Table S1. DFT(B3LYP)/6-311++G(d,p) calculated frequencies [a] and intensities for **Sk'**, **Sk** and **Syn** conformers of 1-phenyl-4-allyl-tetrazolone.

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 1-phenyl-4-allyl-tetrazolone. The calculated frequencies were scaled by a factor of 0.978.

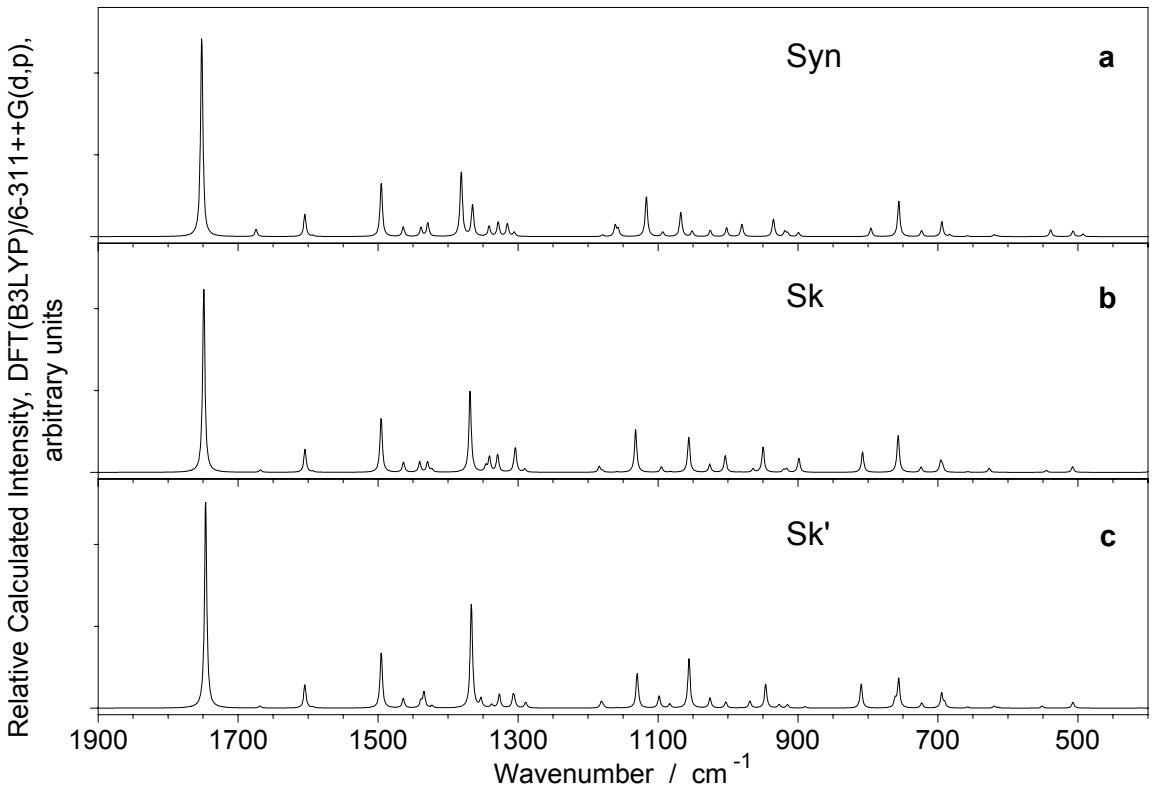

Table S2. Cartesian coordinates for the 1-phenyl-4-allyl-tetrazolone (conformer Sk').

	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

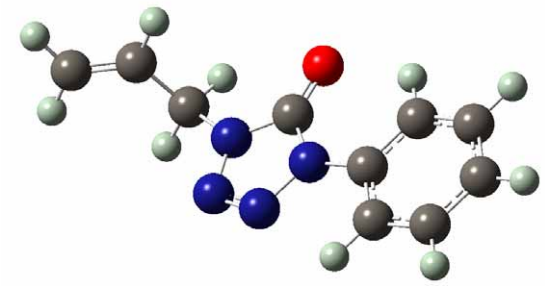

Table S3. Cartesian coordinates for the 1-phenyl-4-allyl-tetrazolone (conformer Sk).

	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

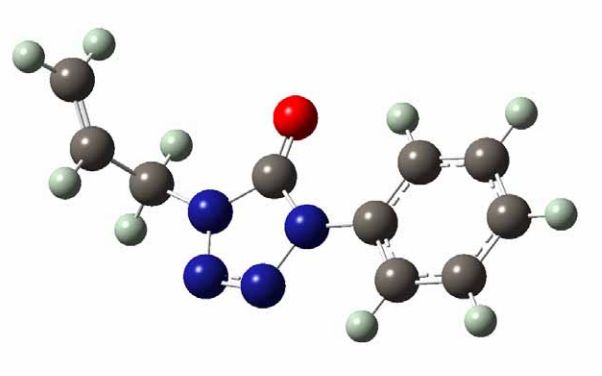

Table S4. Cartesian coordinates for the 1-phenyl-4-allyl-tetrazolone (conformer Syn).

	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