Appendix D

Table S1. Optimized [B3LYP/6-311++G(d,p)] geometries for the five tautomers of PT.[a]

	1-phenyl -1,4-dihydro-5*H*-tetrazol-5-one	**1-phenyl -1*H*-tetrazol-3 ium-5-olate**	**1-phenyl 1,2-dihydro-5*H*-tetrazol-5-one**	**1-phenyl-1*H*-tetrazol-5-ol (form A)**	**1-phenyl-1*H*-tetrazol-5-ol (form B)**
ΔE / kJ mol^{-1}	0.0	60.7	91.9	50.1	68.7
Bond length/ pm					
N_2=N_3	126.6	129.4	135.2	128.1	128.2
N_4-N_3	135.4	131.8	126.6	136.1	136.1
C_5-N_4	138.3	137.7	142.9	131.0	131.0
N_1-C_5	140.0	145.4	140.4	135.1	135.7
C_6-N_1	142.6	142.5	141.7	142.7	142.3
C_7-C_6	139.8	140.0	139.9	139.6	139.5
C_8-C_7	139.1	139.0	139.2	139.1	139.1
C_9-C_8	139.4	139.5	139.3	139.4	139.5
C_{10}-C_9	139.2	139.2	139.4	139.3	139.3
C_{11}-C_{10}	139.3	139.4	139.1	139.3	139.4
H_{12}-C_7	108.1	108.1	108.3	108.2	108.3
H_{13}-C_8	108.4	108.4	108.4	108.4	108.4
H_{14}-C_9	108.4	108.4	108.3	108.4	108.4
H_{15}-C_{10}	108.4	108.4	108.4	108.4	108.4
H_{16}-C_{11}	108.0	108.0	108.1	108.1	108.4
O_{17}-C_5	121.2	121.1	120.5	133.3	133.3
H_{18}-N_4 / H_{18}-N_3 / H_{18}-N_2 /H_{18}-O_{17}	100.8	101.2	101.6	96.7	96.7
Bond angle/°					
N_4-N_3-N_2	108.0	118.9	110.6	111.6	112.3
C_5-N_4-N_3	112.5	104.1	109.7	105.2	105.3
N_1-C_5-N_4	99.9	103.9	104.5	110.1	109.6
C_6-N_1-C_5	128.8	129.3	129.4	132.0	130.0
C_7-C_6-N_1	119.1	119.5	120.3	118.7	119.5
C_8-C_7-C_6	119.3	119.4	119.4	119.2	119.1
C_9-C_8-C_7	120.6	120.5	120.5	120.5	120.4
C_{10}-C_9-C_8	119.4	119.5	119.6	119.7	120.0
C_{11}-C_{10}-C_9	120.9	121.0	120.9	120.5	120.2
H_{12}-C_7-C_6	119.9	120.1	120.5	119.6	119.5
H_{13}-C_8-C_7	119.2	119.2	119.3	119.3	119.5
H_{14}-C_9-C_8	120.3	120.2	120.2	120.1	120.0
H_{15}-C_{10}-C_9	120.1	120.1	120.1	120.2	120.3
H_{16}-C_{11}-C_{10}	120.9	121.3	121.1	120.4	120.5
O_{17}-C_5-N_1	129.1	126.3	127.6	123.1	125.6
H_{18}-N_4-C_5 /H_{18}-N_3-N_4 / H_{18}-N_2-N_3/H_{18}-O_{17}-C_5	126.6	121.6	115.3	107.5	110.5
Dihedral angle/°					
C_5-N_4-N_3-N_2	0.0	0.0	5.2	0.1	-0.2
N_1-C_5-N_4-N_3	0.0	0.0	0.2	-0.1	-0.3
C_6-N_1-C_5-N_4	180.0	180.0	167.2	178.2	177.9
C_7-C_6-N_1-C_5	180.0	180.0	146.6	-150.6	-127.8
C_8-C_7-C_6-N_1	180.0	180.0	178.5	-179.2	179.7
C_9-C_8-C_7-C_6	0.0	0.0	0.0	-0.5	-0.8
C_{10}-C_9-C_8-C_7	0.0	0.0	0.0	0.4	1.0
C_{11}-C_{10}-C_9-C_8	0.0	0.0	0.0	0.2	0.0
H_{12}-C_7-C_6-N_1	0.0	0.0	-3.2	0.4	-0.9
H_{13}-C_8-C_7-C_6	180.0	180.0	180.0	179.9	179.6
H_{14}-C_9-C_8-C_7	180.0	180.0	180.0	-179.7	-179.6
H_{15}-C_{10}-C_9-C_8	180.0	180.0	180.0	179.7	178.8
H_{16}-C_{11}-C_{10}-C_9	180.0	180.0	180.0	179.5	176.2
O_{17}-C_5-N_4-N_3	180.0	180.0	180.0	179.4	179.1
H_{18}-N_4-C_5-N_1 /H_{18}-N_3-N_4-C_5 / H_{18}-N_2-N_3-N_4 /H_{18}-O_{17}-C_5-N_4	180.0	180.0	-143.2	-1.9	-172.8
Rotational constants/MHz					
A	2358.3769	2375.0204	2372.6328	2330.2303	2332.3146
B	671.7657	671.7051	662.8141	667.5893	652.7622
C	522.8390	523.6157	528.6631	532.8130	552.5120

[a] See Figure 1 (Chapter 3 – Part 3) for atom numbering.

Table S2. Definition of internal coordinates used in the normal coordinate analysis of 1-phenyl -1,4-dihydro-5*H*-tetrazole-5-one.

	Definition [a]	**Approximate description**
S_1	$\nu(C_5=O_{17})$	νC=O
S_2	$\nu(N_4-H_{18})$	νN-H
S_3	$\nu(N_1-C_6)$	νN-C
S_4	$\nu(N_2=N_3)$	νN=N
S_5	$\nu(N_3-N_4)$	νN-N
S_6	$\nu(N_4-C_5)$	νN-C
S_7	$\nu(C_5-N_1)$	νC-N
S_8	$\nu(N_1-N_2)$	νN-N
S_9	$\nu(C_6-C_7)+\nu(C_7-C_8)+\nu(C_8-C_9)+\nu(C_9-C_{10})+\nu(C_{10}-C_{11})+\nu(C_{11}-C_6)$	ν(C-C ring 1)
S_{10}	$-\nu(C_6-C_7)+2\nu(C_7-C_8)-\nu(C_8-C_9)-\nu(C_9-C_{10})+2\nu(C_{10}-C_{11})-\nu(C_{11}-C_6)$	ν(C-C ring 2)
S_{11}	$\nu(C_6-C_7)-\nu(C_7-C_8)+\nu(C_8-C_9)-\nu(C_9-C_{10})+\nu(C_{10}-C_{11})-\nu(C_{11}-C_6)$	ν(C-C ring 3)
S_{12}	$\nu(C_6-C_7)-\nu(C_8-C_9)+\nu(C_9-C_{10})-\nu(C_{11}-C_6)$	ν(C-C ring 4)
S_{13}	$\nu(C_6-C_7)-\nu(C_8-C_9)-\nu(C_9-C_{10})+\nu(C_{11}-C_6)$	ν(C-C ring 5)
S_{14}	$\nu(C_7-C_8)-\nu(C_{10}-C_{11})$	ν(C-C ring 6)
S_{15}	$\nu(C_7-H_{12})+\nu(C_8-H_{13})+\nu(C_9-H_{14})+\nu(C_{10}-H_{15})+\nu(C_{11}-H_{16})$	ν(C-H ring 1)
S_{16}	$\nu(C_7-H_{12})+\nu(C_8-H_{13})-\nu(C_{10}-H_{15})-\nu(C_{11}-H_{16})$	ν(C-H ring 2)
S_{17}	$\nu(C_7-H_{12})-2\nu(C_9-H_{14})+\nu(C_{11}-H_{16})$	ν(C-H ring 3)
S_{18}	$\nu(C_7-H_{12})-\nu(C_8-H_{13})+\nu(C_{10}-H_{15})-\nu(C_{11}-H_{16})$	ν(C-Hring 4)
S_{19}	$2\nu(C_7-H_{12})-3\nu(C_8-H_{13})+2\nu(C_9-H_{14})-3\nu(C_{10}-H_{15})+2\nu(C_{11}-H_{16})$	ν(C-H ring 5)
S_{20}	$\delta(H_{18}-N_4-N_3) - \delta(H_{18}-N_4-C_5)$	δNH
S_{21}	$\delta(O_{17}-C_5-N_4) - \delta(O_{17}-N_1-C_5)$	δC=O
S_{22}	$\delta(N_4N_1 C_5) – 0.809\delta(N_3C_5 N_4) – 0.809\delta(C_5N_2 N_1) + 0.309\delta(N_2N_4 N_3) + 0.309\delta(N_1N_3N_2)$	δ(ring1)
S_{23}	$–1.118\delta(N_3C_5 N_4) + 1.118\delta(C_5N_2 N_1) + 1.809\delta(N_2N_4 N_3) – 1.809\delta(N_1N_3N_2)$	δ(ring2)
S_{24}	N_3 out of plane $H_{18}N_3N_4C_5$	γN_2-N_1
S_{25}	N_4 out of plane $O_{17}N_4C_5N_1$	γN_1-C_5
S_{26}	$\tau N_4N_3N_2N_1 – 0.809\tau C_5N_4N_3N_2 – 0.809\tau N_3N_2N_1C_5 + 0.309\tau N_1C_5N_4N_3 + 0.309\tau N_2N_1C_5N_4$	τ(ring1)
S_{27}	$1.118\tau C_5N_4N_3N_2 – 1.118\tau N_3N_2N_1C_5 – 1.809\tau N_1C_5N_4N_3 + 1.809\tau N_2N_1C_5N_4$	τ(ring2)
S_{28}	N_2 out of plane $C_6N_2N_1C_5$	γN_3N_4
S_{29}	$\delta(C_6N_1N_2) - \delta(C_6N_1C_5)$	δN-C
S_{30}	$\delta(C_{11}-C_6-C_7)-\delta(C_6-C_7-C_8)+\delta(C_7-C_8-C_9)-\delta(C_8-C_9-C_{10})+\delta(C_9-C_{10}-C_{11}) -\delta(C_{10}-C_{11}-C_6)$	δ(ring 1)
S_{31}	$\delta(C_6-C_7-C_8)-\delta(C_7-C_8-C_9)+\delta(C_9-C_{10}-C_{11})-\delta(C_{10}-C_{11}-C_6)$	δ(ring 2)
S_{32}	$2\delta(C_{11}-C_6-C_7)-\delta(C_6-C_7-C_8)-\delta(C_7-C_8-C_9)+2\delta(C_8-C_9-C_{10})-\delta(C_9-C_{10}-C_{11}) -\delta(C_{10}-C_{11}-C_6)$	δ(ring 3)
S_{33}	$\tau(C_{11}-C_6-C_7-C_8)+\tau(C_{11}-C_6-C_7-H_{12})+\tau(N_1-C_6-C_7-C_8)+\tau(N_1-C_6-C_7-H_{12})-\tau(C_6-C_7-C_8-C_9)-\tau(C_6-C_7-C_8-H_{13})-\tau(H_{12}-C_7-C_8-C_9)-\tau(H_{12}-C_7-C_8-H_{13})+\tau(C_7-C_8-C_9-C_{10})+\tau(C_7-C_8-C_9-H_{14})+\tau(H_{13}-C_8-C_9-C_{10})+\tau(H_{13}-C_8-C_9-H_{14})-\tau(C_8-C_9-C_{10}-C_{11})-\tau(C_8-C_9-C_{10}-H_{15})-\tau(H_{14}-C_9-C_{10}-C_{11})-\tau(H_{14}-C_9-C_{10}-H_{15})+\tau(C_9-C_{10}-C_{11}-C_6)+\tau(C_9-C_{10}-C_{11}-H_{16})+\tau(H_{15}-C_{10}-C_{11}-C_6)+\tau(H_{15}-C_{10}-C_{11}-H_{16})-\tau(C_{10}-C_{11}-C_6-C_7)-\tau(C_{10}-C_{11}-C_6-N_1)-\tau(H_{16}-C_{11}-C_6-C_7)-\tau(H_{16}-C_{11}-C_6-N_1)$	τ(ring 1)
S_{34}	$\tau(C_{11}-C_6-C_7-C_8)+\tau(C_{11}-C_6-C_7-H_{12})+\tau(N_1-C_6-C_7-C_8)+\tau(N_1-C_6-C_7-H_{12})-\tau(C_7-C_8-C_9-C_{10})-\tau(C_7-C_8-C_9-H_{14})-\tau(H_{13}-C_8-C_9-C_{10})-\tau(H_{13}-C_8-C_9-H_{14})+\tau(C_8-C_9-C_{10}-C_{11})+\tau(C_8-C_9-C_{10}-H_{15})+\tau(H_{14}-C_9-C_{10}-C_{11})+\tau(H_{14}-C_9-C_{10}-H_{15})-\tau(C_{10}-C_{11}-C_6-C_7)-\tau(C_{10}-C_{11}-C_6-N_1)-\tau(H_{16}-C_{11}-C_6-C_7)-\tau(H_{16}-C_{11}-C_6-N_1)$	τ(ring 2)
S_{35}	$-\tau(C_{11}-C_6-C_7-C_8)-\tau(C_{11}-C_6-C_7-H_{12})-\tau(N_1-C_6-C_7-C_8)-\tau(N_1-C_6-C_7-H_{12})+2\tau(C_6-C_7-C_8-C_9)+2\tau(C_6-C_7-C_8-H_{13})+2\tau(H_{12}-C_7-C_8-C_9)+2\tau(H_{12}-C_7-C_8-H_{13})-\tau(C_7-C_8-C_9-C_{10})-\tau(C_7-C_8-C_9-H_{14})-\tau(H_{13}-C_8-C_9-C_{10})-\tau(H_{13}-C_8-C_9-H_{14})-\tau(C_8-C_9-C_{10}-C_{11})-\tau(C_8-C_9-C_{10}-H_{15})-\tau(H_{14}-C_9-C_{10}-C_{11})-\tau(H_{14}-C_9-C_{10}-H_{15})+2\tau(C_9-C_{10}-C_{11}-C_6)+2\tau(C_9-C_{10}-C_{11}-H_{16})+2\tau(H_{15}-C_{10}-C_{11}-C_6)+2\tau(H_{15}-C_{10}-C_{11}-H_{16})-\tau(C_{10}-C_{11}-C_6-C_7)-\tau(C_{10}-C_{11}-C_6-N_1)-\tau(H_{16}-C_{11}-C_6-C_7)-\tau(H_{16}-C_{11}-C_6-N_1)$	τ(ring 3)
S_{36}	$\delta(C_7-C_6-N_1)-\delta(C_{11}-C_6-N_1$	ω(ring)
S_{37}	$\gamma(N_1-C_{11}-C_6-C_7)$	γ(ring)
S_{38}	$\delta(H_{12}-C_7-C_6)-\delta(H_{12}-C_7-C_8)+\delta(H_{13}-C_8-C_7)- \delta(H_{13}-C_8-C_9)+\delta(H_{14}-C_9-C_8)-\delta(H_{14}-C_9-C_{10})+\delta(H_{15}-C_{10}-C_9)-\delta(H_{15}-C_{10}-C_{11})+\delta(H_{16}-C_{11}-C_{10})-\delta(H_{16}-C_{11}-C_6)$	δ(C-H ring 1)
S_{39}	$\delta(H_{12}-C_7-C_6)-\delta(H_{12}-C_7-C_8)+\delta(H_{13}-C_8-C_7)-\delta(H_{13}-C_8-C_9)-\delta(H_{15}-C_{10}-C_9)+\delta(H_{15}-C_{10}-C_{11})-\delta(H_{16}-C_{11}-C_{10})+\delta(H_{16}-C_{11}-C_6)$	δ(C-H ring 2)
S_{40}	$\delta(H_{12}-C_7-C_6)-\delta(H_{12}-C_7-C_8)-2\delta(H_{14}-C_9-C_8)+2\delta(H_{14}-C_9-C_{10})+\delta(H_{16}-C_{11}-C_{10})-\delta(H_{16}-C_{11}-C_6)$	δ(C-H ring 3)
S_{41}	$\delta(H_{12}-C_7-C_6)-\delta(H_{12}-C_7-C_8)-\delta(H_{13}-C_8-C_7)+\delta(H_{13}-C_8-C_9)+\delta(H_{15}-C_{10}-C_9)-\delta(H_{15}-C_{10}-C_{11})-\delta(H_{16}-C_{11}-C_{10})+\delta(H_{16}-C_{11}-C_6)$	δ(C-H ring 4)

S_{42}	$2\delta(H_{12}\text{-}C_7\text{-}C_6)-2\delta(H_{12}\text{-}C_7\text{-}C_8)-3\delta(H_{13}\text{-}C_8\text{-}C_7)+3\delta(H_{13}\text{-}C_8\text{-}C_9)+2\delta(H_{14}\text{-}C_9\text{-}C_8)-2\delta(H_{14}\text{-}C_9\text{-}C_{10})-$ $3\delta(H_{15}\text{-}C_{10}\text{-}C_9)+3\delta(H_{15}\text{-}C_{10}\text{-}C_{11})+2\delta(H_{16}\text{-}C_{11}\text{-}C_{10})-2\delta(H_{16}\text{-}C_{11}\text{-}C_6)$	δ(C-H ring 5)
S_{43}	$\gamma(H_{12}\text{-}C_6\text{-}C_7\text{-}C_8)+\gamma(H_{13}\text{-}C_7\text{-}C_8\text{-}C_9)+\gamma(H_{14}\text{-}C_8\text{-}C_9\text{-}C_{10})+\gamma(H_{15}\text{-}C_9\text{-}C_{10}\text{-}C_{11})+\gamma(H_{16}\text{-}C_{10}\text{-}C_{11}\text{-}C_6)$	γ(C-H ring 1)
S_{44}	$\gamma(H_{12}\text{-}C_6\text{-}C_7\text{-}C_8)+\gamma(H_{13}\text{-}C_7\text{-}C_8\text{-}C_9)-\gamma(H_{15}\text{-}C_9\text{-}C_{10}\text{-}C_{11})-\gamma(H_{16}\text{-}C_{10}\text{-}C_{11}\text{-}C_6)$	γ(C-H ring 2)
S_{45}	$\gamma(H_{12}\text{-}C_6\text{-}C_7\text{-}C_8)-2\gamma(H_{14}\text{-}C_8\text{-}C_9\text{-}C_{10})+\gamma(H_{16}\text{-}C_{10}\text{-}C_{11}\text{-}C_6)$	γ(C-H ring 3)
S_{46}	$\gamma(H_{12}\text{-}C_6\text{-}C_5\text{-}C_8)-\gamma(H_{11}\text{-}C_7\text{-}C_8\text{-}C_9)+\gamma(H_{15}\text{-}C_9\text{-}C_{10}\text{-}C_{11})-\gamma(H_{16}\text{-}C_{10}\text{-}C_{11}\text{-}C_6)$	γ(C-H ring 4)
S_{47}	$2\gamma(H_{12}\text{-}C_6\text{-}C_7\text{-}C_8)-3\gamma(H_{13}\text{-}C_7\text{-}C_8\text{-}C_9)+2\gamma(H_{14}\text{-}C_8\text{-}C_9\text{-}C_{10})-3\gamma(H_{15}\text{-}C_9\text{-}C_{10}\text{-}C_{11})+2\gamma(H_{16}\text{-}C_{10}\text{-}C_{11}\text{-}C_6)$	γ(C-H ring 5)
S_{48}	$\tau(C_{11}\text{-}C_6\text{-}N_1\text{-}C_5)+\tau(C_7\text{-}C_6\text{-}N_1\text{-}C_5)+\tau(C_{11}\text{-}C_6\text{-}N_1\text{-}N_2)+\tau(C_7\text{-}C_6\text{-}N_1\text{-}N_2)$	$\tau(C\text{-}C_\alpha)$

[a] ν, bond stretching, δ, bending, γ rocking, τ torsion, s, symmetric, as, asymmetric.

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 1-phenyl -1,4-dihydro-5*H*-tetrazole-5-one. [a]

Approximate Description	Sym-metry	Calculated frequency	Intensity	PED [b]
νN-H	A'	3585.7	144.1	S_{2}(99.6)
ν(C-H ring 2)	A'	3159.7	6.7	S_{16}(29.7) + S_{15}(26.5) + S_{18}(19.1) + S_{17}(15.6)
ν(C-H ring 1)	A'	3149.3	0.3	S_{15}(29.5) + S_{16}(33.6) + S_{18}(17.0) + S_{17}(13.0)
ν(C-H ring 3)	A'	3122.3	15.1	S_{17}(47.6) + S_{15}(42.3)
ν(C-Hring 4)	A'	3110.4	13.3	S_{18}(63.6) + S_{16}(35.9)
ν(C-H ring 5)	A'	3100.2	0.0	S_{19}(75.5) + S_{17}(23.3)
νC=O	A'	1771.7	507.8	S_{1}(76.3)
ν(C-C ring 2)	A'	1604.8	36.6	S_{10}(66.7) + S_{41}(21.4) + S_{32}(9.8)
ν(C-C ring 4)	A'	1593.9	1.6	S_{12}(70.3) + S_{40}(11.4)
δ(C-H ring 2)	A'	1496.3	90.7	S_{39}(57.9) + S_{13}(31.1)
νN=N	A'	1471.8	23.5	S_{4}(46.8) + S_{40}(14.8) + S_{14}(13.7)
ν(C-C ring 6)	A'	1452.3	8.2	S_{14}(25.8) + S_{4}(25.2) + S_{40}(20.2)
νN-C	A'	1359.7	68.6	S_{3}(17.9) + S_{20}(22.4) + S_{23}(10.0)
δNH	A'	1341.3	70.8	S_{20}(29.0) + S_{4}(14.7) + S_{5}(11.9) + S_{3}(11.1) + S_{38}(10.8)
δ(C-H ring 1)	A'	1330.8	40.1	S_{38}(66.2)
ν(C-C ring 3)	A'	1306.1	6.9	S_{11}(85.0)
νN-C	A'	1196.9	19.0	S_{6}(35.5) + S_{21}(19.9) + S_{5}(9.6)
δ(C-H ring 4)	A'	1179.2	9.7	S_{41}(68.1) + S_{10}(19.6)
δ(C-H ring 5)	A'	1159.5	0.8	S_{42}(67.2) + S_{40}(12.4) + S_{11}(10.4)
νN-N	A'	1137.3	42.7	S_{8}(31.9) + S_{23}(18.9) + S_{5}(11.0)
δ(C-H ring 3)	A'	1083.5	3.5	S_{40}(30.0) + S_{14}(45.8)
ν(C-C ring 5)	A'	1044.3	1.3	S_{13}(48.0) + S_{39}(23.7)
νN-N	A'	1020.7	68.1	S_{5}(26.7) + S_{9}(21.3) + S_{23}(14.2) + S_{30}(13.0) + S_{13}(10.3)
δ(ring 1)	A'	1007.7	28.6	S_{30}(20.8) + S_{5}(16.3) + S_{23}(15.6) + S_{6}(15.4) + S_{20}(10.1)
ν(C-C ring 1)	A'	992.6	0.4	S_{9}(48.3) + S_{30}(48.7)
γ(C-H ring 5)	A"	984.7	0.6	S_{47}(62.0) + S_{33}(12.8) + S_{46}(9.7) + S_{34}(9.6)
τ(ring 3)	A"	971.5	0.0	S_{35}(54.0) + S_{46}(25.4) + S_{33}(14.6)
δ(ring2)	A'	942.2	14.2	S_{23}(24.8) + S_{7}(35.2) + S_{8}(16.8) + S_{6}(12.3)
γ(C-H ring 3)	A"	916.6	7.4	S_{45}(71.5) + S_{34}(16.1)
γ(C-H ring 2)	A"	838.2	0.0	S_{44}(99.2)
δ(ring1)	B	758.5	2.2	S_{22}(34.1) + S_{7}(15.7) + S_{1}(12.2) + S_{8}(11.5)
γ(C-H ring 1)	B	754.0	66.7	S_{43}(64.7) + S_{37}(22.0)
γN_{1}-C_{5}	A	721.7	1.4	S_{25}(78.2) + S_{27}(21.1)
τ(ring 1)	A	690.6	30.4	S_{33}(49.0) + S_{47}(22.5) + S_{43}(14.6) + S_{37}(10.7)
δ(ring 3)	A	686.6	9.1	S_{32}(47.8) + S_{22}(24.1) + S_{3}(11.4)
τ(ring 1)	A	675.1	4.7	S_{26}(92.5)
δ(ring 2)	A'	617.0	0.2	S_{31}(87.5)
δC=O	A'	552.3	7.0	S_{21}(56.9) + S_{29}(9.9)
γ(ring)	A"	510.0	54.1	S_{37}(43.4) + S_{24}(15.5) + S_{34}(11.5)
γN_{2}-N_{1}	A"	480.7	69.3	S_{24}(76.9)
γ(C-H ring 4)	A"	408.4	0.0	S_{46}(48.3) + S_{35}(38.2) + S_{48}(15.8)
ω(ring)	A'	371.4	0.6	S_{36}(19.8) + S_{32}(17.1) + S_{3}(14.7) + S_{29}(13.7) + S_{8}(9.9)
νC-N	A'	318.6	6.3	S_{7}(21.0) + S_{21}(18.2) + S_{3}(16.4) + S_{36}(15.8) + S_{32}(13.5)
τ(ring 2)	A"	286.5	0.8	S_{34}(30.4) + S_{28}(30.5) + S_{27}(13.5)
τ(ring 2)	A"	218.1	1.8	S_{27}(71.3) + S_{34}(18.1)
δN-C	A'	173.7	1.5	S_{29}(54.0) + S_{36}(37.3)
γ$N_{3}N_{4}$	A"	97.7	2.9	S_{28}(66.0) + S_{34}(13.9) + S_{37}(13.0)
τ(C-C_{α})	A"	24.0	0.0	S_{48}(80.4) + S_{46}(20.9)

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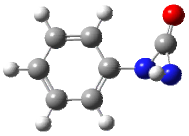
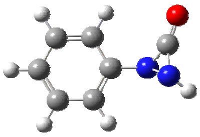
[a] Frequencies in cm^{-1}, calculated intensities in km mol^{-1}. ν, bond stretching, δ, bending, γ rocking, τ torsion, s, symmetric, as, asymmetric. See Table S02 for definition of symmetry coordinates.

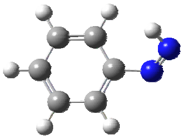
[b] Only PED values greater than 10 % are given.

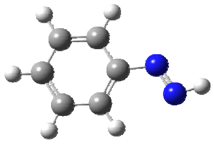
Table S4. DFT/B3LYP/6-311++G(d,p) calculated IR of 1-phenyl-diaziridin-3-one.

Conformer I			***Conformer II***		
Frequency (cm^{-1})	Intensity (km mol^{-1})		Frequency (cm^{-1})	Intensity (km mol^{-1})	
3296.9	9.1		3390.5	31.8	
3128.4	5.8		3127.8	5.7	
3124.7	4.2		3123.7	8.0	
3118.0	8.6		3117.0	10.8	
3108.8	6.8		3107.6	6.5	
3100.2	0.1		3099.1	0.2	
1921.2	645.7		1931.2	669.7	
1597.2	12.9		1599.2	18.1	
1584.5	3.2		1588.9	2.7	
1484.1	34.2		1486.4	36.2	
1449.8	3.8		1450.8	4.4	
1324.5	0.5		1323.9	0.6	
1297.1	2.6		1298.5	0.6	
1242.9	48.8		1236.2	54.1	
1174.8	1.7		1169.6	2.1	
1162.3	1.6		1156.9	0.1	
1155.8	0.7		1126.8	18.4	
1077.6	10.0		1078.6	5.6	
1050.1	10.2		1066.3	30.9	
1041.4	19.6		1037.0	6.1	
1019.8	4.6		1019.9	6.2	
993.1	1.1		993.2	1.1	
982.2	0.1		976.2	0.1	
966.1	0.0		959.7	2.0	
915.6	61.4		945.5	140.1	
910.0	109.8		903.9	19.6	
831.8	0.2		826.4	0.3	
762.3	45.9		762.1	43.4	
758.7	0.8		756.2	51.9	
694.2	55.2		691.8	24.1	
678.6	3.3		681.7	17.9	
613.7	2.0		616.1	2.9	
556.3	12.2		585.3	18.7	
536.9	18.1		560.7	16.6	
521.5	20.1		522.4	6.1	
440.4	3.6		439.7	4.2	
406.0	1.2		404.4	1.0	
331.3	1.1		333.1	2.7	
284.9	0.8		290.8	4.0	
127.5	2.8		132.2	3.0	
113.1	0.8		108.3	2.4	
27.4	2.2		11.6	2.6	

Frequencies were scaled by 0.978. The molecule belongs to the C_1 symmetry point group. Sum of electronic and zero-point energies: -1194608.656 kJ mol^{-1} (conformer I), -1194623.129 kJ mol^{-1} (conformer II). Dipolar moment: 4.1314 Debye (conformer I), 2.7012 (conformer II).

Table S5. DFT/B3LYP/6-311++G(d,p) calculated IR of phenyldiazene.



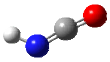


	Isomer Z			***Isomer E***	
Sym	Frequency (cm^{-1})	Intensity ($km\ mol^{-1}$)	Sym	Frequency (cm^{-1})	Intensity ($km\ mol^{-1}$)
A’	3127.2	7.9	A'	3250.3	1.5
A’	3120.3	11.6	A'	3134.8	3.7
A'	3111.1	9.0	A'	3125.8	8.9
A’	3103.1	0.9	A'	3115.9	13.6
A'	3095.2	0.8	A'	3106.5	9.7
A'	3012.0	55.9	A'	3095.6	0.5
A'	1611.2	16.6	A'	1607.1	1.9
A'	1589.9	5.4	A'	1594.2	1.2
A'	1569.8	31.7	A'	1553.7	59.9
A'	1478.4	8.3	A'	1476.2	0.8
A'	1451.7	12.6	A'	1471.3	21.9
A'	1437.9	57.7	A'	1431.6	10.4
A'	1318.7	0.9	A'	1319.0	5.9
A'	1303.9	0.3	A'	1300.8	8.7
A'	1176.3	0.3	A'	1179.2	7.2
A'	1157.3	0.3	A'	1155.6	0.8
A'	1135.4	8.0	A'	1127.1	43.4
A'	1081.2	4.1	A'	1072.4	6.0
A'	1018.8	4.2	A'	1016.5	6.6
A'	995.1	3.8	A'	994.0	0.6
A"	969.8	5.7	A"	984.9	1.4
A"	951.1	10.2	A"	972.9	0.1
A"	966.1	12.1	A"	964.9	42.4
A"	900.7	13.0	A"	909.3	8.6
A"	827.7	2.2	A"	840.2	0.0
A'	788.8	5.0	A'	793.1	12.8
A"	742.6	80.3	A"	746.2	34.0
A"	671.6	23.3	A"	679.9	35.6
A'	620.5	5.3	A'	633.3	29.1
A'	613.8	0.8	A'	614.6	0.1
A'	473.5	2.3	A"	460.6	18.9
A'	429.7	2.8	A'	456.2	0.0
A"	407.3	0.7	A"	409.5	0.2
A"	267.1	9.5	A'	262.8	2.6
A"	211.7	11.5	A"	226.5	3.8
A"	113.5	4.2	A"	70.9	0.3

Frequencies were scaled by 0.978. The molecule belongs to the C_s symmetry point group. Sym: Symmetry. Sum of electronic and zero-point energies: -897091.6753 kJ mol^{-1} (isoomer E), -897068.0345 kJ mol^{-1} (isomer Z). Dipolar moment: 1.1573 Debye (isomer E), 3.7342 (isomer Z).

Table S6. DFT/B3LYP/6-311++G(d,p) **c**alculated IR spectrum of isocyanic acid.

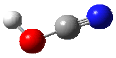
Symmetry	Frequency (cm^{-1})	Intensity ($km\ mol^{-1}$)
A'	3608.2	170.0
A'	2288.1	783.0
A'	1308.0	0.5
A'	747.6	199.7
A'	618.8	3.6
A"	555.4	96.7



Frequencies were scaled by 0.978. The molecule belongs to the C_s symmetry point group. Sum of electronic and zero-point energies: -442967.828 kJ mol^{-1}. Dipolar moment: 2.2682 Debye.

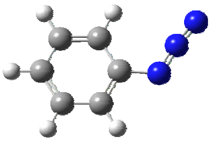
Table S7. DFT/B3LYP/6-311++G(d,p) **c**alculated IR spectrum of cyanic acid.

Symmetry	Frequency (cm^{-1})	Intensity ($km\ mol^{-1}$)
A'	3689.7	160.5
A'	2324.7	143.4
A'	1206.4	91.1
A'	1075.0	76.9
A'	501.2	2.9
A"	443.3	15.2



Frequencies were scaled by 0.978. The molecule belongs to the C_s symmetry point group. Sum of electronic and zero-point energies: -442848.4384 kJ mol^{-1}. Dipolar moment: 3.9809 Debye.

Table S8– DFT/B3LYP/6-311++G(d,p) calculated IR of phenyl azide.

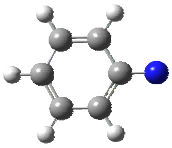


Sym	Frequency (cm^{-1})	Intensity ($km\ mol^{-1}$)
A'	3128.8	4.8
A'	3122.0	13.4
A'	3111.9	11.1
A'	3103.8	2.2
A'	3096.4	2.4
A'	2191.4	843.5
A'	1600.5	59.2
A'	1585.3	6.4
A'	1487.7	86.3
A'	1450.9	1.1
A'	1336.4	151.2
A'	1325.0	29.8
A'	1296.8	18.2
A'	1174.6	2.4
A'	1156.3	0.1
A'	1128.9	18.3
A'	1080.2	9.7
A'	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	0.0
A'	138.1	0.6
A"	70.1	0.0

Frequencies were scaled by 0.978. The molecule belongs to the C_s symmetry point group. Sym: Symmetry. Sum of electronic and zero-point energies: -1039278.444 kJ mol^{-1}. Dipolar moment: 1.9485 Debye.

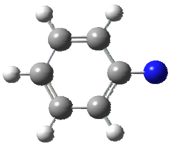
Table S9. DFT/B3LYP/6-311++G(d,p) calculated IR of phenyl nitrene (singlet).

Sym	Frequency (cm^{-1})	Intensity ($km\ mol^{-1}$)
A1	3128.4	3.9
B2	3125.6	5.8
A1	3112.6	10.2
B2	3104.7	6.9
A1	3092.7	0.1
A1	1570.7	102.3
B2	1533.0	0.6
A1	1439.3	22.0
B2	1421.6	45.7
A1	1333.7	85.7
B2	1318.3	51.3
B2	1244.2	4.3
B2	1159.6	6.1
A1	1146.1	21.9
B2	1059.2	4.8
B1	1013.6	0.4
A2	999.8	0
A1	998.3	2.7
A1	985.7	0.9
B1	982.8	1.4
A2	831.7	0
A1	799.7	11.7
B1	783.7	39.4
B1	650.4	48.6
B2	591.7	0.3
A1	528.3	0.3
A2	458.4	0
B1	442.3	<0.1
B2	417.4	3.6
B1	148.6	8.2



Frequencies were scaled by 0.978. The molecule belongs to the C2v symmetry point group. Sum of electronic and zero-point energies: -751525.3804 kJ mol^{-1}. Dipolar moment: 5.9415 Debye.

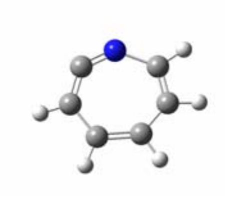
Table S10. DFT/B3LYP/6-311++G(d,p) calculated IR of phenyl nitrene (triplet).



Sym	Frequency (cm^{-1})	Intensity ($km\ mol^{-1}$)
A1	3130.0	2.9
B2	3127.6	7.7
A1	3120.6	8.9
B2	3104.2	7.1
A1	3098.1	0.5
A1	1550.4	10.4
B2	1520.5	2.5
A1	1426.8	1.2
B2	1410.2	2.5
B2	1309.5	0.1
A1	1280.4	14.1
B2	1240.5	0.8
B2	1148.6	0.1
A1	1143.7	4.1
B2	1067.4	7.1
A1	1002.8	2.8
B1	956.5	0.2
A1	952.1	0.7
A2	951.5	0
B1	879.7	3.1
A1	811.9	2.5
A2	795.9	0
B1	733.6	63.6
B1	645.8	31.2
B2	601.5	0.1
A1	513.6	0.3
B1	467.6	2.8
A2	386.9	0
B2	369.9	7.1
B1	197.7	2.0

Frequencies were scaled by 0.978. The molecule belongs to the C2v symmetry point group. Sum of electronic and zero-point energies: -751658.339 kJ mol^{-1}. Dipolar moment: 3.2180 Debye.

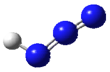
Table S11. DFT/B3LYP/6-311++G(d,p) **c**alculated IR spectrum of 1-aza-1,2,4,6-cycloheptatetraene.



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 molecule belongs to the C1 symmetry point group. Sum of electronic and zero-point energies: -751604.5681 kJ mol^{-1}. Dipolar moment: 2.0789 Debye.

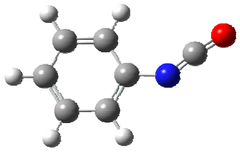
Table S12. DFT/B3LYP/6-311++G(d,p) calculated IR spectrum of azide.



Symmetry	Frequency (cm^{-1})	Intensity ($km\ mol^{-1}$)
A'	3412.2	45.2
A'	2218.4	405.2
A'	1265.8	0.2
A'	1148.0	222.2
A"	578.1	0.6
A"	524.1	16.3

Frequencies were scaled by 0.978. The molecule belongs to the C_s symmetry point group. Sum of electronic and zero-point energies: -432720.9782 kJ mol^{-1}. Dipolar moment: 1.9542 Debye.

Table S13. DFT/B3LYP/6-311++G(d,p) calculated IR spectrum of phenylisocyanate.

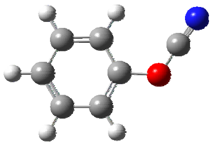


Symmetry	Frequency (cm^{-1})	Intensity ($km\ mol^{-1}$)
A’	3129.7	3.3
A’	3122.2	12.9
A’	3113.4	14.7
A’	3105.0	2.6
A’	3097.7	1.7
A’	2307.6	1757.5
A’	1603.3	68.8
A’	1583.7	8.9
A’	1519.4	59.6
A’	1451.4	2.4
A’	1446.5	4.8
A’	1322.3	0.4
A’	1289.4	5.7
A’	1171.7	0.1
A’	1156.3	0.1
A’	1120.2	53.5
A’	1076.0	11.0
A’	1022.1	6.9
A’	993.9	0.2
A’’	966.2	0.2
A’’	951.5	0.1
A’’	896.4	5.9
A’’	822.3	0.1
A’	756.6	13.9
A’’	748.5	65.2
A’’	678.1	26.6
A’	632.8	31.0
A’	617.0	2.3
A’’	564.8	23.4
A’’	491.7	5.4
A’	457.6	0.9
A’’	407.6	0.0
A’	378.0	11.2
A’’	234.6	0.0
A’	87.0	2.3
A’’	56.9	0.0

Frequencies were scaled by 0.978. The molecule belongs to the C_s symmetry point group. Sum of electronic and zero-point energies: -1049518.333 kJ mol^{-1}. Dipolar moment: 2.6461 Debye.

Table S14. DFT/B3LYP/6-311++G(d,p) calculated IR spectrum of phenylcyanate.

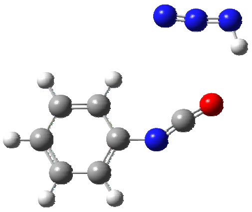
Symmetry	Frequency (cm^{-1})	Intensity ($km\ mol^{-1}$)
A’	3135.0	1.4
A’	3129.0	4.8
A’	3122.1	5.8
A’	3114.1	7.8
A’	3105.3	0.0
A’	2306.2	259.7
A’	1610.9	12.0
A’	1594.4	50.4
A’	1484.7	93.7
A’	1457.7	2.6
A’	1321.9	1.7
A’	1307.0	0.5
A’	1191.4	264.9
A’	1163.7	48.4
A’	1156.4	6.5
A’	1079.0	13.7
A’	1072.9	1.2
A’	1018.9	7.2
A’	994.9	2.5
A’’	969.5	0.1
A’’	955.4	0.0
A’’	895.3	6.6
A’’	817.6	0.0
A’	775.3	29.7
A’’	748.7	76.5
A’’	676.8	20.0
A’	639.6	2.5
A’	612.7	0.3
A’’	495.8	2.7
A’’	487.9	13.4
A’	450.6	1.2
A’’	410.4	0.0
A’	361.1	3.0
A’’	223.8	0.2
A’	134.4	5.0
A’’	49.2	1.8



Frequencies were scaled by 0.978. The molecule belongs to the C_s symmetry point group. Sum of electronic and zero-point energies: -1049382.852 kJ mol^{-1}. Dipolar moment: 4.7228 Debye.

Table S15. DFT/B3LYP/6-311++G(d,p) calculated IR spectrum of the azide / phenylisocyanate complex.

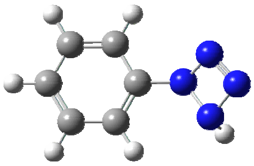
Symmetry	Frequency (cm^{-1})	Intensity ($km\ mol^{-1}$)
A’	3398.0	94.1
A’	3129.9	4.1
A’	3123.2	11.7
A’	3114.8	6.9
A’	3106.6	4.4
A’	3099.8	0.4
A’	2322.0	1839.7
A’	2214.5	279.9
A’	1602.4	44.4
A’	1585.1	7.5
A’	1518.6	31.9
A’	1452.4	10.3
A’	1447.9	9.2
A’	1324.0	0.2
A’	1290.6	4.8
A’	1277.3	9.1
A’	1173.5	0.4
A’	1167.0	267.8
A’	1157.2	0.2
A’	1116.2	52.5
A’	1078.0	9.7
A’	1022.0	7.5
A’	994.0	0.2
A’’	977.1	0.1
A’’	961.1	0.0
A’’	904.4	5.7
A’’	827.3	<0.1
A’’	750.9	63.7
A’’	750.1	13.2
A’’	685.5	27.3
A’	623.6	26.4
A’	614.2	16.1
A’’	579.5	0.7
A’’	556.1	25.1
A’	523.5	22.3
A’’	493.0	4.8
A’	454.3	0.4
A’’	409.5	<0.1
A’	378.0	14.7
A’’	260.1	125.2
A’’	237.8	0.1
A’	111.8	2.5
A’	76.7	7.5
A’’	59.8	0.4
A’’	40.4	1.3
A’’	29.4	0.2
A’’	16.1	<0.1
A’’	9.3	2.6



Frequencies were scaled by 0.978. The molecule belongs to the C_s symmetry point group. Sum of electronic and zero-point energies: -1482249.417 kJ mol^{-1}. Dipolar moment: 3.3409 Debye.

Table S 16. DFT/B3LYP/6-311++G(d,p) calculated IR spectrum of 1-phenyl-1,2-dihydrotetrazete.

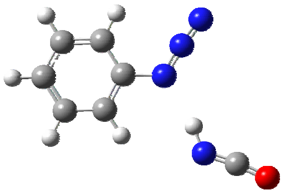
Frequency (cm^{-1})	Intensity ($km\ mol^{-1}$)
3370.1	16.7
3129.9	2.3
3127.3	4.5
3119.7	13.4
3107.6	9.2
3099.5	0.3
1602.7	42.31
1593.9	5.2
1490.5	52.3
1455.3	4.2
1427.8	8.9
1325.9	0.6
1311.7	43.1
1303.1	14.0
1281.6	26.6
1171.3	0.2
1157.0	0.9
1127.0	66.9
1099.0	25.7
1073.9	7.0
1064.1	8.6
1021.7	12.4
991.5	0.4
971.5	0.1
955.9	<0.1
929.2	48.5
893.3	6.1
834.0	80.3
823.2	3.4
748.3	67.3
696.7	8.3
683.7	21.4
634.7	46.3
615.9	0.1
506.2	11.6
445.4	4.5
404.0	0.1
391.2	1.6
261.6	8.6
172.3	1.4
109.9	5.8
39.5	4.2



Frequencies were scaled by 0.978. The molecule belongs to the C_1 symmetry point group. Sum of electronic and zero-point energies: -1184400.618 kJ mol^{-1}. Dipolar moment: 3.2497 Debye.

Table S17. Observed and calculated IR bands of the complex phenylazide / isocyanic acid (1:1).

Sym	Frequency (cm^{-1})	Intensity ($km\ mol^{-1}$)
A’	3399.3	1092.2
A’	3129.4	3.4
A’	3123.4	6.4
A’	3113.9	10.5
A’	3106.0	1.0
A’	3098.4	2.4
A’	2286.6	994.0
A’	2197.1	722.6
A’	1600.2	47.4
A’	1588.5	6.9
A’	1488.8	72.6
A’	1453.1	1.4
A’	1332.3	9.7
A’	1315.3	147.9
A’	1309.0	13.9
A’	1299.0	32.2
A’	1179.0	2.5
A’	1158.8	0.2
A’	1129.3	26.3
A’	1085.2	8.6
A’	1024.0	4.7
A’	992.1	0.6
A’’	978.0	0.1
A’’	954.6	0.1
A’’	894.0	5.6
A’	831.1	297.3
A’’	820.8	0.3
A’	810.3	43.5
A’’	747.2	68.7
A’’	683.6	26.6
A’	670.7	26.7
A’’	637.7	0.1
A’	626.8	21.5
A’	616.0	2.3
A’’	509.6	15.4
A’’	491.0	3.0
A’’	461.0	4.6
A’’	422.3	102.1
A’’	405.3	8.4
A’	375.2	1.0
A’’	228.7	2.3
A’	148.7	1.1
A’	116.0	4.3
A’’	71.0	0.5
A’	69.3	0.1
A’’	26.7	0.3
A’	21.1	1.2
A’’	6.8	0.3



Frequencies were scaled by 0.978. The complex belongs to the Cs symmetry point group. Sym: Symmetry. Sum of electronic and zero-point energies: -1482258.3 kJ mol^{-1}. Dipole moment: 4.4878 Debye.

Table S18. DFT(B3LYP)/6-311++G(d,p) calculated frequencies and intensities for **Sk'**, **Sk** and **Syn** conformers of 4-allyl-1-phenyl-tetrazolone. [a]

Sk'		Sk		Syn	
Frequency cm^{-1}	Intensity (km mol^{-1})	Frequency cm^{-1}	Intensity (km mol^{-1})	Frequency cm^{-1}	Intensity (km mol^{-1})
3157.2	6.9	3158.2	7.0	3157.7	6.2
3149.2	0.3	3149.3	0.3	3157.1	12.4
3147.7	9.2	3148.0	8.6	3148.9	0.3
3121.9	17.3	3122.4	17.3	3122.1	17.0
3109.5	14.0	3109.8	14.1	3109.7	13.9
3099.5	0.0	3099.9	0.0	3099.8	0.0
3080.1	3.1	3079.1	3.1	3079.9	3.2
3062.6	8.0	3063.1	6.0	3069.1	14.8
3043.2	2.3	3046.3	0.3	3014.6	1.0
2991.1	12.0	2991.1	15.3	2977.8	16.5
1746.4	396.5	1749.0	353.1	1752.0	381.1
1669.0	3.9	1668.1	4.9	1674.3	13.8
1604.6	45.1	1604.4	44.3	1604.5	43.3
1593.1	1.8	1593.4	1.7	1593.1	1.8
1495.5	106.5	1495.7	104.0	1495.5	102.4
1463.9	18.1	1463.7	19.3	1464.0	18.4
1438.8	12.1	1440.6	20.1	1438.6	17.3
1434.4	30.1	1429.3	19.5	1428.9	26.0
1423.0	4.4	1423.1	5.6	1416.6	0.3
1366.7	198.4	1368.5	156.4	1381.2	124.7
1353.0	16.8	1346.1	11.4	1365.0	60.0
1337.7	6.1	1340.8	28.6	1341.3	19.4
1326.8	26.2	1329.2	33.6	1328.4	27.6
1307.0	20.2	1306.1	4.8	1315.2	24.7
1305.2	12.2	1303.9	45.0	1305.4	8.2
1289.0	11.2	1290.4	6.2	1291.4	0.2
1181.0	12.2	1184.0	11.5	1179.2	3.2
1178.3	3.5	1179.5	3.1	1161.2	21.2
1158.5	0.8	1158.5	1.1	1156.9	14.1
1129.8	66.4	1132.0	82.0	1116.7	76.9
1098.4	23.2	1095.2	10.4	1093.2	8.7
1083.4	7.4	1082.3	1.3	1067.5	46.0
1055.8	94.4	1056.1	67.5	1051.2	10.6
1025.7	19.5	1026.1	15.5	1025.3	12.2
1003.3	11.7	1004.0	31.9	1002.1	16.9
993.0	0.1	993.0	0.2	993.0	0.1
981.8	0.5	982.6	0.6	981.8	0.5
969.2	0.0	969.7	0.0	980.1	23.0
968.8	13.2	964.3	6.5	968.9	0.0
946.2	45.4	950.0	48.9	935.2	33.5
927.0	6.5	920.2	5.1	918.9	9.6
915.1	6.7	916.1	6.6	915.1	6.7
890.1	2.7	898.7	26.6	899.3	7.7
836.0	0.0	837.2	0.0	835.8	0.0

809.7	45.6	807.7	39.4	795.8	16.5
761.2	15.1	757.1	46.0	756.1	32.8
756.2	56.4	756.5	26.1	755.9	35.5
723.3	9.9	724.1	9.9	723.4	11.5
694.8	28.2	696.2	20.5	694.4	28.8
690.5	9.3	693.3	10.8	683.3	3.3
657.8	2.2	657.2	1.5	657.8	1.8
619.7	3.8	626.9	8.0	619.7	3.7
614.0	1.4	615.6	0.3	614.6	1.4
551.0	4.0	545.2	3.9	539.0	13.0
507.2	11.3	507.7	11.0	507.1	11.1
411.8	0.5	407.4	0.0	492.8	5.2
406.9	0.0	398.8	2.1	406.2	0.0
363.9	1.8	366.1	0.8	359.8	2.0
347.9	5.6	343.9	6.6	317.6	2.8
306.3	3.7	307.3	2.6	307.0	2.8
301.7	3.8	299.7	1.8	293.8	1.1
262.5	3.9	273.6	5.2	277.2	6.6
207.4	3.5	207.0	3.2	195.9	2.5
147.0	1.1	148.5	1.1	157.3	1.3
124.6	0.1	122.4	0.2	115.4	0.5
74.7	0.8	74.0	0.6	104.0	0.2
48.6	1.2	41.9	1.1	51.8	1.3
26.1	0.2	27.3	0.1	33.2	0.4
20.3	0.0	15.8	0.0	19.3	0.0

[a] Frequencies were scaled by 0.978.

Figure S1. Calculated spectra for **Sk'**, **Sk** and **Syn** conformers of 4-allyl-1-phenyl-tetrazolone. The calculated frequencies were scaled by a factor of 0.978.

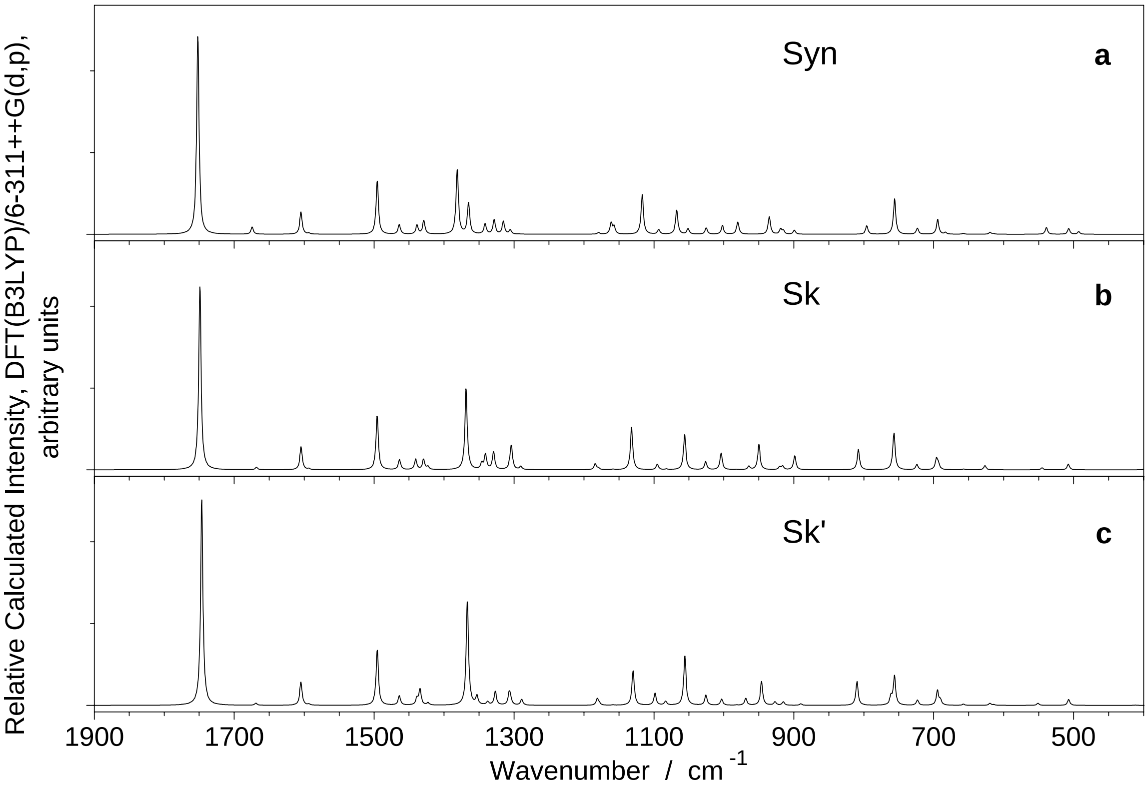


Table S19. Cartesian coordinates for the 4-allyl-1-phenyl-tetrazolone (conformer Sk’).

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--------------------------------------------------------------
                             Coordinates (Angstroms)
                         X              Y              Z
--------------------------------------------------------------
 N                   0.28492500   -0.30391200   -0.18815500
 N                  -0.26771200   -1.55636100   -0.23724600
 N                  -1.52055200   -1.44428700   -0.39397400
 N                  -1.83291200   -0.12753400   -0.45930500
 C                  -0.70751000    0.66788900   -0.32739000
 C                   1.68841700   -0.13354600   -0.01443600
 C                   2.23766600    1.15005600    0.05139800
 C                   3.61351600    1.28843100    0.22376700
 C                   4.43664300    0.17060300    0.32971100
 C                   3.87382200   -1.10346700    0.26188800
 C                   2.50345200   -1.26512600    0.09004500
 H                   1.59792700    2.01648600   -0.03114300
 H                   4.03866400    2.28424600    0.27461800
 H                   5.50551200    0.28903700    0.46355600
 H                   4.50335200   -1.98216400    0.34290400
 H                   2.06427000   -2.25141800    0.03770800
 O                  -0.63710600    1.88188400   -0.33794100
 C                  -3.20644300    0.34392600   -0.61738000
 C                  -3.96064400    0.39758400    0.68398300
 C                  -5.10106200   -0.24868200    0.90280400
 H                  -3.70174200   -0.31161900   -1.33510300
 H                  -3.12132000    1.34248800   -1.05462100
 H                  -3.52532900    1.02541400    1.45732600
 H                  -5.55098100   -0.88395000    0.14597400
 H                  -5.62689300   -0.16493100    1.84673200
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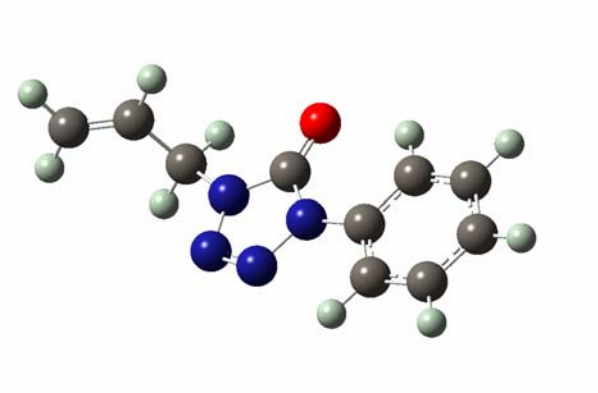

Table S20. Cartesian coordinates for the 4-allyl-1-phenyl-tetrazolone (conformer Sk).

	Coordinates (Angstroms)		
	X	Y	Z
N	0.27696600	-0.43149700	-0.15505800
N	-0.15865000	-1.72505400	-0.05117200
N	-1.41417300	-1.74789900	-0.22933600
N	-1.84297700	-0.48410500	-0.45884100
C	-0.79705000	0.42247700	-0.41888900
C	1.65718900	-0.11373600	-0.00338100
C	2.09020300	1.20983900	-0.12198800
C	3.44598000	1.49372200	0.02995200
C	4.36310300	0.48067400	0.29613800
C	3.91580800	-0.83497700	0.41191100
C	2.56744500	-1.14123300	0.26401900
H	1.37778200	1.99508900	-0.32812100
H	3.78084900	2.52051300	-0.06235900
H	5.41541100	0.71198800	0.41249000
H	4.61912200	-1.63337600	0.61903100
H	2.21794700	-2.16020700	0.35301000
O	-0.83339400	1.62576700	-0.58456500
C	-3.25449500	-0.16318700	-0.65540800
C	-4.00768800	-0.03666200	0.64266700
C	-4.64252100	1.06789400	1.02118100
H	-3.67363400	-0.95809300	-1.27752400
H	-3.28205800	0.77222800	-1.21617100
H	-4.01869700	-0.92291600	1.27217000
H	-4.63554500	1.96637300	0.41211000
H	-5.19003600	1.11328600	1.95551800

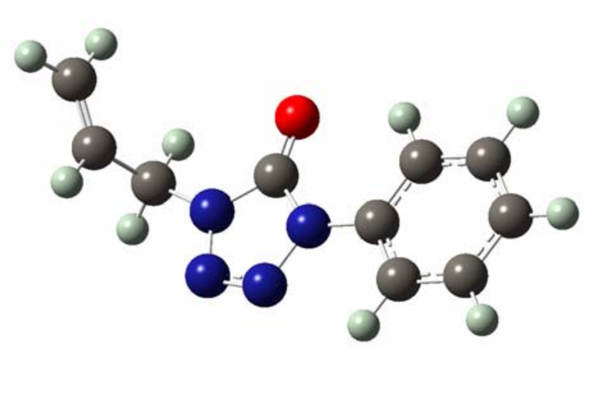

Table S21. Cartesian coordinates for the 4-allyl-1-phenyl-tetrazolone (conformer Syn).

	Coordinates (Angstroms)		
	X	Y	Z
N	0.19178700	-0.32299100	-0.23570100
N	-0.33155200	-1.58713400	-0.29072000
N	-1.58299300	-1.50449500	-0.47435700
N	-1.92498800	-0.19405200	-0.54500200
C	-0.81758600	0.62737800	-0.40588600
C	1.58872100	-0.12129100	-0.04233800
C	2.10675100	1.17414800	0.04207100
C	3.47659500	1.34297100	0.23412600
C	4.32417200	0.24375900	0.34194700
C	3.79232200	-1.04244500	0.25584300
C	2.42857300	-1.23443500	0.06371900
H	1.44835600	2.02623000	-0.04301500
H	3.87757200	2.34794700	0.29898400
H	5.38809000	0.38591800	0.49122900
H	4.44109400	-1.90691600	0.33805200
H	2.01354600	-2.23027800	-0.00305200
O	-0.76879300	1.84068300	-0.43861000
C	-3.29079400	0.24408100	-0.76977100
C	-4.15539200	0.29336200	0.46353400
C	-3.79794300	-0.05424800	1.69403800
H	-3.73239800	-0.41996000	-1.51878600
H	-3.21872900	1.24048100	-1.21583900
H	-5.16270000	0.65656500	0.27316500
H	-2.80634900	-0.42546800	1.92636000
H	-4.49643600	0.02104300	2.51855400