19}-H_{23}	109.2	109.2	109.1
C_{19}-H_{24}	109.2	109.1	109.3
Bond angles/ degrees			
N_2-N_1-C_5	106.4	106.4	106.4
N_2-N_1-C_6	121.5	121.5	121.5
C_5-N_1-C_6	132.1	132.0	132.1
N_1-N_2=N_3	106.9	106.9	106.9
N_2=N_3-N_4	111.7	111.7	111.7
N_3-N_4=C_5	105.4	105.4	105.4
N_1-C_5=N_4	109.6	109.6	109.6
N_1-C_5-O_{17}	122.4	122.2	122.2
N_4=C_5-O_{17}	128.0	128.3	128.3
N_1-C_6-C_7	118.7	118.7	118.6
N_1-C_6-C_{11}	120.5	120.5	120.5
C_7-C_6-C_{11}	120.8	120.8	120.8
C_6-C_7-C_8	119.3	119.3	119.3
C_6-C_7-H_{12}	119.5	119.5	119.5
C_8-C_7-H_{12}	121.2	121.2	121.2
C_7-C_8-C_9	120.5	120.5	120.5
C_7-C_8-H_{13}	119.3	119.3	119.3
C_9-C_8-H_{13}	120.2	120.2	120.2
C_8-C_9-C_{10}	119.7	119.7	119.6
C_8-C_9-H_{14}	120.2	120.2	120.2
C_{10}-C_9-H_{14}	120.2	120.2	120.2
C_9-C_{10}-C_{11}	120.6	120.6	120.6
C_9-C_{10}-H_{15}	120.2	120.1	120.2
C_{11}-C_{10}-H_{15}	119.3	119.3	119.3
C_6-C_{11}-C_{10}	119.2	119.2	119.2
C_6-C_{11}-H_{16}	120.3	120.3	120.3
C_{10}-C_{11}-H_{16}	120.5	120.5	120.5
C_5-O_{17}-C_{18}	115.7	116.5	116.5
O_{17}-C_{18}-C_{19}	107.3	111.7	111.7
O_{17}-C_{18}-H_{20}	108.1	108.3	103.2
O_{17}-C_{18}-H_{21}	108.2	103.2	108.3
C_{19}-C_{18}-H_{20}	112.4	111.9	111.8

C_{19}-C_{18}-H_{21}	112.5	111.8	111.8
H_{20}-C_{18}-H_{21}	108.3	109.6	109.5
C_{18}-C_{19}-H_{22}	109.3	109.1	109.1
C_{18}-C_{19}-H_{23}	111.2	110.9	111.1
C_{18}-C_{19}-H_{24}	111.1	111.1	111.0
H_{22}-C_{19}-H_{23}	108.2	108.2	108.1
H_{22}-C_{19}-H_{24}	108.3	108.0	108.2
H_{23}-C_{19}-H_{24}	108.7	109.3	109.3
Dihedral angles/ degrees			
C_5-N_1-N_2=N_3	0.0	0.0	-0.1
C_6-N_1-N_2=N_3	-178.1	-178.3	-178.1
N_2-N_1-C_5=N_4	0.0	-0.1	0.2
N_2-N_1-C_5-O_{17}	-179.5	179.9	-179.0
C_6-N_1-C_5=N_4	177.8	177.9	177.9
C_6-N_1-C_5-O_{17}	-1.8	-2.1	-1.2
N_2-N_1-C_6-C_7	26.9	27.3	26.1
N_2-N_1-C_6-C_{11}	-152.1	-151.7	-152.9
C_5-N_1-C_6-C_7	-150.5	-150.4	-151.3
C_5-N_1-C_6-C_{11}	30.4	30.5	29.7
N_1-N_2=N_3-N_4	0.0	0.1	0.0
N_2=N_3-N_4=C_5	0.0	-0.1	0.2
N_3-N_4=C_5-N_1	0.0	0.1	-0.2
N_3-N_4=C_5-O_{17}	179.5	-179.8	178.9
N_1-C_5-O_{17}-C_{18}	176.6	176.0	177.6
N_4=C_5-O_{17}-C_{18}	-2.8	-4.1	-1.4
N_1-C_6-C_7-C_8	-179.1	-179.1	-178.9
N_1-C_6-C_7-H_{12}	0.5	0.4	0.6
C_{11}-C_6-C_7-C_8	0.0	0.0	0.0
C_{11}-C_6-C_7-H_{12}	179.5	179.4	179.5
N_1-C_6-C_{11}-C_{10}	179.6	179.6	179.4
N_1-C_6-C_{11}-H_{16}	-0.6	-0.6	-0.8
C_7-C_6-C_{11}-C_{10}	0.5	0.6	0.5
C_7-C_6-C_{11}-H_{16}	-179.6	-179.6	-179.7
C_6-C_7-C_8-C_9	-0.5	-0.4	-0.4
C_6-C_7-C_8-H_{13}	179.8	179.9	179.9
H_{12}-C_7-C_8-C_9	-180.0	-179.9	-179.9
H_{12}-C_7-C_8-H_{13}	0.3	0.4	0.4
C_7-C_8-C_9-C_{10}	0.4	0.4	0.3
C_7-C_8-C_9-H_{14}	-179.7	-179.7	-179.7
H_{13}-C_8-C_9-C_{10}	-179.9	-179.9	-180.0
H_{13}-C_8-C_9-H_{14}	0.0	0.0	0.0
C_8-C_9-C_{10}-C_{11}	0.2	0.2	0.2
C_8-C_9-C_{10}-H_{15}	179.7	179.7	179.7
H_{14}-C_9-C_{10}-C_{11}	-179.7	-179.75	-179.7
H_{14}-C_9-C_{10}-H_{15}	-0.2	-0.2	-0.2
C_9-C_{10}-C_{11}-C_6	-0.6	-0.6	-0.6
C_9-C_{10}-C_{11}-H_{16}	179.6	179.5	179.6
H_{15}-C_{10}-C_{11}-C_6	179.9	179.8	179.9
H_{15}-C_{10}-C_{11}-H_{16}	0.1	0.0	0.1
C_5-O_{17}-C_{18}-C_{19}	-179.4	-80.7	82.6
C_5-O_{17}-C_{18}-H_{20}	-56.0	43.0	-157.0
C_5-O_{17}-C_{18}-H_{21}	59.0	159.1	-40.9
O_{17}-C_{18}-C_{19}-H_{22}	179.6	-175.8	176.0
O_{17}-C_{18}-C_{19}-H_{23}	-61.0	-56.6	-65.0
O_{17}-C_{18}-C_{19}-H_{24}	60.2	65.2	56.9
H_{20}-C_{18}-C_{19}-H_{22}	60.9	62.7	60.8
H_{20}-C_{18}-C_{19}-H_{23}	-179.7	-178.2	179.8
H_{20}-C_{18}-C_{19}-H_{24}	-58.5	-56.3	-58.3
H_{21}-C_{18}-C_{19}-H_{22}	-61.6	-60.6	-62.5
H_{21}-C_{18}-C_{19}-H_{23}	57.8	58.5	56.5
H_{21}-C_{18}-C_{19}-H_{24}	179.0	-179.6	178.4

Table S9. Definition of internal coordinates used in the normal coordinate analysis of 5-ethoxy-1-phenyl-1*H*-tetrazole.[a]

	Definition	Approximate description
S_1	$\nu(C_5\text{-}O_{17})$	νC-O
S_2	$\nu(O_{17}\text{-}C_{18})$	νO-C
S_3	$\nu(N_1\text{-}C_6)$	νN-C
S_4	$\nu(N_2\text{=}N_3)$	νN=N
S_5	$\nu(N_3\text{-}N_4)$	νN-N
S_6	$\nu(N_4\text{=}C_5)$	νN=C
S_7	$\nu(C_5\text{-}N_1)$	νC-N
S_8	$\nu(N_1\text{-}N_2)$	νN-N'
S_9	$\nu(C_6\text{-}C_7)+\nu(C_7\text{-}C_8)+\nu(C_8\text{-}C_9)+\nu(C_9\text{-}C_{10})+\nu(C_{10}\text{-}C_{11})+\nu(C_{11}\text{-}C_6)$	ν(C-C P-ring 1)
S_{10}	$-\nu(C_6\text{-}C_7)+2\nu(C_7\text{-}C_8)-\nu(C_8\text{-}C_9)-\nu(C_9\text{-}C_{10})+2\nu(C_{10}\text{-}C_{11})-\nu(C_{11}\text{-}C_6)$	ν(C-C P-ring 2)
S_{11}	$\nu(C_6\text{-}C_7)-\nu(C_7\text{-}C_8)+\nu(C_8\text{-}C_9)-\nu(C_9\text{-}C_{10})+\nu(C_{10}\text{-}C_{11})-\nu(C_{11}\text{-}C_6)$	ν(C-C P-ring 3)
S_{12}	$\nu(C_6\text{-}C_7)-\nu(C_8\text{-}C_9)+\nu(C_9\text{-}C_{10})-\nu(C_{11}\text{-}C_6)$	ν(C-C P-ring 4)
S_{13}	$\nu(C_6\text{-}C_7)-\nu(C_8\text{-}C_9)-\nu(C_9\text{-}C_{10})+\nu(C_{11}\text{-}C_6)$	ν(C-C P-ring 5)
S_{14}	$\nu(C_7\text{-}C_8)-\nu(C_{10}\text{-}C_{11})$	ν(C-C P-ring 6)
S_{15}	$\nu(C_7\text{-}H_{12})+\nu(C_8\text{-}H_{13})+\nu(C_9\text{-}H_{14})+\nu(C_{10}\text{-}H_{15})+\nu(C_{11}\text{-}H_{16})$	ν(C-H P-ring 1)
S_{16}	$\nu(C_7\text{-}H_{12})+\nu(C_8\text{-}H_{13})-\nu(C_{10}\text{-}H_{15})-\nu(C_{11}\text{-}H_{16})$	ν(C-H P-ring 2)
S_{17}	$\nu(C_7\text{-}H_{12})-2\nu(C_9\text{-}H_{14})+\nu(C_{11}\text{-}H_{16})$	ν(C-H P-ring 3)
S_{18}	$\nu(C_7\text{-}H_{12})-\nu(C_8\text{-}H_{13})+\nu(C_{10}\text{-}H_{15})-\nu(C_{11}\text{-}H_{16})$	ν(C-H P-ring 4)
S_{19}	$2\nu(C_7\text{-}H_{12})-3\nu(C_8\text{-}H_{13})+2\nu(C_9\text{-}H_{14})-3\nu(C_{10}\text{-}H_{15})+2\nu(C_{11}\text{-}H_{16})$	ν(C-H P-ring 5)
S_{20}	$\nu(C_{18}\text{-}H_{20})+\nu(C_{18}\text{-}H_{21})$	νCH_2 s
S_{21}	$\nu(C_{18}\text{-}H_{20})\text{-}\nu(C_{18}\text{-}H_{21})$	νCH_2 as
S_{22}	$\nu(C_{19}\text{-}H_{22})+\nu(C_{19}\text{-}H_{23})+\nu(C_{19}\text{-}H_{24})$	νCH_3 s
S_{23}	$2\nu(C_{19}\text{-}H_{22})-\nu(C_{19}\text{-}H_{23})-\nu(C_{19}\text{-}H_{24})$	νCH_3 as'
S_{24}	$\nu(C_{19}\text{-}H_{23})-\nu(C_{19}\text{-}H_{24})$	νCH_3 as''
S_{25}	$\delta(C_{18}O_{17}C_5)$	$\delta C\text{-}O\text{-}CH_3$
S_{26}	$\delta(O_{17}C_5N_4)-\delta(O_{17}C_5N_1)$	δCO
S_{27}	$\delta(H_{23}C_{19}H_{22})+\delta(H_{22}C_{19}H_{24})+\delta(H_{23}C_{19}H_{24})-\delta(H_{23}C_{19}O_{17})-\delta(H_{22}C_{19}O_{17})-\delta(H_{24}C_{19}O_{17})$	δCH_3 s
S_{28}	$2\delta(H_{23}C_{19}H_{24})-\delta(H_{22}C_{19}H_{24})-\delta(H_{23}C_{19}H_{22})$	δCH_3 as'
S_{29}	$\delta(H_{22}C_{19}H_{24})-\delta(H_{23}C_{19}H_{22})$	δCH_3 as''
S_{30}	$2\delta(H_{22}C_{19}O_{17})-\delta(H_{24}C_{19}O_{17})-\delta(H_{23}C_{19}O_{17})$	γCH_3'
S_{31}	$\delta(H_{24}C_{19}O_{17})-\delta(H_{23}C_{19}O_{17})$	γCH_3''
S_{32}	$5\delta(H_{20}C_{18}H_{21})-\delta(H_{20}C_{18}O_{17})-\delta(H_{21}C_{18}O_{17})-\delta(H_{20}C_{18}C_{19})-\delta(H_{21}C_{18}C_{19})-\delta(C_{19}C_{18}O_{17})$	δCH_2
S_{33}	$-\delta(H_{20}C_{18}O_{17})-\delta(H_{21}C_{18}O_{17})-\delta(H_{20}C_{18}C_{19})-\delta(H_{21}C_{18}C_{19})+4\delta(C_{19}C_{18}O_{17})$	δOCC
S_{34}	$\delta(H_{20}C_{18}O_{17})+\delta(H_{21}C_{18}O_{17})-\delta(H_{20}C_{18}C_{19})-\delta(H_{21}C_{18}C_{19})$	ωCH_2
S_{35}	$\delta(H_{20}C_{18}O_{17})-\delta(H_{21}C_{18}O_{17})-\delta(H_{20}C_{18}C_{19})+\delta(H_{21}C_{18}C_{19})$	$tw CH_2$
S_{36}	$\delta(H_{20}C_{18}O_{17})-\delta(H_{21}C_{18}O_{17})+\delta(H_{20}C_{18}C_{19})-\delta(H_{21}C_{18}C_{19})$	γCH_2
S_{37}	$\delta(N_4C_5N_1)-0.809\delta(N_3N_4C_5)-0.809\delta(C_5N_1N_2)+0.309\delta(N_2N_3N_4)+0.309\delta(N_1N_2N_3)$	δ(T-ring 1)
S_{38}	$-1.118\delta(N_3N_4C_5)+1.118\delta(C_5\,N_1N_2)+1.809\delta(N_2N_3N_4)-1.809\delta(N_1N_2N_3)$	δ(T-ring 2)
S_{39}	$\tau(C_{11}C_6N_1C_5)+\tau(C_7C_6N_1C_5)+\tau(C_{11}C_6N_1N_2)+\tau(C_7C_6N_1N_2)$	τC-N
S_{40}	C_5 out of plane $O_{17}N_4N_1$	γCO
S_{41}	$\tau(N_4N_3N_2N_1)-0.809\tau(C_5N_4N_3N_2)-0.809\tau(N_3N_2N_1C_5)+0.309\tau(N_1C_5N_4N_3)+0.309\tau(N_2N_1C_5N_4)$	τ(T-ring 1)
S_{42}	$1.118\tau(C_5N_4N_3N_2)-1.118\tau(N_3N_2N_1C_5)-1.809\tau(N_1C_5N_4N_3)+1.809\tau(N_2N_1C_5N_4)$	τ(T-ring 2)
S_{43}	$\tau(H_{22}C_{19}C_{18}O_{17})+\tau(H_{23}C_{19}C_{18}O_{17})+\tau(H_{24}C_{19}C_{18}O_{17})$	τCH_3
S_{44}	$\nu(C_{18}\text{-}C_{19})$	νC-C
S_{45}	$\tau(C_{19}C_{18}O_{17}C_5)$	τO-C
S_{46}	$\tau(C_{18}O_{17}C_5N_4)+\tau(C_{18}O_{17}C_5N_1)$	τC-O
S_{47}	N_1 out of plane $C_6N_2C_5$	γCN
S_{48}	$\delta(C_6N_1N_2)-\delta(C_6N_1C_5)$	δNC
S_{49}	$\delta(C_{11}C_6C_7)-\delta(C_6C_7C_8)+\delta(C_7C_8C_9)-\delta(C_8C_9C_{10})+\delta(C_9C_{10}C_{11})-\delta(C_{10}C_{11}C_6)$	δ(P-ring 1)
S_{50}	$\delta(C_6C_7C_8)-\delta(C_7C_8C_9)+\delta(C_9C_{10}C_{11})-\delta(C_{10}C_{11}C_6)$	δ(P-ring 2)
S_{51}	$2\delta(C_{11}C_6C_7)-\delta(C_6C_7C_8)-\delta(C_7C_8C_9)+2\delta(C_8C_9C_{10})-\delta(C_9C_{10}C_{11})-\delta(C_{10}C_{11}C_6)$	δ(P-ring 3)
S_{52}	$\tau(C_{11}C_6C_7C_8)+\tau(C_{11}C_6C_7H_{12})+\tau(N_1C_6C_7C_8)+\tau(N_1C_6C_7H_{12})-\tau(C_6C_7C_8C_9)-\tau(C_6C_7C_8H_{13})$ $-\tau(H_{12}C_7C_8C_9)-\tau(H_{12}C_7C_8H_{13})+\tau(C_7C_8C_9C_{10})+\tau(C_7C_8C_9H_{14})+\tau(H_{13}C_8C_9C_{10})$ $+\tau(H_{13}C_8C_9H_{14})-\tau(C_8C_9C_{10}C_{11})-\tau(C_8C_9C_{10}H_{15})-\tau(H_{14}C_9C_{10}C_{11})-\tau(H_{14}C_9C_{10}H_{15})$	τ(P-ring 1)

	$+\tau(C_9C_{10}C_{11}C_6)+\tau(C_9C_{10}C_{11}H_{16})+\tau(H_{15}C_{10}C_{11}C_6)+\tau(H_{15}C_{10}C_{11}H_{16})-\tau(C_{10}C_{11}C_6C_7)$ $-\tau(C_{10}C_{11}C_6N_1)-\tau(H_{16}C_{11}C_6C_7)-\tau(H_{16}C_{11}C_6N_1)$	
S_{53}	$\tau(C_{11}C_6C_7C_8)+\tau(C_{11}C_6C_7H_{12})+\tau(N_1C_6C_7C_8)+\tau(N_1C_6C_7H_{12})-\tau(C_7C_8C_9C_{10})-\tau(C_7C_8C_9H_{14})$ $-\tau(H_{13}C_8C_9C_{10})-\tau(H_{13}C_8C_9H_{14})+\tau(C_8C_9C_{10}C_{11})+\tau(C_8C_9C_{10}H_{15})+\tau(H_{14}C_9C_{10}C_{11})$ $+\tau(H_{14}C_9C_{10}H_{15})-\tau(C_{10}C_{11}C_6C_7)-\tau(C_{10}C_{11}C_6N_1)-\tau(H_{16}C_{11}C_6C_7)-\tau(H_{16}C_{11}C_6N_1)$	τ(P-ring 2)
S_{54}	$-\tau(C_{11}C_6C_7C_8)-\tau(C_{11}C_6C_7H_{12})-\tau(N_1C_6C_7C_8)-\tau(N_1C_6C_7H_{12})+2\tau(C_6C_7C_8C_9)+2\tau(C_6C_7C_8H_{13})$ $+2\tau(H_{12}C_7C_8C_9)+2\tau(H_{12}C_7C_8H_{13})-\tau(C_7C_8C_9C_{10})-\tau(C_7C_8C_9H_{14})-\tau(H_{13}C_8C_9C_{10})-\tau(H_{13}C_8C_9H_{14})$ $-\tau(C_8C_9C_{10}C_{11})-\tau(C_8C_9C_{10}H_{15})-\tau(H_{14}C_9C_{10}C_{11})-\tau(H_{14}C_9C_{10}H_{15})+2\tau(C_9C_{10}C_{11}C_6)$ $+2\tau(C_9C_{10}C_{11}H_{16})+2\tau(H_{15}C_{10}C_{11}C_6)+2\tau(H_{15}C_{10}C_{11}H_{16})-\tau(C_{10}C_{11}C_6C_7)-\tau(C_{10}C_{11}C_6N_1)$ $-\tau(H_{16}C_{11}C_6C_7)-\tau(H_{16}C_{11}C_6N_1)$	τ(P-ring 3)
S_{55}	$\delta(C_7C_6N_1)-\delta(C_{11}C_6N_1)$	δCN
S_{56}	C_6 out of plane $N_1C_{11}C_7$	γNC
S_{57}	$\delta(H_{12}C_7C_6)-\delta(H_{12}C_7C_8)+\delta(H_{13}C_8C_7)-\delta(H_{13}C_8C_9)+\delta(H_{14}C_9C_8)-\delta(H_{14}C_9C_{10})+\delta(H_{15}C_{10}C_9)$ $-\delta(H_{15}C_{10}C_{11})+\delta(H_{16}C_{11}C_{10})-\delta(H_{16}C_{11}C_6)$	δ(C-H P-ring 1)
S_{58}	$\delta(H_{12}C_7C_6)-\delta(H_{12}C_7C_8)+\delta(H_{13}C_8C_7)-\delta(H_{13}C_8C_9)-\delta(H_{15}C_{10}C_9)+\delta(H_{15}C_{10}C_{11})-\delta(H_{16}C_{11}C_{10})$ $+\delta(H_{16}C_{11}C_6)$	δ(C-H P-ring 2)
S_{59}	$\delta(H_{12}C_7C_6)-\delta(H_{12}C_7C_8)-2\delta(H_{14}C_9C_8)+2\delta(H_{14}C_9C_{10})+\delta(H_{16}C_{11}C_{10})-\delta(H_{16}C_{11}C_6)$	δ(C-H P-ring 3)
S_{60}	$\delta(H_{12}C_7C_6)-\delta(H_{12}C_7C_8)-\delta(H_{13}C_8C_7)+\delta(H_{13}C_8C_9)+\delta(H_{15}C_{10}C_9)-\delta(H_{15}C_{10}C_{11})-\delta(H_{16}C_{11}C_{10})$ $+\delta(H_{16}C_{11}C_6)$	δ(C-H P-ring 4)
S_{61}	$2\delta(H_{12}C_7C_6)-2\delta(H_{12}C_7C_8)-3\delta(H_{13}C_8C_7)+3\delta(H_{13}C_8C_9)+2\delta(H_{14}C_9C_8)-2\delta(H_{14}C_9C_{10})$ $-3\delta(H_{15}C_{10}C_9)+3\delta(H_{15}C_{10}C_{11})+2\delta(H_{16}C_{11}C_{10})-2\delta(H_{16}C_{11}C_6)$	δ(C-H P-ring 5)
S_{62}	$\gamma(H_{12}C_6C_7C_8)+\gamma(H_{13}C_7C_8C_9)+\gamma(H_{14}C_8C_9C_{10})+\gamma(H_{15}C_9C_{10}C_{11})+\gamma(H_{16}C_{10}C_{11}C_6)$	γ(C-H P-ring 1)
S_{63}	$\gamma(H_{12}C_6C_7C_8)+\gamma(H_{13}C_7C_8C_9)-\gamma(H_{15}C_9C_{10}C_{11})-\gamma(H_{16}C_{10}C_{11}C_6)$	γ(C-H P-ring 2)
S_{64}	$\gamma(H_{12}C_6C_7C_8)-2\gamma(H_{14}C_8C_9C_{10})+\gamma(H_{16}C_{10}C_{11}C_6)$	γ(C-H P-ring 3)
S_{65}	$\gamma(H_{12}C_6C_7C_8)-\gamma(H_{11}C_7C_8C_9)+\gamma(H_{15}C_9C_{10}C_{11})-\gamma(H_{16}C_{10}C_{11}C_6)$	γ(C-H P-ring 4)
S_{66}	$2\gamma(H_{12}C_6C_7C_8)-3\gamma(H_{13}C_7C_8C_9)+2\gamma(H_{14}C_8C_9C_{10})-3\gamma(H_{15}C_9C_{10}C_{11})+2\gamma(H_{16}C_{10}C_{11}C_6)$	γ(C-H P-ring 5)

[a] ν, bond stretching, δ, bending, γ rocking, τ torsion, s, symmetric, as, antisymmetric; P-ring, phenyl ring; T-ring, tetrazole ring. Normalizing factors (N) are not provided; they can be calculated as $N_j = \sqrt{\sum_i {}^{1}/_{c_i^2}}$, where j refer to the vibrational coordinate and c_i are the coefficients associated with each coordinate in which the vibrational coordinate expands.

Table S10. DFT(B3LYP)/6-311++G(d,p) calculated frequencies and intensities, and normal coordinate analysis for conformer **T** of 5-ethoxy-1-phenyl-1*H*-tetrazole.[a]

Calculated frequency	Intensity	PED[b]
3149.9	0.7	$S_{15}(31.5) + S_{16}(31.6) + S_{18}(16.5) + S_{17}(13.5)$
3144.6	0.3	$S_{16}(35.7) + S_{15}(31.4) + S_{18}(16.0) + S_{17}(11.2)$
3123.2	15.1	$S_{17}(53.0) + S_{15}(35.6) + S_{19}(10.7)$
3111.6	11.1	$S_{18}(67.4) + S_{16}(31.9)$
3101.7	0.0	$S_{19}(77.1) + S_{17}(21.8)$
3052.8	30.4	$S_{24}(59.6) + S_{21}(40.2)$
3039.4	21.5	$S_{23}(97.9)$
3028.3	0.1	$S_{21}(59.1) + S_{24}(40.6)$
2992.1	14.3	$S_{20}(98.2)$
2973.0	12.1	$S_{22}(100.0)$
1605.5	24.0	$S_{10}(65.4) + S_{60}(20.3) + S_{51}(9.7)$
1598.0	33.0	$S_{12}(66.0) + S_{59}(9.7) + S_{50}(8.0)$
1555.5	284.9	$S_{1}(36.7) + S_{6}(22.6) + S_{7}(12.8) + S_{37}(8.4)$
1499.2	115.2	$S_{58}(49.6) + S_{13}(29.1) + S_{3}(10.7)$
1484.2	26.0	$S_{32}(77.8) + S_{28}(17.3)$
1466.6	3.4	$S_{28}(77.9) + S_{32}(17.6)$
1456.0	29.2	$S_{14}(34.9) + S_{59}(30.5) + S_{57}(11.2) + S_{61}(7.3)$
1452.8	9.0	$S_{29}(82.4) + S_{31}(17.0)$
1441.8	102.0	$S_{7}(26.4) + S_{6}(13.5) + S_{58}(9.9) + S_{3}(8.8) + S_{26}(7.4) + S_{38}(6.6) + S_{44}(6.3)$
1392.6	69.9	$S_{27}(70.2) + S_{34}(18.3)$
1363.1	52.4	$S_{34}(64.9) + S_{27}(25.4)$
1342.2	35.9	$S_{4}(68.1) + S_{57}(18.0) + S_{37}(4.5)$
1326.1	3.9	$S_{57}(56.0) + S_{11}(15.1) + S_{14}(8.8) + S_{4}(8.2) + S_{61}(6.4)$
1299.6	5.6	$S_{11}(68.9) + S_{4}(12.0) + S_{57}(9.5)$
1287.3	37.4	$S_{6}(26.8) + S_{3}(23.6) + S_{58}(7.1) + S_{1}(6.3)$
1271.8	1.2	$S_{35}(85.6) + S_{31}(10.7)$
1176.9	1.8	$S_{60}(75.5) + S_{10}(23.5)$
1158.9	0.3	$S_{61}(67.3) + S_{59}(12.5) + S_{11}(12.2) + S_{12}(7.9)$
1150.0	3.6	$S_{36}(52.2) + S_{31}(22.6) + S_{29}(9.8) + S_{43}(9.3)$
1119.4	14.2	$S_{5}(30.5) + S_{8}(9.9) + S_{6}(9.4) + S_{30}(8.8) + S_{33}(8.2) + S_{1}(7.9) + S_{44}(6.0)$
1103.0	39.1	$S_{30}(22.5) + S_{44}(10.1) + S_{33}(13.8) + S_{8}(8.7) + S_{59}(8.6) + S_{14}(7.9) + S_{2}(6.4)$
1089.5	5.5	$S_{59}(14.0) + S_{5}(26.5) + S_{14}(17.7) + S_{38}(14.8) + S_{59}(14.0) + S_{30}(8.2)$
1064.4	85.8	$S_{38}(33.9) + S_{14}(21.4) + S_{59}(9.1)$
1041.8	9.7	$S_{13}(40.4) + S_{58}(20.5) + S_{8}(18.9)$
1017.5	95.8	$S_{44}(24.6) + S_{2}(27.8) + S_{32}(17.6) + S_{5}(7.8) + S_{13}(6.6) + S_{38}(6.3)$
1014.0	11.2	$S_{9}(25.2) + S_{49}(24.0) + S_{44}(13.3) + S_{2}(8.6) + S_{13}(8.2)$
994.9	0.1	$S_{49}(52.2) + S_{9}(46.5)$
982.9	0.1	$S_{66}(62.8) + S_{52}(28.6)$
974.1	5.0	$S_{8}(11.7) + S_{38}(29.0) + S_{5}(16.6) + S_{7}(14.8) + S_{37}(8.6)$
966.1	0.1	$S_{54}(50.7) + S_{65}(47.8)$
909.9	4.7	$S_{64}(71.0) + S_{53}(10.7) + S_{66}(7.3)$
889.6	32.8	$S_{2}(31.1) + S_{44}(18.7) + S_{30}(20.4) + S_{37}(17.6)$
830.5	0.1	$S_{63}(99.8)$
798.5	0.6	$S_{31}(41.5) + S_{36}(47.6) + S_{35}(9.1)$
767.2	1.5	$S_{37}(9.0) + S_{1}(18.3) + S_{30}(13.9) + S_{25}(10.8) + S_{26}(8.1)$
754.1	59.2	$S_{62}(63.4) + S_{56}(20.9) + S_{64}(7.0)$
717.9	4.4	$S_{42}(45.9) + S_{40}(36.5) + S_{41}(14.5)$
690.0	13.5	$S_{52}(30.0) + S_{41}(39.3) + S_{66}(13.4)$
681.5	15.0	$S_{51}(30.1) + S_{52}(10.6) + S_{37}(9.9) + S_{41}(9.4)$
679.1	15.7	$S_{41}(34.7) + S_{51}(19.0) + S_{52}(8.5) + S_{62}(8.0)$
616.3	0.2	$S_{50}(86.0) + S_{12}(7.9)$
563.4	4.2	$S_{26}(19.0) + S_{48}(17.7) + S_{8}(10.2) + S_{2}(7.7) + S_{25}(6.9)$

498.0	11.2	$S_{56}(40.7) + S_{53}(15.1) + S_{66}(6.3) + S_{52}(6.0) + S_{47}(5.9)$
405.3	0.2	$S_{65}(51.1) + S_{54}(47.3)$
385.2	2.3	$S_{33}(18.6) + S_{55}(18.8) + S_{51}(8.8) + S_{26}(8.5) + S_3(7.2)$
353.5	4.2	$S_{40}(18.3) + S_{33}(12.5) + S_{42}(14.3) + S_{53}(10.0) + S_{47}(6.1)$
325.0	5.6	$S_{33}(23.9) + S_3(13.8) + S_{51}(12.8) + S_{37}(9.1)$
298.5	2.3	$S_{55}(16.2) + S_{42}(16.7) + S_{40}(13.8) + S_{25}(10.8) + S_7(8.9)$
258.2	0.7	$S_{53}(27.2) + S_{48}(13.1) + S_{42}(9.6) + S_{47}(9.1) + S_{25}(8.7) + S_{43}(7.8)$
242.5	0.1	$S_{43}(77.3)$
176.1	1.8	$S_{25}(23.4) + S_{55}(18.7) + S_{48}(11.1) + S_{26}(10.9) + S_{53}(8.8)$
114.2	2.0	$S_{47}(34.4) + S_{46}(36.4) + S_{53}(6.7)$
88.0	0.9	$S_{46}(36.7) + S_{48}(16.2) + S_{26}(12.1) + S_{25}(10.2) + S_{47}(10.1) + S_{55}(6.7)$
76.2	0.4	$S_{48}(13.4) + S_{47}(19.9) + S_{46}(15.2) + S_{56}(10.1) + S_{39}(7.8) + S_{53}(7.2)$
58.1	0.9	$S_{45}(84.1)$
29.1	0.8	$S_{39}(85.4)$

[a] Frequencies in cm^{-1}, calculated intensities in km mol^{-1}. See Table S10 for definition of internal coordinates. [b] Only PED values greater than 5.0 % are given.

Table S11. DFT(B3LYP)/6-311++G(d,p) calculated frequencies and intensities, and normal coordinate analysis for conformer **G** of 5-ethoxy-1-phenyl-1*H*-tetrazole.[a]

Calculated frequency	Intensity	PED[b]
3148.7	0.7	$S_{15}(32.1) + S_{16}(31.3) + S_{18}(15.8) + S_{17}(13.6) + S_{19}(6.7)$
3143.9	0.3	$S_{16}(36.1) + S_{15}(30.9) + S_{18}(16.3) + S_{17}(11.1) + S_{19}(5.2)$
3122.5	15.3	$S_{17}(52.8) + S_{15}(35.6) + S_{19}(10.9)$
3110.9	11.1	$S_{18}(67.6) + S_{16}(32.0)$
3100.9	0.0	$S_{19}(77.0) + S_{17}(22.1)$
3069.6	17.1	$S_{21}(67.9) + S_{24}(30.2)$
3047.0	2.1	$S_{24}(53.6) + S_{21}(29.8) + S_{23}(15.3)$
3033.8	27.6	$S_{23}(75.9) + S_{24}(15.5)$
3008.3	19.3	$S_{20}(92.3)$
2971.3	13.5	$S_{22}(97.9)$
1605.6	24.1	$S_{10}(65.4) + S_{60}(20.3) + S_{51}(9.7)$
1598.2	31.8	$S_{12}(66.2) + S_{59}(9.7) + S_{50}(8.1)$
1555.9	291.9	$S_{1}(36.4) + S_{6}(22.4) + S_{7}(10.9) + S_{37}(8.5) + S_{32}(5.2)$
1499.8	113.4	$S_{58}(49.8) + S_{13}(29.3) + S_{3}(10.8)$
1472.6	6.5	$S_{28}(76.9) + S_{32}(9.0) + S_{29}(6.8)$
1460.8	4.8	$S_{32}(48.9) + S_{14}(13.7) + S_{59}(12.5) + S_{28}(6.3)$
1456.5	1.0	$S_{29}(49.8) + S_{31}(10.3) + S_{14}(6.9)$
1451.9	33.4	$S_{14}(14.1) + S_{32}(30.1) + S_{29}(17.2) + S_{59}(11.8)$
1437.8	132.5	$S_{7}(28.9) + S_{6}(10.8) + S_{3}(9.9) + S_{58}(9.3) + S_{26}(7.3) + S_{38}(7.2)$
1387.6	43.8	$S_{27}(71.6) + S_{44}(22.7)$
1363.3	23.1	$S_{34}(63.5) + S_{27}(25.2)$
1342.3	48.2	$S_{4}(65.5) + S_{57}(14.8)$
1325.9	3.3	$S_{57}(57.8) + S_{11}(14.6) + S_{14}(8.8) + S_{4}(7.2) + S_{61}(6.1)$
1300.3	2.7	$S_{11}(57.1) + S_{35}(17.6) + S_{57}(8.4)$
1298.4	6.1	$S_{35}(65.1) + S_{11}(13.0) + S_{4}(9.9)$
1286.9	29.0	$S_{3}(25.2) + S_{6}(24.0) + S_{37}(8.0) + S_{58}(7.4)$
1176.8	2.1	$S_{60}(75.5) + S_{10}(23.4)$
1169.0	8.9	$S_{36}(45.5) + S_{31}(21.7) + S_{43}(10.3) + S_{29}(10.1)$
1158.5	0.1	$S_{61}(67.5) + S_{59}(12.3) + S_{11}(12.1) + S_{12}(7.8)$
1110.9	41.4	$S_{5}(32.5) + S_{8}(16.9) + S_{1}(7.5) + S_{7}(7.5) + S_{59}(6.6)$
1091.7	17.0	$S_{59}(17.8) + S_{5}(25.8) + S_{14}(21.2) + S_{38}(19.8)$
1087.3	29.4	$S_{30}(43.8) + S_{44}(20.2) + S_{33}(25.0)$
1064.1	87.4	$S_{38}(32.2) + S_{14}(22.1) + S_{59}(9.6)$
1042.2	9.2	$S_{13}(41.4) + S_{58}(21.1) + S_{8}(17.6)$
1015.8	26.1	$S_{9}(24.8) + S_{49}(26.1) + S_{13}(14.0) + S_{8}(8.5)$
1006.0	64.0	$S_{2}(31.5) + S_{32}(17.2) + S_{44}(30.8) + S_{38}(10.2) + S_{9}(7.2)$
994.9	0.1	$S_{49}(53.0) + S_{9}(45.6)$
981.5	0.2	$S_{66}(62.9) + S_{52}(28.4)$
974.5	8.8	$S_{8}(13.6) + S_{38}(24.8) + S_{7}(12.6) + S_{5}(12.4) + S_{37}(12.3) + S_{44}(10.7)$
964.8	0.2	$S_{54}(50.5) + S_{65}(48.4)$
909.2	4.6	$S_{64}(71.3) + S_{53}(10.7) + S_{66}(7.2)$
873.3	22.2	$S_{44}(25.4) + S_{30}(24.1) + S_{2}(28.7) + S_{37}(13.1)$
829.2	0.1	$S_{63}(99.9)$
805.4	1.0	$S_{31}(43.4) + S_{36}(34.1) + S_{35}(9.5)$
753.8	57.4	$S_{62}(62.2) + S_{56}(21.7) + S_{64}(7.1)$
726.0	3.0	$S_{51}(17.3) + S_{1}(13.3) + S_{36}(10.4) + S_{3}(9.3) + S_{26}(7.5)$
718.2	4.3	$S_{42}(44.8) + S_{40}(36.5) + S_{41}(13.6)$
689.9	14.4	$S_{52}(31.0) + S_{41}(40.0) + S_{66}(13.8)$
679.7	14.3	$S_{41}(44.2) + S_{52}(17.9) + S_{62}(13.9) + S_{66}(7.5) + S_{56}(6.1)$
665.4	17.7	$S_{37}(21.8) + S_{51}(36.5) + S_{1}(11.7)$
616.7	0.2	$S_{50}(85.5) + S_{12}(7.9)$
576.7	4.6	$S_{26}(17.3) + S_{48}(14.4) + S_{25}(10.6) + S_{2}(7.3)$

500.2	11.5	$S_{56}(42.6) + S_{53}(16.0) + S_{66}(6.9)$
439.1	4.8	$S_{33}(43.0) + S_{30}(12.3) + S_{55}(9.7) + S_{40}(6.6) + S_{48}(6.3)$
405.8	0.2	$S_{65}(51.0) + S_{54}(47.5)$
354.2	3.9	$S_{3}(20.8) + S_{51}(21.8) + S_{55}(12.5) + S_{8}(8.4) + S_{37}(7.7)$
325.6	0.9	$S_{40}(20.3) + S_{53}(19.6) + S_{42}(12.5) + S_{33}(12.4) + S_{47}(9.7) + S_{48}(6.6)$
312.8	3.8	$S_{55}(12.8) + S_{25}(19.4) + S_{33}(6.6) + S_{7}(8.6) + S_{43}(8.4) + S_{42}(7.5)$
264.6	2.3	$S_{43}(26.8) + S_{42}(13.8) + S_{26}(11.1) + S_{40}(10.6) + S_{25}(10.3) + S_{55}(10.2)$
234.6	0.4	$S_{53}(19.4) + S_{43}(21.7) + S_{42}(8.3) + S_{47}(6.1)$
196.5	2.9	$S_{25}(25.3) + S_{43}(32.9) + S_{26}(14.9) + S_{55}(6.9) + S_{53}(6.3)$
118.0	1.0	$S_{47}(34.3) + S_{48}(24.2) + S_{55}(16.5) + S_{26}(8.1)$
103.1	1.2	$S_{48}(14.5) + S_{47}(20.6) + S_{56}(13.6) + S_{45}(13.5) + S_{53}(13.5) + S_{46}(12.4)$
85.9	0.5	$S_{45}(67.5) + S_{46}(17.5)$
48.8	0.3	$S_{46}(49.0) + S_{47}(13.7) + S_{39}(13.4) + S_{45}(11.9)$
30.4	1.3	$S_{39}(81.0) + S_{46}(11.8)$

[a] Frequencies in cm^{-1}, calculated intensities in km mol^{-1}. See Table S10 for definition of internal coordinates. [b] Only PED values greater than 5.0 % are given.

Table S12. DFT(B3LYP)/6-311++G(d,p) calculated frequencies and intensities, and normal coordinate analysis for conformer **G'** of 5-ethoxy-1-phenyl-1*H*-tetrazole.[a]

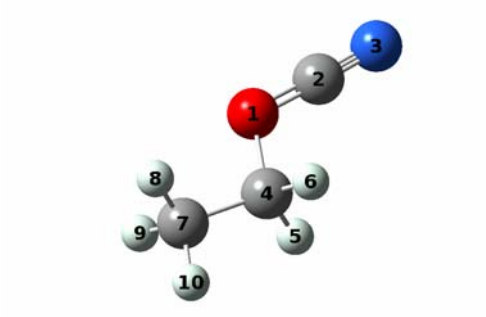
Calculated frequency	Intensity	PED[b]
3149.9	0.8	$S_{15}(31.4) + S_{16}(31.7) + S_{18}(16.1) + S_{17}(13.6) + S_{19}(6.8)$
3145.0	0.3	$S_{16}(35.3) + S_{15}(30.8) + S_{18}(16.4) + S_{17}(11.5)$
3123.1	15.3	$S_{17}(53.1) + S_{15}(36.2) + S_{19}(10.1)$
3111.2	11.2	$S_{18}(67.2) + S_{16}(32.4)$
3101.4	0.0	$S_{19}(77.6) + S_{17}(21.4)$
3069.7	16.7	$S_{21}(68.2) + S_{24}(29.5)$
3047.4	2.3	$S_{24}(51.3) + S_{21}(29.2) + S_{23}(18.0)$
3032.5	28.4	$S_{23}(72.7) + S_{24}(18.3) + S_{20}(7.4)$
3008.1	18.6	$S_{20}(91.0) + S_{23}(7.1)$
2970.7	14.2	$S_{22}(97.8)$
1605.7	24.2	$S_{10}(65.3) + S_{60}(20.3) + S_{51}(9.7)$
1598.4	33.2	$S_{12}(66.0) + S_{59}(9.7) + S_{50}(8.1)$
1556.4	291.2	$S_{1}(36.5) + S_{6}(22.3) + S_{7}(10.8) + S_{37}(8.4) + S_{32}(5.2)$
1499.7	113.7	$S_{58}(50.1) + S_{13}(29.4) + S_{3}(10.6)$
1472.6	6.1	$S_{28}(76.3) + S_{32}(9.5) + S_{29}(6.6)$
1460.4	3.1	$S_{32}(43.6) + S_{14}(15.8) + S_{59}(14.3) + S_{28}(7.5)$
1456.3	1.7	$S_{29}(51.8) + S_{31}(10.7) + S_{32}(7.5)$
1451.9	35.7	$S_{14}(13.4) + S_{32}(32.6) + S_{29}(16.2) + S_{59}(11.3)$
1437.2	134.4	$S_{7}(28.9) + S_{6}(11.0) + S_{3}(10.0) + S_{58}(9.1) + S_{26}(7.3) + S_{38}(7.2)$
1388.0	47.9	$S_{27}(72.2) + S_{34}(22.2)$
1363.1	24.2	$S_{34}(64.0) + S_{27}(24.6)$
1343.0	47.1	$S_{4}(65.2) + S_{57}(15.5)$
1326.2	3.3	$S_{57}(57.3) + S_{11}(14.7) + S_{14}(8.7) + S_{4}(7.7)$
1300.3	3.0	$S_{11}(58.5) + S_{35}(15.2) + S_{57}(8.8)$
1298.3	6.1	$S_{35}(67.2) + S_{11}(11.5) + S_{4}(9.2)$
1286.3	30.2	$S_{6}(23.6) + S_{3}(25.1) + S_{37}(8.0) + S_{58}(7.3)$
1177.1	2.3	$S_{60}(75.4) + S_{10}(23.4)$
1169.0	9.2	$S_{36}(45.5) + S_{31}(21.8) + S_{43}(10.3) + S_{29}(10.2)$
1158.7	0.2	$S_{61}(67.5) + S_{59}(12.2) + S_{11}(12.1) + S_{12}(7.7)$
1111.0	40.7	$S_{5}(32.8) + S_{8}(16.8) + S_{1}(7.4) + S_{7}(7.3)$
1092.2	12.8	$S_{59}(18.0) + S_{5}(23.8) + S_{14}(21.3) + S_{38}(18.7)$
1086.8	30.4	$S_{44}(19.5) + S_{30}(42.9) + S_{33}(24.2)$
1063.9	91.0	$S_{38}(32.8) + S_{14}(21.6) + S_{59}(9.2)$
1042.2	9.1	$S_{13}(41.5) + S_{58}(21.1) + S_{8}(17.4)$
1015.8	26.8	$S_{9}(25.1) + S_{49}(25.4) + S_{13}(13.9) + S_{8}(8.5)$
1006.0	63.2	$S_{2}(31.6) + S_{44}(30.8) + S_{38}(9.9) + S_{9}(6.6)$
994.9	0.0	$S_{49}(52.8) + S_{9}(45.9)$
982.7	0.1	$S_{66}(62.6) + S_{52}(28.5)$
974.7	8.8	$S_{8}(13.6) + S_{38}(24.9) + S_{7}(12.7) + S_{5}(12.5) + S_{37}(12.2)$
965.6	0.2	$S_{54}(50.8) + S_{65}(47.7)$
909.6	4.2	$S_{64}(71.1) + S_{53}(10.7) + S_{66}(7.4)$
873.5	22.2	$S_{30}(23.7) + S_{34}(42.4) + S_{2}(28.7) + S_{44}(25.5) + S_{37}(13.3)$
829.9	0.1	$S_{63}(99.8)$
805.2	0.8	$S_{31}(43.4) + S_{36}(34.0) + S_{35}(9.6)$
754.1	57.7	$S_{62}(63.3) + S_{56}(21.3) + S_{64}(6.9)$
726.5	2.1	$S_{51}(17.0) + S_{44}(14.6) + S_{1}(12.6) + S_{36}(9.3) + S_{3}(8.9) + S_{26}(7.0)$
717.3	5.7	$S_{42}(43.3) + S_{40}(35.5) + S_{41}(11.5)$
690.0	13.3	$S_{52}(30.6) + S_{41}(40.9) + S_{66}(13.7)$
680.3	13.8	$S_{41}(43.0) + S_{52}(18.7) + S_{62}(13.6) + S_{66}(7.8) + S_{56}(6.4)$
665.5	17.8	$S_{37}(21.4) + S_{51}(37.0) + S_{1}(11.4)$
616.9	0.2	$S_{50}(85.5) + S_{12}(7.9)$
576.7	3.9	$S_{26}(17.5) + S_{48}(14.3) + S_{25}(10.7) + S_{8}(9.7) + S_{2}(7.4)$

503.3	13.8	$S_{56}(42.0) + S_{53}(15.0) + S_{52}(7.0) + S_{66}(7.0)$
421.0	2.3	$S_{33}(49.8) + S_{30}(12.9) + S_{48}(7.8)$
406.2	0.2	$S_{65}(51.0) + S_{54}(47.3)$
374.7	4.9	$S_{40}(16.5) + S_{55}(18.2) + S_{42}(10.8) + S_{47}(8.1)$
342.8	3.2	$S_{3}(24.8) + S_{51}(24.9) + S_{8}(6.9) + S_{37}(6.2)$
284.9	3.5	$S_{43}(20.1) + S_{25}(23.6) + S_{53}(13.1) + S_{33}(10.9) + S_{48}(8.5)$
266.0	0.2	$S_{55}(19.4) + S_{42}(24.7) + S_{40}(20.8) + S_{33}(15.4)$
236.4	0.1	$S_{53}(18.8) + S_{43}(34.5) + S_{26}(9.9) + S_{47}(6.4)$
194.7	3.3	$S_{25}(26.6) + S_{43}(32.6) + S_{26}(14.1) + S_{55}(6.6)$
124.1	1.1	$S_{48}(21.6) + S_{47}(30.0) + S_{55}(15.1) + S_{45}(8.4) + S_{26}(6.9)$
96.2	1.0	$S_{47}(24.3) + S_{48}(16.5) + S_{56}(14.1) + S_{53}(13.0) + S_{46}(10.5) + S_{45}(7.9)$
82.5	0.6	$S_{45}(64.4) + S_{46}(10.1) + S_{39}(6.2)$
48.3	0.4	$S_{46}(59.4) + S_{45}(15.4) + S_{47}(11.6)$
30.7	1.2	$S_{39}(87.4) + S_{46}(7.0)$

[a] Frequencies in cm^{-1}, calculated intensities in km mol^{-1}. See Table S10 for definition of internal coordinates. [b] Only PED values greater than 5.0 % are given.

Table S13. Calculated IR spectrum of ethylcyanate at the DFT(B3LYP)/6-311++G(d,p) level. (Conformer **T**).

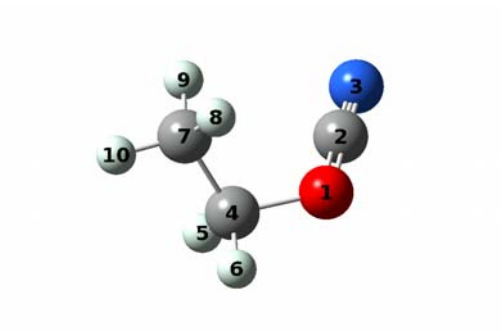
Symmetry	Frequency (cm^{-1})	Intensity (km mol^{-1})
A"	3059.0	26.7
A'	3042.9	15.8
A"	3032.8	2.3
A'	2988.5	15.7
A"	2976.5	7.7
A'	2297.1	237.9
A"	1482.4	6.8
A'	1467.4	2.8
A'	1450.2	8.6
A'	1395.7	32.1
A'	1369.0	8.0
A"	1268.7	0.8
A"	1143.2	4.6
A'	1138.3	152.6
A'	1096.6	49.9
A"	986.0	41.5
A'	803.8	30.2
A'	801.1	1.3
A'	579.2	5.9
A'	514.7	8.4
A'	369.7	6.6
A"	243.5	0.1
A'	171.3	5.0
A"	58.0	1.6



Frequencies were scaled by 0.978. The compound belongs to the C_S symmetry point group. Sum of electronic and zero-point energies: −247.33801134 a.u. Dipole moment: 5.2 Debye.

Table S14. Calculated IR spectrum of ethylcyanate at the DFT(B3LYP)/6-311++G(d,p) level. (conformer **G**).

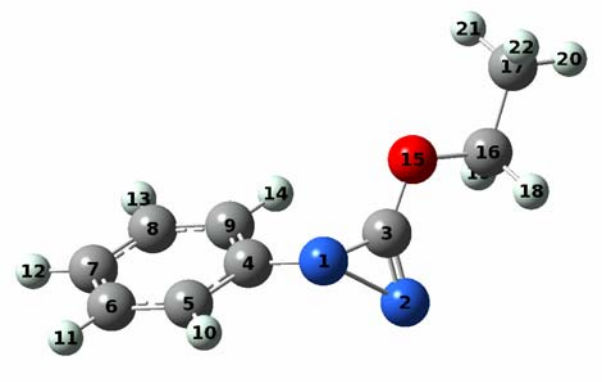
Symmetry	Frequency (cm^{-1})	Intensity (km mol^{-1})
A	3076.2	16.2
A	3044.7	9.5
A	3035.2	13.0
A	3001.9	18.8
A	2971.1	5.8
A	2294.6	213.0
A	1477.1	6.2
A	1463.7	0.9
A	1453.4	8.7
A	1390.9	18.5
A	1364.5	2.2
A	1286.8	15.9
A	1174.4	51.4
A	1102.2	124.2
A	1081.0	11.5
A	961.9	26.7
A	808.9	11.6
A	778.3	25.9
A	603.6	4.6
A	518.7	10.7
A	386.6	1.0
A	265.6	1.8
A	183.5	5.5
A	77.2	0.8



Frequencies were scaled by 0.978. The compound belongs to the C_1 symmetry point group. Sum of electronic and zero-point energies: −247.33765649 a.u. Dipole moment: 5.0 Debye.

Table S15. Calculated IR bands of 3-ethoxy-1-phenyl-1*H*-diazirene at the DFT(B3LYP)/6-311++G(d,p) level. (conformer **T**).

Frequency (cm^{-1})	**Intensity (km mol^{-1})**
3128.8	6.4
3121.8	11.2
3115.0	14.1
3105.0	6.8
3096.0	0.9
3050.9	26.7
3039.4	19.7
3017.7	5.0
2978.3	13.4
2973.7	14.5
1770.4	468.2
1594.1	0.5
1579.0	0.5
1486.0	10.9
1479.7	11.6
1467.2	4.9
1451.9	8.2
1448.6	7.8
1401.9	8.5
1377.1	10.8
1338.0	163.6
1321.7	7.7
1296.9	12.2
1273.3	1.8
1192.0	54.2
1160.2	23.4
1154.1	6.8
1150.6	3.2
1110.2	9.5
1079.0	4.6
1028.3	203.2
1019.1	58.1
992.8	0.7
976.5	14.6
976.0	11.1
960.1	0.5
906.9	2.5
835.9	5.7
822.1	1.1
806.0	4.8
800.5	0.7
763.8	37.7
712.2	11.5
677.7	35.2
619.8	1.0
578.4	9.6
559.0	4.4
485.0	8.1

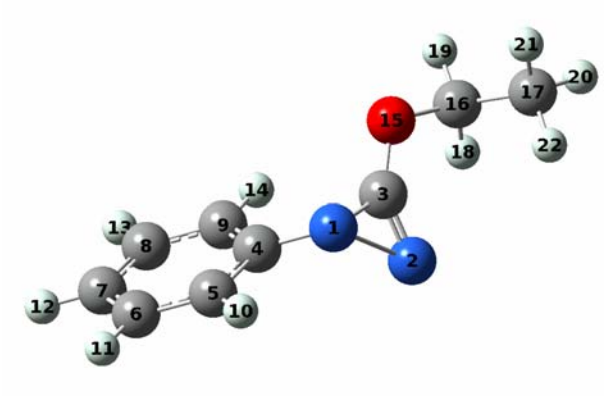


407.7	3.0
395.8	13.4
339.3	58.6
307.2	2.2
249.3	11.0
244.4	49.4
178.5	1.6
152.6	0.4
107.1	0.9
68.6	2.4
40.6	1.3
30.8	0.4

Frequencies were scaled by 0.978. The compound belongs to the C_1 symmetry point group. Sum of electronic and zero-point energies: −533.74244438 a.u.. Dipole moment: 3.3 Debye.

Table S16. Calculated IR bands of 3-ethoxy-1-phenyl-1*H*-diazirene at the DFT(B3LYP)/6-311++G(d,p) level. (conformer **G**).

Frequency (cm^{-1})	**Intensity (km mol^{-1})**
3128.8	6.3
3122.0	10.9
3115.1	14.1
3105.1	7.2
3096.0	0.8
3064.5	24.7
3040.7	3.4
3035.4	20.6
2994.6	15.6
2971.1	13.4
1768.4	470.3
1594.4	0.4
1579.2	0.6
1480.0	11.2
1476.1	10.0
1464.1	<0.1
1454.4	10.4
1448.9	7.4
1390.0	13.4
1371.1	12.2
1340.9	136.1
1321.6	7.0
1297.9	2.6
1296.6	16.6
1191.1	48.4
1172.9	26.1
1159.6	19.2
1153.8	7.3
1087.4	21.0
1079.0	6.9
1023.7	77.8
1016.8	153.2
992.8	0.2
975.4	<0.1
959.0	0.3
943.2	27.8
906.9	2.6
829.5	4.2
821.2	1.2
808.4	2.2
778.8	15.8
762.9	31.7
711.2	10.0
677.7	36.1
620.7	1.1
585.5	7.9
558.5	4.9
487.1	8.8
424.2	2.1

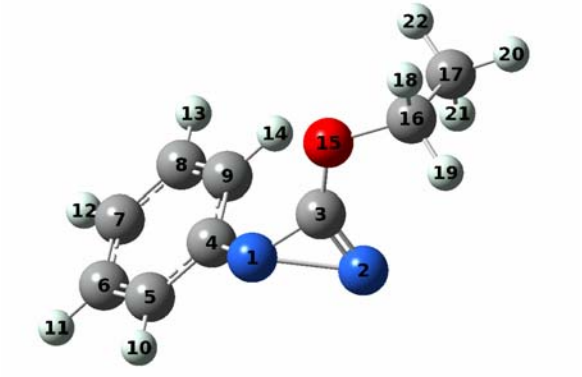


357.8	65.7
407.7	0.7
305.0	15.0
273.3	30.2
239.3	33.2
184.3	1.3
152.8	0.7
104.5	1.3
55.8	1.9
42.6	<0.1
38.8	2.3

Frequencies were scaled by 0.978. The compound belongs to the C_1 symmetry point group. Sum of electronic and zero-point energies: −533.74165279 a.u. Dipole moment: 3.0 Debye.

Table S17. Calculated IR bands of 3-ethoxy-1-phenyl-1*H*-diazirene at the DFT(B3LYP)/6-311++G(d,p) level. (conformer **G'**).

Frequency (cm^{-1})	**Intensity (km mol^{-1})**
3129.1	6.1
3122.4	10.0
3115.4	14.4
3105.3	7.4
3096.0	0.6
3062.8	25.8
3037.6	2.5
3032.9	27.6
2993.8	18.5
2969.2	10.4
1767.0	451.6
1594.2	0.6
1579.0	0.4
1479.6	12.7
1475.3	7.2
1463.0	1.5
1455.9	10.6
1448.9	8.2
1390.3	8.9
1372.5	14.2
1343.3	131.6
1321.4	5.4
1299.5	3.9
1296.8	13.5
1191.7	52.6
1173.0	22.5
1159.4	18.8
1153.9	7.3
1086.8	29.5
1078.8	4.1
1024.7	115.1
1017.9	91.8
992.8	0.3
975.5	0.0
959.4	0.4
945.7	30.5
906.6	2.4
829.0	4.9
821.3	1.5
806.6	2.0
780.2	12.5
763.6	34.6
710.8	11.0
677.5	35.2
620.9	1.7
588.9	6.7
558.1	4.8
489.9	10.6
406.6	1.0



403.1	10.6
353.5	50.6
311.8	5.8
277.8	35.3
238.1	36.2
194.1	1.7
158.0	1.1
104.8	1.6
63.3	1.3
46.8	1.8
33.4	0.6

Frequencies were scaled by 0.978. The compound belongs to the C_1 symmetry point group. Sum of electronic and zero-point energies: −533.74151629 a.u. Dipole moment: 3.2 Debye.