10.1071/CH10340_AC
CSIRO 2010
Aust. J. Chemistry 2010, 63(12), 1694-1702

Accessory Publication

Thioketenes and Iminopropadienethiones RN=C=C=C=S from Isoxazolones

David Kvaskoff[A] and *Curt Wentrup*[A,B]

[A]School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, Qld 4072, Australia.

[B]Corresponding author. Email: wentrup@uq.edu.au

Contents:

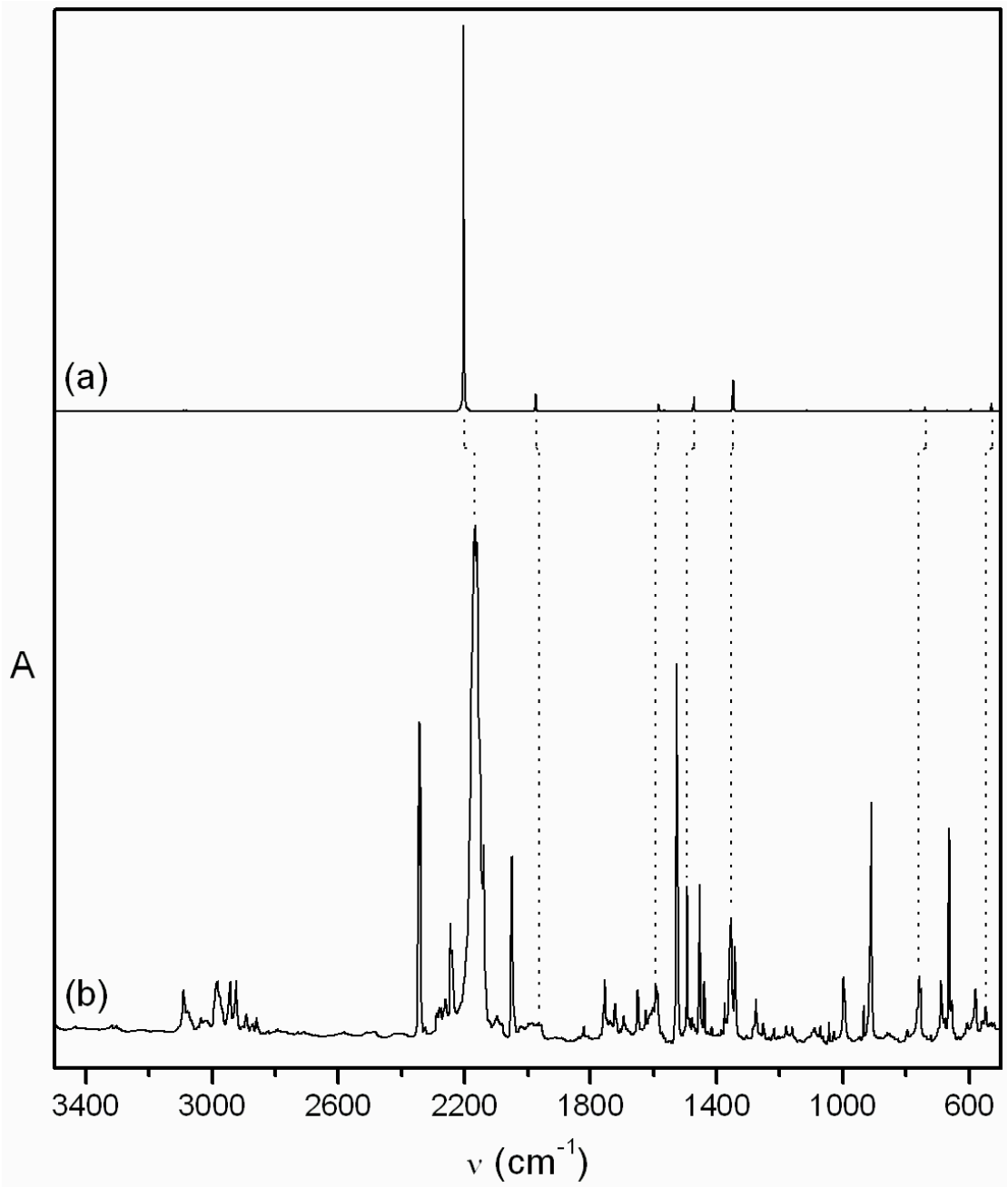


Figure S1. (a) Calculated spectrum (B3LYP/6-31G**; wavenumbers scaled by a factor 0.9613). (b) Ar matrix IR spectrum of the products of FVT of **6a** at 900 ^{o}C. The peaks due to PhNCCCS **8a** are at 2167 vs, ca 2000 vw 1593 w, 1493 m, 1355 m, 753 w and 546 vw cm^{-1}. Bands (cm^{-1}) due to CO_2 (2344, 663), CS_2 (2178, 1528), OCS (2050), propene (3091, 3036, 2983, 2942, 2923, 2859, 1650, 1454, 1439, 1374, 998, 909, 579), and CS_2 (1528 cm^{-1}) are also present. See also ref. 4.

Table S1. Calculated[†] and experimental IR bands of iminopropadienethiones **8a-e** and thioketenes **7a-e** and **10d-e**

	Calculated Frequency[†] (cm^{-1})	Intensity ($km.mol^{-1}$)	Mode	Experimental Frequency (cm^{-1})
8a	2203	4720	$\nu_{N=C=C=C=S}$	2167
8b	2199	4568	$\nu_{N=C=C=C=S}$	2163
8c	2194	5567	$\nu_{N=C=C=C=S}$	2167
8d	2218	3967	$\nu_{N=C=C=C=S}$	2175
8e	2227	4312	$\nu_{N=C=C=C=S}$	2201
7a	1733 1821	874 480	$\nu_{C=C=S}$ $\nu_{C=O}$	1727 1810
7b	1732 1819	863 512	$\nu_{C=C=S}$ $\nu_{C=O}$	1729 1819
7c	1733 1824	870 510	$\nu_{C=C=S}$ $\nu_{C=O}$	1733 1817
7d	1737 1820	955 387	$\nu_{C=C=S}$ $\nu_{C=O}$	1736 1811
7e	1736 1819	918 398	$\nu_{C=C=S}$ $\nu_{C=O}$	1736 1819
10d	1750 2236	496 50	$\nu_{C=C=S}$ $\nu_{C\equiv N}$	1752 2223
10e	1749 2234	344 48	$\nu_{C=C=S}$ $\nu_{C\equiv N}$	1757 2236

[†] B3LYP/6-31G** vibrational frequencies scaled by 0.9613

Peak listings of compounds observed in the FVT/matrix-IR of compounds 6

FVT/IR of 4-[bis((1-methylethyl)thio)methylene]-3-phenyl-isoxazol-5(4H)-one ***6a***

Compound **6a** was sublimed at 80°C (10^{-5} hPa) using the external quartz oven. The IR spectra showed the following absorptions, in each case normalized to the strongest peak in the spectrum (absorbance = 1):

FVT 500°C, IR (Ar, 8 K/cm^{-1})(relative intensity):

Starting material, **6a**: 2979 (0.21), 2937 (0.14), 2872 (0.13), 1738 (0.59), 1505 (**1.0**), 1454 (0.21), 1370 (0.36), 1244 (0.09), 1155 (0.27), 975 (0.25), 875 (0.36), 760 (0.43), 697 (0.23), 651 (0.18).

Carbon dioxide: 2345 (0.23), 2340 (0.32), 663 (0.07).

Carbon disulfide: 1528 (0.57).

FVT 600°C, IR (Ar, 10 K/cm^{-1}) (relative intensity):

Thioketene, **7a**: 1806 (0.46), 1728 (0.92), 1478 (0.08), 1375 (0.28), 1160 (0.12), 1126 (0.08), 940 (0.09), 879 (0.21), 740 (0.07), 693 (0.12), 635 (0.06).

N-(phenylimino)propa-1,2-diene-1-thione, **8a**: 2173/2166/2151 (0.29), 1991 (0.03), 1594 (0.11), 1498 (0.18), 1356 (0.12), 1275 (0.13), 753 (0.07).

Benzonitrile: 2243 (0.06), 2237 (0.12), 1494 (0.20), 760 (0.17), 690 (0.12), 548 (0.05).

Carbon dioxide: 2340 (0.73), 663 (0.32).

Carbon disulfide: 1528 (**1.0**).

Carbon monoxide: 2138 (0.16).

Carbon oxysulfide, OCS : 2050 (0.30).

Compound absorbing at 2024 (0.13), probably *N*-phenylketenimine.

Propene: 3086 (0.13), 2984 (0.23), 2969 (0.23), 2946 (0.16), 2934 (0.19), 2859 (0.07), 1650 (0.17), 1454 (0.56), 1438 (0.21), 1415 (0.09), 1370 (0.21), 1222 (0.05), 1044 (0.09), 992 (0.23), 935 (0.21), 910 (0.55), 581 (0.12).

Unassigned: 2275 (0.06), 1891 (0.04), 1502 (0.19), 653 (0.12).

FVT 700°C, IR (Ar, 8K/cm^{-1}) (relative intensity):

N-(phenylimino)propa-1,2-diene-1-thione, **8a**: 2167 (0.74), 2152 (0.50), 1987 (0.14), 1594 (0.19), 1493 (0.29), 1355 (0.25), 1275 (0.15), 753 (0.17).

Thioketene **7a**: 1810 (0.15), 1727 (0.25), 1478 (0.14), 1370 (0.15), 1160 (0.13).

Benzonitrile: 2244 (0.18), 2238 (0.17), 1494 (0.29), 763 (0.14), 688 (0.14), 547 (0.14).

Carbon dioxide: 2344 (0.90), 2340 (**1.0**), 663 (0.32).

Carbon disulfide: 1527 (0.76).

Carbon monoxide: 2138 (0.25).

OCS : 2050 (0.32).

Cyano(phenyl)thioketene **10a**: 2259 (0.14), 1754 (0.18).

Propene: 3090 (0.18), 3035 (0.15), 2983 (0.19), 2941 (0.19), 2923 (0.18), 2859 (0.15), 1650 (0.17), 1454 (0.29), 1439 (0.18), 1415 (0.08), 1374 (0.17), 1217 (0.14), 1043 (0.14), 997 (0.17), 933 (0.15), 909 (0.38), 579 (0.17).

Unassigned: 2275 (0.14), 2096 (0.14).

FVT 800°C, IR (Ar, 9 K/cm^{-1}) (relative intensity):

N-(phenylimino)propa-1,2-diene-1-thione, **8a**: 2167 (**1.0**), 2152 (0.59), 1987 (0.07), 1593 (0.12), 1493 (0.28), 1355 (0.22), 1275 (0.10), 753 (0.12).

Benzonitrile: 2244 (0.17), 2238 (0.12), 1494 (0.28), 763 (0.07), 688 (0.08), 547 (0.08).

Carbon dioxide: 2344 (0.82), 663 (0.31).

Carbon disulfide: 1527 (0.59).

Carbon monoxide: 2143 (0.26), 2138 (0.24).

OCS : 2050 (0.31).

Propene: 3091 (0.11), 3036 (0.07), 2983 (0.12), 2942 (0.12), 2923 (0.12), 2859 (0.08), 1650 (0.11), 1454 (0.24), 1439 (0.12), 1374 (0.09), 1217 (0.06), 1043 (0.07), 998 (0.12), 933 (0.08), 909 (0.36), 579 (0.09).

Unassigned: 1957 (0.07) (possibly OC_3S).[1]

FVT 900°C, IR (Ar, 9 K) (relative intensity) cm^{-1}:

N-(phenylimino)propa-1,2-diene-1-thione, **8a**: 2167/2160 (**1.0**), 2152 (0.62), 1987 (0.08), 1593 (0.15), 1493 (0.33), 1355 (0.27), 1275 (0.12), 753 (0.14).

Benzonitrile: 2244 (0.26), 2238 (0.21), 1493 (0.33), 757 (0.17), 688 (0.16), 547 (0.11).

Carbon dioxide: 2343 (0.64), 2339 (0.51), 663 (0.44).

Carbon disulfide: 1526 (0.74).

Carbon monoxide: 2143 (0.35), 2138 (0.41).

OCS: 2050 (0.39).

Cyano(phenyl)thioketene **10a**: 2260 (0.12), 1754 (0.16).

Propene: 3090 (0.14), 3035 (0.09), 2983 (0.16), 2942 (0.16), 2923 (0.16), 2859 (0.09), 1650 (0.14), 1454 (0.34), 1439 (0.15), 1374 (0.12), 1217 (0.07), 1043 (0.08), 997 (0.16), 933 (0.11), 909 (0.49), 579 (0.14).

Unassigned: 1957 (0.07) (possibly OC_3S).[1]

FVT 1000°C, IR (Ar, 10 K) (relative intensity) cm^{-1}:

N-(phenylimino)propa-1,2-diene-1-thione, **8a**: 2167 (0.45), 2152 (0.42), 1982 (0.04), 1593 (0.18), 1493 (0.23), 1355 (0.25), 1275 (0.11), 753 (0.09).

Benzonitrile: 2244 (0.46), 2238 (0.30), 1493 (0.23), 757 (0.24), 688 (0.24), 547 (0.13).

Carbon dioxide: 2347 (0.66), 2339 (0.37), 663 (0.69).

Carbon disulfide: 1525 (0.88).

Carbon monoxide: 2138 (**1.0**).

OCS : 2050 (0.56).

Cyano(phenyl)thioketene **10a**: 2260 (0.22), 1754 (0.24).

Propene: 3090 (0.19), 3035 (0.10), 2983 (0.19), 2942 (0.21), 2923 (0.20), 2859 (0.09), 1650 (0.20), 1454 (0.49), 1439 (0.21), 1415 (0.09), 1374 (0.12), 1217 (0.06), 1043 (0.09), 998 (0.22), 933 (0.12), 909 (0.77), 579 (0.16).

Unassignd : 1957 (0.05) (possibly OC_3S).[1]

FVT/IR of 4-[bis((1-methylethyl)thio)methylene]-3-(4-methoxyphenyl)-isoxazol-5(4H)-one ***6b***

Compound **6b** was sublimed at 95-100°C (10^{-5} hPa) using the external quartz oven. The infrared spectra showed the following absorptions:

FVT 500°C, IR (Ar, 8 K/cm^{-1}) (relative intensity):

Starting material, **6b**: 2977 (0.16), 2938 (0.10), 2872 (0.05), 2845 (0.05), 1741 (0.62), 1615 (0.38), 1504 (0.79), 1466 (0.20), 1370 (0.44), 1306 (0.16), 1256 (**1.0**), 1177 (0.33), 1157 (0.23), 1107 (0.16), 1045 (0.24), 978 (0.19), 877 (0.40), 834 (0.24), 777 (0.13), 728 (0.02), 597 (0.19)

Carbon dioxide: 2345 (0.64), 2340 (0.73).

Carbon disulfide: 1528 (0.46).

FVT 600°C, IR (Ar, 8 K/cm^{-1}) (relative intensity):

Thioketene **7b**: 1819 (0.07), 1729 (0.15), 1615 (0.14), 1515 (0.18), 1507 (0.17), 1469 (0.08), 1374 (0.08), 1305 (0.08), 1261 (0.23), 1177 (0.09), 877 (0.08), 834 (0.07).

N-(4-methoxyphenylimino)propa-1,2-diene-1-thione, **8b**: 2178 (0.11), 2163 (0.16), 2151 (0.16).

Carbon dioxide: 2340 (0.79), 663 (0.17).

Carbon disulfide: 1528 (**1.0**).

OCS: 2050 (0.16).

Propene: 3090 (0.05), 2982 (0.09), 2942 (0.08), 2923 (0.08), 2859 (0.03), 1651 (0.08), 1454 (0.18), 1439 (0.08), 1044 (0.10), 997 (0.06), 933 (0.04), 909 (0.26), 578 (0.05).

Unassigned: 1957 (0.01) (possibly OC_3S).[1]

FVT 700°C, IR (Ar, 8 K/cm^{-1}) (relative intensity):

N-(4-methoxyphenylimino)propa-1,2-diene-1-thione, **8b**: 2163 (**1.0**), 1993 (0.04), 1507 (0.49), 1356 (0.10), 1254 (0.33), 834 (0.09), 547 (0.02).

Carbon dioxide: 2343 (0.75), 663 (0.31).

Carbon disulfide: 1526 (0.65).

OCS: 2050 (0.25).

4-Methoxybenzonitrile: 2244 (0.11), 2238 (0.11), 1612 (0.13), 1304 (0.12), 1265 (0.10), 1173 (0.11).

Propene: 3090 (0.07), 2983 (0.09), 2942 (0.10), 2923 (0.10), 2859 (0.04), 1650 (0.12), 1454 (0.22), 1439 (0.11), 1044 (0.12), 997 (0.07), 933 (0.04), 909 (0.35), 578 (0.07).

Unassigned: 1957 (0.02) (possibly OC_3S).[1]

FVT 800°C, IR (Ar, 8 K/cm^{-1}) (relative intensity):

N-(4-methoxyphenylimino)propa-1,2-diene-1-thione, **8b**: 2165 (0.84), 1982 (0.05), 1509 (0.27), 1356 (0.14), 1263 (0.19), 836 (0.10).

Carbon dioxide: 2343 (**1.0**), 663 (0.44).

Carbon disulfide: 1527 (0.97).

Carbon monoxide: 2138 (0.52).

OCS: 2050 (0.40).

Cyano(4-methoxyphenyl)thioketene **10b**: 2260 (0.06), 1755 (0.14).

4-Methoxybenzonitrile: 2244 (0.20), 2238 (0.17), 1615 (0.15), 1305 (0.08), 1263 (0.19), 1176 (0.11).

Propene: 3090 (0.11), 2983 (0.14), 2942 (0.14), 2923 (0.14), 2859 (0.07), 1651 (0.19), 1454 (0.30), 1439 (0.17), 1044 (0.08), 997 (0.13), 933 (0.08), 909 (0.48), 578 (0.10).

Unassigned: 1957 (0.04) (possibly OC_3S).[1]

There was not much further change at 900°C. The intensities of peaks due to **2b** decreased ca. fourfold at 1000°C.

*FVT/IR of 4-[bis((1-methylethyl)thio)methylene]-3-(4-cyanophenyl)-isoxazol-5(4H)-one **6c**.*

Compound **6c** was sublimed at 90-95°C (10^{-5} hPa) using the external quartz oven. The infrared spectra showed the following absorptions:

FVT 200 and 400°C, IR (Ar, 20 K/cm^{-1}) (relative intensity):

Starting material, **6c**: 2979 (0.25), 2938 (0.19), 2874 (0.15), 2238 (0.22), 1749 (0.86), 1501 (**1.0**), 1455 (0.24), 1370 (0.40), 1237 (0.17), 1156 (0.33), 1103 (0.27), 1055 (0.22), 977

(0.30), 890 (0.45), 875 (0.32), 862 (0.31), 843 (0.33), 776 (0.23), 732 (0.11), 562 (0.26), 537 (0.15), 419 (0.24).

FVT 520°C, IR (Ar, 20 K) (relative intensity) cm^{-1}:

Starting material, **6c**: 2873 (0.11), 2239 (0.16), 1749 (0.53), 1502 (0.53), 1370 (0.28), 1244 (0.07), 1154 (0.21), 1103 (0.12), 1054 (0.09), 978 (0.14), 891 (0.29), 877 (0.26), 863 (0.13), 843 (0.27), 777 (0.12), 562 (0.14).

Thioketene **7c**: 2241 (0.11), 1817 (0.24), 1733 (0.88), 1478 (0.07), 1374 (0.23), 1124 (0.11), 1023 (0.18).

N-(4-Cyanophenylimino)propa-1,2-diene-1-thione, **8c**: 2178 (0.08), 2168 (0.13), 2157 (0.10).

Carbon dioxide: 2345 (0.43), 2340 (0.36), 663 (0.11).

Carbon disulfide: 1528 (**1.0**).

Propene: 3091 (0.12), 3036 (0.08), 2984 (0.23), 2941 (0.21), 2923 (0.16), 2859 (0.08), 1651 (0.11), 1454 (0.34), 1439 (0.12), 1043 (0.07), 998 (0.12), 933 (0.07), 909 (0.60), 578 (0.09).

FVT 570°C, IR (Ar, 20 K) (relative intensity) cm^{-1}:

Thioketene **7c**: 2239 (0.09), 1817 (0.25), 1733 (0.83), 1478 (0.06), 1374 (0.11), 1119 (0.08), 1022 (0.16), 893 (0.13), 847 (0.11).

N-(4-cyanophenylimino)propa-1,2-diene-1-thione, **8c**: 2245 (0.10), 2178 (0.11), 2168 (0.41), 2158 (0.27), 1604 (0.06), 1506 (0.14), 1362 (0.13), 1275 (0.07), 1243 (0.07), 842 (0.11).

Carbon dioxide: 2345 (0.59), 2340 (0.52), 663 (0.17).

Carbon disulfide: 1528 (**1.0**).

Carbon monoxide: 2143 (0.09), 2138 (0.10).

Propene: 3091 (0.11), 3037 (0.07), 2984 (0.13), 2941 (0.13), 2923 (0.12), 2859 (0.06), 1650 (0.10), 1453 (0.25), 1439 (0.11), 998 (0.13), 933 (0.07), 909 (0.45), 578 (0.09).

FVT 670°C, IR (Ar, 20 K) (relative intensity) cm^{-1}:

N-(4-cyanophenylimino)propa-1,2-diene-1-thione, **8c**: 2244 (0.08), 2167 (**1.0**), 2159 (0.60), 1982 (0.01), 1604 (0.09), 1506 (0.17), 1362 (0.20), 1275 (0.03), 1253 (0.02), 840 (0.05), 500 (0.02).

Thioketene **7c**: 2239 (0.04), 1817 (0.03), 1733 (0.12), 1374 (0.03), 1119 (0.01), 1022 (0.02), 893 (0.01).

Carbon dioxide: 2344 (0.39), 2340 (0.45), 663 (0.11).

Carbon disulfide: 1528 (0.30).

OSC: 2050 (0.11).

Propene: 3091 (0.04), 3036 (0.02), 2984 (0.05), 2942 (0.05), 2923 (0.04), 2859 (0.02), 1650 (0.04), 1453 (0.10), 1439 (0.04), 998 (0.04), 933 (0.02), 909 (0.18), 578 (0.03).

Unassigned: 1957 (0.01) (possibly OC_3S).[1]

FVT 820°C, IR (Ar, 20 K) (relative intensity) cm^{-1}:

N-(4-cyanophenylimino)propa-1,2-diene-1-thione, **8c**: 2245 (0.09), 2167 (**1.0**), 1605 (0.09), 1506 (0.17), 1362 (0.21), 1275 (0.02), 1253 (0.02), 839 (0.05), 500 (0.03).

Carbon dioxide: 2345 (0.38), 2340 (0.39), 663 (0.11).

Carbon disulfide: 1528 (0.28).

OCS: 2050 (0.11).

Propene: 3091 (0.03), 2984 (0.04), 2941 (0.04), 2923 (0.04), 1650 (0.03), 1453 (0.09), 998 (0.05), 909 (0.18), 579 (0.03).

Unassigned: 1957 (0.01) (possibly OC_3S).[1]

FVT/IR of 4-[bis((1-methylethyl)thio)methylene]-3-(isopropyl)-isoxazol-5(4H)-one ***6d***

Compound **6d** was sublimed at 60°C (10^{-5} hPa) using the internal quartz oven. The infrared spectra showed the following absorptions:

FVT 400°C, IR (Ar, 20 K/cm^{-1}) (relative intensity):

Starting material, **6d**: 2979 (0.69), 2938 (0.34), 2876 (0.18), 2805 (0.07), 1746 (0.70), 1507 (0.73), 1465 (0.34), 1370 (0.30), 1236 (0.17), 1171 (0.14), 1145 (0.34), 1104 (0.30), 1055 (0.26), 916 (0.20), 903 (0.38), 861 (0.30), 780 (0.06), 742 (0.03), 595 (0.04).

Thioketene **7d**: 1811 (0.22), 1733 (**1.0**), 1558 (0.24), 1472 (0.27), 1387 (0.23), 1370 (0.30), 1280 (0.12), 1157 (0.31), 861 (0.03).

N-(isopropyl)propa-1,2-diene-1-thione, **8d**: 2170/2164 (0.02).

Carbon dioxide: 2340 (0.19).

FVT 600°C, IR (Ar, 20 K/cm^{-1}) (relative intensity):

Thioketene **7d**: 2879 (0.06), 2804 (0.05), 1811 (0.10), 1733 (0.21), 1559 (0.05), 1472 (0.08), 1386 (0.08), 1370 (0.08), 1275 (0.04), 1156 (0.05), 862 (0.06).

N-(isopropyl)iminopropa-1,2-diene-1-thione, **8d**: 2170 (0.07).

Carbon dioxide: 2340 (**1.0**), 663 (0.13).

Carbon disulfide: 1528 (0.39).

Carbon monoxide: 2139 (0.08).

Propene: 3090 (0.03), 2982 (0.18), 2941 (0.09), 1650 (0.05), 1454 (0.10), 909 (0.07), 579 (0.02).

FVT 700°C, IR (Ar, 20 K/cm^{-1}) (relative intensity):

N-(isopropyl)iminopropa-1,2-diene-1-thione, **8d**: 2175 (0.13), 2160 (0.16).

Carbon dioxide: 2342 (**1.0**), 2336 (**1.0**), 663 (0.25).

Carbon disulfide: 1528 (**1.0**).

Carbon monoxide: 2138 (0.41).

OCS: 2050 (0.01).

Cyano(isopropyl)thioketene **10d**: 2223 (0.26), 1752 (0.55).

Propene: 3080 (0.12), 2977 (0.40), 2941 (0.26), 1645 (0.24), 1453 (0.39), 1438 (0.21), 1373 (0.18), 1044 (0.11), 996 (0.20), 935 (0.15), 913 (0.35), 587 (0.11).

Unassigned: 2274 (0.11), 2041 (0.26; possibly *N*-isopropylketenimine), 1713 (0.15).

*FVT/IR of 4-[bis((1-methylethyl)thio)methylene]-3-(neopentyl)-isoxazol-5(4H)-one **6e***

Compound **6e** was sublimed at 70°C (10^{-5} hPa) using the internal quartz oven. The infrared spectra (BaF_2 optical window) showed the following absorptions:

FVT 400°C, IR (Ar, 15 K/cm^{-1}) (relative intensity):

Starting material, **6e**: 2972 (0.62), 2937 (0.47), 2873 (0.26), 1739 (**1.0**), 1519 (0.76), 1478 (0.25), 1467 (0.32), 1446 (0.21), 1370 (0.42), 1236 (0.19), 1173 (0.15), 1156 (0.25), 1133 (0.27), 1055 (0.21), 1042 (0.40), 1026 (0.16), 935 (0.23), 924 (0.42), 900 (0.20), 871 (0.31), 788 (0.24).

Carbon dioxide: 2345 (0.20), 2340 (0.18).

OCS: 2050 (0.05).

FVT 600°C, IR (Ar, 15 K/cm^{-1}) (relative intensity):

Thioketene **7e**: 1819 (0.05), 1736 (0.20), 1560 (0.06), 1274 (0.08), 889 (0.06).

N-(Neopentyl)iminopropa-1,2-diene-1-thione, **8e**: 2202 (0.26), 2012 (0.07).

3,3-Dimethylbutyronitrile: 2361 (0.13).

Carbon dioxide: 2340 (**1.0**).

Carbon disulfide: 1528 (0.82).

Carbon monoxide: 2141 (0.12).

OCS: 2050 (0.09).

Propene: 3087 (0.05), 2942 (0.19), 1650 (0.09), 1454 (0.18), 1439 (0.09), 1372 (0.11), 1046 (0.05), 997 (0.08), 910 (0.21).

FVT 700°C, IR (Ar, 15 K/cm^{-1}) (relative intensity):

N-(Neopentyl)iminopropa-1,2-diene-1-thione, **8e**: 2972 (0.18), 2201 (0.39), 2012 (0.07).

Carbon dioxide: 2342 (**1.0**).

Carbon disulfide: 1528 (0.79).

Carbon monoxide: 2142 (0.14).

Cyano(neopentyl)thioketene **10e**: 2244 (0.10), 1755 (0.10).

Propene: 3089 (0.06), 2943 (0.14), 2923 (0.10), 1650 (0.07), 1454 (0.21), 1439 (0.09), 1374 (0.10), 1044 (0.05), 998 (0.09), 933 (0.05), 909 (0.30).

FVT 850°C, IR (Ar, 15 K/cm^{-1}) (relative intensity):

Carbon dioxide: 2345 (**1.0**).

Carbon disulfide: 1527 (0.91).

Carbon monoxide: 2138 (0.22).

OCS: 2050 (0.20).

Cyano(neopentyl)thioketene **10e**: 2236 (0.14), 1757 (0.26).

Propene: 2983 (0.22), 2943 (0.19), 2923 (0.15), 1650 (0.13), 1454 (0.24), 1439 (0.15), 1374 (0.14), 1044 (0.09), 997 (0.13), 934 (0.11), 910 (0.26).

Reference: 1. F. M. Nicolaisen, J. J. Christiansen, J. Mol. Struct. **1979**, *52*, 157.

Reference Spectra:

Benzonitrile IR (Ar, 15 K/cm^{-1}): 3062(w), 2241(m), 2237(m), 1494(m), 1450(w), 1288(m), 1181(w), 1041(m), 761(s), 688(s), 548(m).

Carbon disulfide IR (1% in Ar, 7 K/cm^{-1}): 1528(vs).

Dimethylamine (≥ 99.0%) IR (2% in Ar, 10 K/cm^{-1}): 3223(m), 2965(m), 2817(s), 2775(s), 1453(w), 1142(m), 1029(w), 883(m).

Hydrogen sulfide (99.6%) IR (5.5% in Ar, 10 K/cm^{-1}): 2629(w), 2581(s), 2569(s; dimer), 1180 (w). For further details, see A. J. Barnes, J. D. R. Howells, *J. Chem. Soc,. Faraday Trans 2* 1972, *68*, 729.

p-Methoxybenzonitrile IR (Ar, 22 K/cm^{-1}) (relative intensity): 2979 (0.04), 2963 (0.04), 2949 (0.05), 2926 (0.03), 2852 (0.08), 2245 (0.08), 2238 (0.27), 1615 (0.59), 1581 (0.16), 1515 (0.98), 1471 (0.19), 1445 (0.15), 1306 (0.44), 1265(1.0), 1172 (0.40), 1045 (0.35), 835 (0.42).

3-(4-Methoxyphenyl)-isoxazol-5(4H)-one IR (Ar, 7 K/cm^{-1}) (relative intensity): 1819 (1.0), 1614 (0.27), 1523 (0.25), 1429 (0.16), 1375 (0.17), 1266 (0.39), 1259 (0.34), 1177 (0.20), 1160 (0.30), 1051 (0.19), 899 (0.36), 878 (0.40), 837 (0.12), 831 (0.14).

Propene IR (Ar, 20 K/cm^{-1}): 3091(s), 3036(s), 2983(s), 2941(s), 2923(s), 2859(m), 1650(s), 1453(vs), 1439(s), 1415(m), 1373(w), 1212(m), 1043(s), 998(s), 932(m), 908(vs), 578(s) (see also A. J. Barnes, J. D. R. Howells, *J. Chem. Soc,. Faraday Trans 2* 1973, *69*, 532).

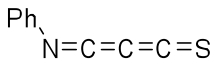
Terephthalonitrile IR (Ar, 16 K/cm^{-1}): 2244(w), 1506(m), 1412(m), 1278(m), 1022(w), 841(s), 640(w) (see also N. Akai, S. Kudoh, M. Nakata, *Chem. Phys. Lett.* 2003, *371*, 655).

Cartesian Coordinates and Energies

All geometries, energies and IR frequencies calculated at B3LYP/6-31G**, unless specified otherwise. Gaussian 03, Revision B.05.

The Onsager SCRF model was used for calculations of solvated systems. An estimate for the solvent cavity parameter a_0 was produced using the *Volume* keyword. The inclusion of diffuse functions was essential to model the charges correctly.

3-(Phenylimino)-propa-1,2-diene-1-thione *(8a)*



Point group: Cs; State = 1-A'
HF = -798.8481284 Hartree
Zero-point correction= 0.111683 (Hartree/Particle)
The Cartesian coordinates and IR spectrum have been reported previousy.[4]
Strongest calculated IR band:

37	A'	2202.5	4719.6	100

3-(4-Methoxyphenylimino)-propa-1,2-diene-1-thione *(8b)*

Point group: Cs; State = 1-A'
HF = -913.3737557 Hartree
Zero-point correction = 0.144259 (Hartree/Particle)

Cartesian coordinates and vibrational frequencies have been reported.[4]
Strongest calculated IR band:

47	A'	2198.8	4568.1	100

3-(4-Cyanophenylimino)-propa-1,2-diene-1-thione *(8c)*

Point group: Cs; State = 1-A'
HF = -891.087864 Hartree
Zero-point correction = 0.110165 (Hartree/Particle)

Atom type	Coordinates (angstroms): X	Y	Z
C	2.256397	2.529474	0.000000
C	0.968864	3.093836	0.000000
C	-0.151330	2.275006	0.000000
C	0.000000	0.879126	0.000000
C	1.287712	0.309574	0.000000
C	2.405047	1.130545	0.000000
N	-1.134267	0.090465	0.000000
C	-1.523534	-1.057056	0.000000
C	-2.055969	-2.229013	0.000000
C	-2.568617	-3.393711	0.000000

S	-3.200969	-4.833333	0.000000
H	3.399317	0.697285	0.000000
H	0.856399	4.172335	0.000000
H	-1.150013	2.696689	0.000000
H	1.395909	-0.769839	0.000000
C	3.412854	3.374668	0.000000
N	4.352174	4.061272	0.000000

Vibrational frequencies (cm^{-1}) (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A'	28.5	1.3	0
2	A"	30.2	1.0	0
3	A"	91.8	3.0	0
4	A'	119.6	2.6	0
5	A"	149.7	2.1	0
6	A'	152.5	14.3	0
7	A"	267.6	0.2	0
8	A'	281.6	2.9	0
9	A'	383.5	17.4	0
10	A"	399.2	0.0	0
11	A"	425.7	0.2	0
12	A'	453.4	30.5	1
13	A"	454.4	0.0	0
14	A'	500.6	39.7	1
15	A"	504.4	11.8	0
16	A'	535.7	0.3	0
17	A"	543.4	17.2	0
18	A'	558.3	32.8	1
19	A'	637.4	6.4	0
20	A'	698.6	35.2	1
21	A"	698.8	0.7	0
22	A"	807.9	3.1	0
23	A'	809.7	10.3	0
24	A"	824.5	45.8	1
25	A"	933.9	0.0	0
26	A"	940.2	0.0	0
27	A'	992.6	1.5	0
28	A'	1093.1	10.0	0
29	A'	1119.7	8.2	0
30	A'	1160.0	16.7	0
31	A'	1182.0	0.3	0
32	A'	1277.8	13.5	0
33	A'	1280.1	0.0	0
34	A'	1356.6	578.6	10
35	A'	1399.4	7.3	0
36	A'	1483.1	255.5	5
37	A'	1535.6	35.7	1
38	A'	1589.1	209.4	4
39	A'	1959.3	121.1	2
40	A'	2193.6	5566.5	100
41	A'	2256.2	8.5	0
42	A'	3083.7	2.6	0
43	A'	3090.4	2.3	0
44	A'	3097.6	1.2	0
45	A'	3104.1	1.3	0

3-(Isopropylimino)-propa-1,2-diene-1-thione *(8d)*

Point group: C1; State = 1-A
HF = -685.7389684 Hartree
Zero-point correction = 0.115553 (Hartree/Particle)

Atom type	Coordinates (angstroms): X	Y	Z
C	2.688231	0.000251	-0.318487
N	1.324504	-0.002418	-0.811760
C	0.164989	-0.002293	-0.496806
C	-1.113986	-0.002796	-0.280316
C	-2.359616	-0.000854	-0.049926
S	-3.914067	0.001068	0.237681
C	2.959950	1.279515	0.483995
H	2.746969	2.168734	-0.114553
H	2.337870	1.308701	1.383972
H	4.010743	1.309718	0.787809
C	2.963411	-1.275976	0.487662
H	2.753257	-2.167481	-0.108478
H	4.014177	-1.302247	0.791943
H	2.341081	-1.304479	1.387485
H	3.331574	-0.000187	-1.205487

Vibrational frequencies (cm^{-1}) (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	21.1	0.6	0
2	A	51.1	6.1	0
3	A	111.8	0.1	0
4	A	133.2	13.1	0
5	A	229.1	0.0	0
6	A	258.3	1.0	0
7	A	329.9	2.8	0
8	A	385.0	3.1	0
9	A	424.9	1.3	0
10	A	430.0	0.8	0
11	A	464.3	5.3	0
12	A	506.2	19.0	0
13	A	511.9	62.6	2
14	A	541.7	56.5	1
15	A	780.5	8.6	0
16	A	876.7	16.1	0
17	A	905.9	0.7	0
18	A	920.0	0.2	0
19	A	1093.9	64.3	2
20	A	1095.7	6.7	0
21	A	1145.0	5.7	0
22	A	1283.5	491.3	12
23	A	1306.9	3.6	0
24	A	1347.0	11.4	0
25	A	1358.2	5.1	0
26	A	1377.9	9.6	0
27	A	1439.2	2.4	0
28	A	1442.0	0.0	0
29	A	1450.6	9.9	0
30	A	1463.2	0.7	0
31	A	1987.9	161.9	4
32	A	2217.8	3967.4	100
33	A	2933.4	12.8	0

34	A	2936.3	21.6	1
35	A	2943.2	20.0	1
36	A	3005.9	0.0	0
37	A	3012.6	56.9	1
38	A	3018.0	14.9	0
39	A	3019.4	20.3	1

3-(Neopentylimino)-propa-1,2-diene-1-thione ***(8e)***

Point group: C1; State = 1-A
HF = -764.3699803 Hartree
Zero-point correction = 0.171619 (Hartree/Particle)

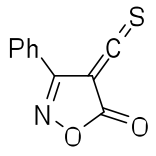
Atom type	Coordinates (angstroms): X	Y	Z
C	-1.542519	-0.857242	-0.002219
N	-0.318277	-0.095994	-0.001531
C	0.881232	-0.137855	0.000411
C	2.175888	-0.067999	0.001882
C	3.441799	-0.013525	0.000593
S	5.020684	0.053432	-0.000517
H	-1.547309	-1.503947	-0.889730
H	-1.546425	-1.507327	0.882821
C	-2.802991	0.036155	0.000038
C	-4.025955	-0.899374	-0.001084
H	-4.038686	-1.545336	0.884151
H	-4.952135	-0.316411	0.000560
H	-4.039664	-1.541914	-0.888790
C	-2.817414	0.919979	-1.259686
H	-1.939804	1.572565	-1.293648
H	-2.823056	0.312430	-2.171838
H	-3.710389	1.553150	-1.274440
C	-2.816186	0.915362	1.262993
H	-3.709135	1.548489	1.280911
H	-2.820957	0.304512	2.172941
H	-1.938546	1.567833	1.298483

Vibrational frequencies (cm^{-1}) (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	10.4	0.0	0
2	A	35.2	3.3	0
3	A	101.6	0.5	0
4	A	125.7	5.5	0
5	A	139.1	2.3	0
6	A	208.1	0.2	0
7	A	212.7	37.0	1
8	A	256.3	0.1	0
9	A	257.2	0.3	0
10	A	285.2	0.1	0
11	A	319.3	0.5	0
12	A	376.6	2.3	0
13	A	397.1	0.2	0
14	A	425.9	0.1	0
15	A	442.3	35.7	1
16	A	448.3	0.3	0
17	A	504.3	15.6	0
18	A	514.7	53.0	1

19	A	610.7	2.2	0
20	A	718.5	12.5	0
21	A	862.5	52.5	1
22	A	869.0	0.0	0
23	A	909.7	1.4	0
24	A	913.9	0.7	0
25	A	932.4	0.9	0
26	A	932.5	0.2	0
27	A	1015.1	9.2	0
28	A	1031.3	0.2	0
29	A	1164.1	0.4	0
30	A	1195.0	64.9	2
31	A	1232.2	42.8	1
32	A	1271.2	2.4	0
33	A	1303.5	517.9	12
34	A	1323.0	107.9	3
35	A	1361.9	7.8	0
36	A	1363.3	5.7	0
37	A	1392.3	54.3	1
38	A	1426.9	32.8	1
39	A	1437.1	0.0	0
40	A	1443.3	0.1	0
41	A	1444.1	0.0	0
42	A	1463.0	9.8	0
43	A	1463.3	5.1	0
44	A	1475.2	20.1	0
45	A	1992.5	209.9	5
46	A	2226.5	4311.7	100
47	A	2901.2	28.5	1
48	A	2918.6	29.4	1
49	A	2921.7	32.6	1
50	A	2928.1	9.8	0
51	A	2945.5	14.7	0
52	A	2983.6	16.4	0
53	A	2989.6	33.0	1
54	A	2990.4	17.7	0
55	A	2997.6	41.3	1
56	A	3000.8	1.3	0
57	A	3005.1	74.7	2

3-Phenyl-4-thiocarbonylisoxazol-5-(4*H*)-one *(7a)*



Point group: C1; State = 1-A
HF = -987.3933014 Hartree
Zero-point correction= 0.127314 (Hartree/Particle)

Atom type	Coordinates (angstroms): X	Y	Z
N	0.369132	-2.135856	0.133439
O	1.762845	-2.320522	0.128023
C	2.431847	-1.108118	0.082450
C	1.344491	-0.085721	0.037737
C	0.107903	-0.863371	0.079297

C	-1.280121	-0.375697	0.050119
O	3.628451	-1.015987	0.077874
C	1.573565	1.209626	-0.103027
S	1.939591	2.704772	-0.273866
C	-1.611305	0.901469	0.524538
C	-2.934608	1.339240	0.501342
C	-3.939247	0.506531	0.007752
C	-3.616412	-0.769735	-0.460846
C	-2.296993	-1.210941	-0.442627
H	-0.842093	1.546237	0.936836
H	-3.179964	2.328587	0.874988
H	-4.394573	-1.420469	-0.847843
H	-2.036629	-2.196983	-0.811275
H	-4.969203	0.849644	-0.012508

Vibrational frequencies (cm^{-1}) (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	32.7	0.3	0
2	A	65.7	0.3	0
3	A	75.7	0.1	0
4	A	118.3	0.7	0
5	A	135.9	1.3	0
6	A	210.2	2.9	0
7	A	287.8	0.3	0
8	A	303.2	2.7	0
9	A	343.6	0.7	0
10	A	398.4	0.0	0
11	A	428.3	0.2	0
12	A	445.8	0.4	0
13	A	471.8	1.7	0
14	A	512.1	2.3	0
15	A	599.7	1.2	0
16	A	609.6	5.5	1
17	A	616.9	10.0	1
18	A	650.0	21.6	2
19	A	680.0	23.4	3
20	A	711.0	31.4	4
21	A	733.7	5.4	1
22	A	754.4	17.3	2
23	A	826.7	1.5	0
24	A	874.4	115.0	13
25	A	902.0	5.2	1
26	A	914.2	48.0	5
27	A	943.1	0.2	0
28	A	968.4	0.1	0
29	A	977.5	2.7	0
30	A	1000.0	148.5	17
31	A	1014.6	15.4	2
32	A	1070.6	3.7	0
33	A	1078.9	28.2	3
34	A	1144.7	0.1	0
35	A	1157.0	14.3	2
36	A	1164.7	4.4	1
37	A	1286.0	5.0	1
38	A	1313.4	0.9	0
39	A	1336.8	114.7	13
40	A	1429.3	11.7	1
41	A	1480.5	12.2	1
42	A	1524.9	45.6	5
43	A	1575.9	3.7	0

44	A	1595.9	1.7	0
45	A	1732.6	874.3	100
46	A	1820.6	479.5	55
47	A	3063.7	0.6	0
48	A	3072.5	5.5	1
49	A	3081.0	24.1	3
50	A	3089.0	10.4	1
51	A	3097.7	3.5	0

3-(4-Methoxyphenyl)-4-thiocarbonylisoxazol-5-(4*H*)-one *(7b)*

Point group: C1; State = 1-A
HF = -1101.9200431 Hartree
Zero-point correction= 0.159862 (Hartree/Particle)

Atom type	Coordinates (angstroms): X	Y	Z
N	-1.270135	-2.149150	-0.147489
O	-2.674173	-2.259224	-0.104070
C	-3.275376	-1.015027	-0.044963
C	-2.134903	-0.050378	-0.028456
C	-0.940306	-0.891386	-0.099288
C	0.466640	-0.474330	-0.097487
O	-4.465266	-0.857835	-0.011267
C	-2.294325	1.254212	0.116870
S	-2.579746	2.766566	0.296566
C	0.862361	0.792713	-0.560216
C	2.198169	1.162784	-0.565784
C	3.179712	0.269421	-0.108942
C	2.800401	-1.000627	0.349711
C	1.456134	-1.360371	0.352839
H	0.123558	1.488778	-0.943603
H	2.510940	2.136645	-0.926276
H	3.538005	-1.706536	0.711311
H	1.160613	-2.339465	0.713843
O	4.458166	0.727609	-0.148628
C	5.502037	-0.131985	0.292176
H	6.426130	0.433695	0.169737
H	5.380904	-0.403264	1.347973
H	5.553644	-1.045403	-0.312664

Vibrational frequencies (cm^{-1}) (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	29.7	1.1	0
2	A	48.7	0.4	0
3	A	66.0	0.8	0
4	A	83.6	1.1	0
5	A	113.6	3.1	0
6	A	118.7	3.1	0
7	A	179.5	0.7	0
8	A	213.7	1.1	0
9	A	226.2	0.2	0
10	A	265.2	2.9	0
11	A	276.6	1.2	0
12	A	326.5	3.2	0
13	A	378.8	1.0	0

14	A	407.6	0.2	0
15	A	431.3	0.1	0
16	A	449.5	0.7	0
17	A	456.4	0.2	0
18	A	500.4	2.7	0
19	A	525.0	5.9	1
20	A	584.6	49.3	6
21	A	597.7	1.3	0
22	A	611.9	6.5	1
23	A	630.3	3.2	0
24	A	698.9	3.5	0
25	A	717.4	19.3	2
26	A	727.0	8.2	1
27	A	784.6	11.7	1
28	A	797.1	1.7	0
29	A	817.0	44.4	5
30	A	874.3	139.1	16
31	A	913.1	54.8	6
32	A	922.9	3.1	0
33	A	933.1	1.0	0
34	A	985.7	7.5	1
35	A	1002.3	167.5	19
36	A	1028.5	50.8	6
37	A	1078.8	30.3	4
38	A	1100.8	5.7	1
39	A	1131.4	0.8	0
40	A	1155.2	48.7	6
41	A	1159.9	36.8	4
42	A	1163.8	13.4	2
43	A	1257.8	322.9	37
44	A	1283.6	1.9	0
45	A	1299.4	14.3	2
46	A	1340.9	263.6	31
47	A	1404.5	6.7	1
48	A	1431.8	7.8	1
49	A	1447.0	6.4	1
50	A	1458.0	47.7	6
51	A	1497.9	94.7	11
52	A	1524.1	18.9	2
53	A	1563.6	24.8	3
54	A	1603.0	185.3	21
55	A	1731.9	863.5	100
56	A	1818.9	512.2	59
57	A	2906.6	58.9	7
58	A	2969.8	35.5	4
59	A	3035.5	21.7	3
60	A	3077.9	10.1	1
61	A	3089.5	2.0	0
62	A	3095.5	3.9	0
63	A	3105.2	7.3	1

3-(4-Cyanophenyl)-4-thiocarbonylisoxazol-5-(4*H*)-one *(7c)*

Point group: C1; State = 1-A
HF = -1079.6321289 Hartree
Zero-point correction= 0.125727 (Hartree/Particle)

Atom type	Coordinates (angstroms):		
	X	Y	Z

N	1.212767	-2.135160	0.123676
O	2.611999	-2.179825	0.119734
C	3.158242	-0.902573	0.076808
C	1.973204	0.004424	0.034757
C	0.824643	-0.894862	0.074156
C	-0.608350	-0.560749	0.052087
O	4.338589	-0.693046	0.072287
C	2.073333	1.317951	-0.099927
S	2.291801	2.841036	-0.263121
C	-1.072826	0.682753	0.504776
C	-2.430993	0.979045	0.488602
C	-3.348877	0.026930	0.018546
C	-2.889918	-1.224480	-0.429453
C	-1.532730	-1.512238	-0.413360
C	-4.749797	0.331457	-0.005644
N	-5.885954	0.579882	-0.025767
H	-0.376903	1.417279	0.894698
H	-2.787173	1.939916	0.843049
H	-3.601262	-1.957673	-0.793265
H	-1.171446	-2.472140	-0.764162

Vibrational frequencies (cm^{-1}) (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	31.0	0.3	0
2	A	46.4	4.3	0
3	A	66.0	1.8	0
4	A	89.8	1.8	0
5	A	108.5	4.9	1
6	A	151.7	0.3	0
7	A	167.0	2.1	0
8	A	226.2	4.4	1
9	A	258.3	0.9	0
10	A	297.8	2.1	0
11	A	342.1	0.3	0
12	A	394.8	0.1	0
13	A	424.9	1.0	0
14	A	441.0	0.7	0
15	A	459.9	0.9	0
16	A	483.1	2.6	0
17	A	532.2	5.4	1
18	A	542.0	4.6	1
19	A	556.9	12.9	1
20	A	600.6	2.4	0
21	A	613.0	12.1	1
22	A	636.6	2.0	0
23	A	704.3	12.3	1
24	A	721.6	9.6	1
25	A	723.2	9.8	1
26	A	765.7	10.3	1
27	A	818.2	8.1	1
28	A	833.2	28.0	3
29	A	877.4	159.8	18
30	A	912.7	43.3	5
31	A	935.4	1.1	0
32	A	954.3	0.1	0
33	A	994.8	37.7	4
34	A	1002.0	121.1	14
35	A	1077.0	34.2	4
36	A	1101.8	3.5	0
37	A	1155.9	8.1	1

38	A	1165.5	7.6	1
39	A	1185.0	0.9	0
40	A	1283.3	5.3	1
41	A	1286.4	1.3	0
42	A	1339.8	103.8	12
43	A	1392.8	24.1	3
44	A	1489.1	15.6	2
45	A	1512.7	23.3	3
46	A	1552.9	19.7	2
47	A	1600.6	0.9	0
48	A	1733.4	870.1	100
49	A	1824.3	510.4	59
50	A	2259.0	24.3	3
51	A	3084.6	5.5	1
52	A	3090.6	0.8	0
53	A	3099.2	2.8	0
54	A	3105.3	0.3	0

3-Isopropyl-4-thiocarbonylisoxazol-5-(4*H*)-one *(7d)*

Point group: C1; State = 1-A
HF = -874.285634 Hartree
Zero-point correction= 0.130929 (Hartree/Particle)

Atom type	Coordinates (angstroms): X	Y	Z
N	-1.290928	1.531451	-0.030358
O	-0.186452	2.402254	0.102576
C	1.007353	1.700978	0.100257
C	0.597774	0.273337	-0.047079
C	-0.861477	0.314006	-0.112924
O	2.081534	2.227721	0.199653
C	1.429633	-0.751348	-0.120413
S	2.442090	-1.921446	-0.204961
C	-1.792281	-0.865113	-0.239363
H	-1.388225	-1.493838	-1.045711
C	-1.783917	-1.699715	1.058728
H	-2.186156	-1.115342	1.892127
H	-2.407463	-2.589844	0.933458
H	-0.777192	-2.030202	1.331275
C	-3.215571	-0.437042	-0.621176
H	-3.846038	-1.322347	-0.745163
H	-3.656326	0.194020	0.155144
H	-3.225279	0.130110	-1.555251

Vibrational frequencies (cm^{-1}) (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	39.4	0.0	0
2	A	71.8	0.3	0
3	A	83.9	0.0	0
4	A	140.0	1.3	0
5	A	175.4	1.5	0
6	A	217.2	0.1	0
7	A	234.1	0.8	0
8	A	256.1	0.4	0
9	A	301.2	1.7	0
10	A	355.3	1.3	0

11	A	415.2	1.1	0
12	A	427.8	3.1	0
13	A	453.3	1.2	0
14	A	467.3	0.8	0
15	A	590.3	2.7	0
16	A	612.5	7.4	1
17	A	635.3	7.1	1
18	A	717.0	11.2	1
19	A	730.7	5.8	1
20	A	841.6	5.9	1
21	A	872.9	88.1	9
22	A	904.7	1.3	0
23	A	936.6	0.4	0
24	A	952.9	11.7	1
25	A	1002.8	191.2	20
26	A	1070.3	13.2	1
27	A	1085.9	1.9	0
28	A	1134.8	19.2	2
29	A	1154.5	7.4	1
30	A	1239.6	68.7	7
31	A	1284.2	0.5	0
32	A	1346.7	7.7	1
33	A	1363.7	2.3	0
34	A	1382.9	6.2	1
35	A	1441.6	0.6	0
36	A	1446.4	2.8	0
37	A	1456.9	8.1	1
38	A	1466.1	8.1	1
39	A	1557.6	62.2	7
40	A	1736.8	955.5	100
41	A	1819.7	386.8	40
42	A	2905.6	11.4	1
43	A	2932.2	17.8	2
44	A	2941.6	17.6	2
45	A	3004.7	27.0	3
46	A	3007.1	6.6	1
47	A	3013.3	28.4	3
48	A	3019.8	18.2	2

3-Neopentyl-4-thiocarbonylisoxazol-5-(4*H*)-one *(7e)*

Point group: C1; State = 1-A
HF = -952.9175951 Hartree
Zero-point correction= 0.187215 (Hartree/Particle)

Atom type	Coordinates (angstroms): X	Y	Z
N	-0.083828	-2.057554	-0.493705
O	-1.383398	-2.390844	-0.051538
C	-2.144667	-1.255586	0.168407
C	-1.228197	-0.126217	-0.165332
C	0.024702	-0.767814	-0.554084
O	-3.284285	-1.288519	0.544927
C	-1.559676	1.153488	-0.130777
S	-1.995856	2.638903	-0.080607
C	1.299138	-0.106786	-0.994495
H	1.043187	0.843285	-1.477900
H	1.752489	-0.745172	-1.759779

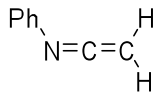
C	2.363036	0.161111	0.117617
C	2.879716	-1.171124	0.690100
H	2.075649	-1.757826	1.142472
H	3.337215	-1.786435	-0.092200
H	3.638212	-0.985704	1.458088
C	1.774642	1.022167	1.250089
H	0.960275	0.509223	1.771453
H	2.545826	1.251191	1.993061
H	1.389383	1.975990	0.871464
C	3.529389	0.919402	-0.544466
H	3.202847	1.884934	-0.947430
H	4.323905	1.113372	0.183565
H	3.964462	0.340627	-1.366610

Vibrational frequencies (cm^{-1}) (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	27.3	0.3	0
2	A	55.6	0.1	0
3	A	70.2	0.4	0
4	A	91.9	0.6	0
5	A	118.5	1.4	0
6	A	205.5	1.2	0
7	A	212.4	0.5	0
8	A	231.5	0.3	0
9	A	255.5	0.3	0
10	A	269.7	0.1	0
11	A	281.8	0.6	0
12	A	322.2	0.6	0
13	A	331.5	1.9	0
14	A	376.0	0.5	0
15	A	391.2	0.1	0
16	A	418.6	0.4	0
17	A	440.0	1.3	0
18	A	458.2	1.5	0
19	A	475.0	0.4	0
20	A	562.4	7.7	1
21	A	599.7	7.0	1
22	A	663.5	9.5	1
23	A	701.1	7.3	1
24	A	734.8	4.6	0
25	A	759.3	11.1	1
26	A	850.5	50.4	5
27	A	869.4	8.8	1
28	A	889.2	33.0	4
29	A	907.8	0.8	0
30	A	910.0	3.4	0
31	A	931.8	0.0	0
32	A	970.0	8.8	1
33	A	1003.5	144.4	16
34	A	1015.4	10.3	1
35	A	1028.0	22.9	2
36	A	1130.6	4.8	1
37	A	1145.7	21.1	2
38	A	1185.9	6.6	1
39	A	1212.8	25.6	3
40	A	1254.8	27.5	3
41	A	1289.5	11.3	1
42	A	1329.1	45.5	5
43	A	1362.2	6.3	1
44	A	1365.2	7.3	1

45	A	1393.6	4.0	0
46	A	1429.2	2.9	0
47	A	1437.8	0.6	0
48	A	1441.8	1.0	0
49	A	1442.3	1.0	0
50	A	1462.1	3.5	0
51	A	1465.2	11.1	1
52	A	1471.2	14.2	2
53	A	1552.0	64.6	7
54	A	1735.7	917.9	100
55	A	1818.9	398.4	43
56	A	2916.9	25.0	3
57	A	2920.9	22.6	2
58	A	2927.2	17.4	2
59	A	2934.2	10.3	1
60	A	2980.8	0.2	0
61	A	2983.6	4.6	1
62	A	2987.9	35.5	4
63	A	2989.7	15.3	2
64	A	2994.3	34.8	4
65	A	2997.1	48.2	5
66	A	3010.4	26.3	3

_N_-phenylketenimine



Point group: CS; State = 1-A’
HF = -363.7777636 Hartree
Zero-point correction= 0.125577 (Hartree/Particle)

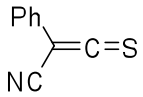
Atom type	Coordinates (angstroms): X	Y	Z
N	1.203941	1.125603	0.000000
C	2.341087	0.661206	0.000000
C	3.595138	0.270945	0.000000
H	4.122045	0.105467	0.933198
H	4.122045	0.105467	-0.933198
C	0.000000	0.371382	0.000000
C	-0.027145	-1.030822	0.000000
C	-1.198420	1.092023	0.000000
C	-1.248393	-1.698637	0.000000
H	0.908597	-1.582364	0.000000
C	-2.418353	0.416589	0.000000
H	-1.151748	2.175962	0.000000
C	-2.446993	-0.978584	0.000000
H	-1.266990	-2.784681	0.000000
H	-3.346120	0.980917	0.000000
H	-3.396950	-1.504596	0.000000

Vibrational frequencies (cm^{-1}) (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	40.9	1.9	0
2	A'	117.1	1.4	0
3	A"	208.2	0.8	0

4	A"	334.6	0.6	0
5	A'	361.0	4.4	1
6	A"	405.5	0.0	0
7	A'	441.4	0.7	0
8	A"	445.0	1.4	0
9	A"	586.3	3.2	1
10	A'	605.9	0.3	0
11	A'	616.6	30.5	6
12	A"	679.8	21.6	5
13	A'	681.8	86.1	18
14	A"	757.3	34.3	7
15	A'	769.3	4.6	1
16	A"	825.1	0.0	0
17	A"	902.0	4.3	1
18	A"	940.8	0.0	0
19	A"	958.2	1.0	0
20	A"	961.8	0.1	0
21	A'	979.4	0.9	0
22	A'	1009.7	4.0	1
23	A'	1061.2	6.2	1
24	A'	1079.6	4.6	1
25	A'	1140.5	0.1	0
26	A'	1152.2	0.4	0
27	A'	1246.9	8.3	2
28	A'	1286.5	9.3	2
29	A'	1309.7	2.7	1
30	A'	1407.8	0.6	0
31	A'	1437.4	2.3	0
32	A'	1476.4	36.5	8
33	A'	1575.9	7.2	2
34	A'	1589.8	21.7	5
35	A'	2043.7	471.2	100
36	A'	3048.7	3.0	1
37	A'	3058.2	1.0	0
38	A'	3066.6	5.2	1
39	A'	3074.7	12.9	3
40	A'	3082.9	23.0	5
41	A'	3091.8	8.5	2
42	A"	3130.7	0.0	0

(Phenyl)cyanothioketene ***(10a)***

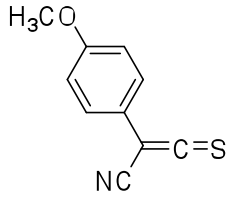


Point group: Cs; State = 1-A’
HF = -798.8583384 Hartree
Zero-point correction = 0.111592 (Hartree/Particle)

Atom type	Coordinates (angstroms): X	Y	Z
C	0.636758	-0.741118	0.000000
C	-0.041798	-1.891224	0.000000
S	-0.833889	-3.227608	0.000000
C	0.000000	0.602330	0.000000
C	0.802217	1.753083	0.000000
C	-1.397128	0.742933	0.000000
C	0.214935	3.017190	0.000000

H	1.883141	1.657199	0.000000
C	-1.975542	2.008402	0.000000
H	-2.033065	-0.137332	0.000000
C	-1.173247	3.152050	0.000000
H	0.849382	3.898302	0.000000
H	-3.057427	2.100823	0.000000
H	-1.627463	4.137966	0.000000
C	2.061384	-0.868022	0.000000
N	3.223169	-0.952711	0.000000

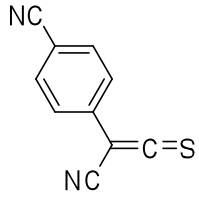
(4-Methoxyphenyl)cyanothioketene ***(10b)***



Point group: Cs; State = 1-A’
HF = -913.3841254 Hartree
Zero-point correction = 0.144212 (Hartree/Particle)

Atom type	Coordinates (angstroms): X	Y	Z
C	0.488177	1.727952	0.000000
C	1.776945	2.077620	0.000000
S	3.278818	2.480647	0.000000
C	0.000000	0.325729	0.000000
C	-1.373517	0.058343	0.000000
C	0.893653	-0.761407	0.000000
C	-1.854032	-1.251468	0.000000
H	-2.082401	0.880142	0.000000
C	0.425898	-2.064345	0.000000
H	1.965339	-0.585840	0.000000
C	-0.954854	-2.323350	0.000000
H	-2.924087	-1.418530	0.000000
H	1.110928	-2.905372	0.000000
C	-0.441902	2.814704	0.000000
N	-1.216867	3.684500	0.000000
O	-1.309540	-3.637555	0.000000
C	-2.692931	-3.962057	0.000000
H	-2.745589	-5.051309	0.000000
H	-3.197755	-3.575415	0.894067
H	-3.197755	-3.575415	-0.894067

(4-Cyanophenyl)cyanothioketene ***(10c)***

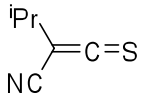


Point group: Cs; State = 1-A’

HF = 891.0984324 Hartree
Zero-point correction = 0.110079 (Hartree/Particle)

Atom type	Coordinates (angstroms): X	Y	Z
C	1.193410	1.150237	0.000000
C	2.452357	0.699027	0.000000
S	3.912303	0.177755	0.000000
C	0.000000	0.270533	0.000000
C	-1.284448	0.838388	0.000000
C	0.127638	-1.129378	0.000000
C	-2.413805	0.029323	0.000000
H	-1.398380	1.917004	0.000000
C	-0.996540	-1.941495	0.000000
H	1.111157	-1.588015	0.000000
C	-2.280929	-1.368577	0.000000
H	-3.402225	0.475176	0.000000
H	-0.890444	-3.020628	0.000000
C	1.043633	2.572653	0.000000
N	0.900500	3.728449	0.000000
C	-3.443555	-2.206371	0.000000
N	-4.386720	-2.887544	0.000000

(Isopropyl)cyanothioketene *(10d)*



Point group: C1; State = 1-A
HF = -685.7509042 Hartree
Zero-point correction= 0.115139 (Hartree/Particle)

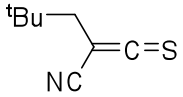
Atom type	Coordinates (angstroms): X	Y	Z
C	0.091859	0.195581	0.000000
C	-1.227571	0.322474	0.000000
S	-2.782719	0.426984	0.000000
C	0.766818	-1.191359	0.000000
C	0.901765	1.368902	0.000000
N	1.603184	2.299800	0.000000
H	-0.042717	-1.930052	0.000000
C	1.603184	-1.381311	1.274921
H	2.062878	-2.374976	1.277393
H	2.404613	-0.637698	1.331646
H	0.986762	-1.286399	2.173245
C	1.603184	-1.381311	-1.274921
H	2.062878	-2.374976	-1.277393
H	0.986762	-1.286399	-2.173245
H	2.404613	-0.637698	-1.331646

Vibrational frequencies (cm^{-1}) (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	38.5	0.1	0
2	A'	98.3	2.1	0
3	A"	128.7	1.5	0

4	A'	130.8	2.8	1
5	A"	226.9	0.0	0
6	A'	252.9	0.0	0
7	A'	309.8	0.5	0
8	A"	333.2	0.0	0
9	A'	396.3	0.8	0
10	A"	400.6	3.6	1
11	A'	474.8	3.7	1
12	A'	552.5	2.1	0
13	A"	603.5	4.2	1
14	A'	619.8	4.2	1
15	A'	844.7	2.0	0
16	A"	902.6	1.3	0
17	A"	926.4	0.0	0
18	A'	1002.2	29.7	6
19	A'	1014.1	11.7	2
20	A"	1082.2	1.9	0
21	A'	1146.0	61.5	12
22	A'	1155.6	5.1	1
23	A"	1287.1	2.3	0
24	A'	1306.1	7.8	2
25	A"	1358.6	4.9	1
26	A'	1378.3	1.4	0
27	A"	1441.0	1.0	0
28	A"	1446.3	1.1	0
29	A'	1454.2	9.9	2
30	A'	1465.3	5.0	1
31	A'	1749.8	495.6	100
32	A'	2235.7	49.8	10
33	A"	2928.4	17.3	3
34	A'	2932.0	18.8	4
35	A'	2940.0	7.1	1
36	A"	2998.3	0.9	0
37	A'	3003.5	39.2	8
38	A"	3008.5	17.9	4
39	A'	3010.4	21.0	4

(Neopentyl)cyanothioketene *(10e)*



Point group: C1; State = 1-A
HF = -764.377447 Hartree
Zero-point correction= 0.171354 (Hartree/Particle)

Atom type	Coordinates (angstroms): X	Y	Z
C	-0.838804	0.692814	-0.000014
C	-1.366793	-0.524631	-0.000003
S	-2.057960	-1.923045	0.000002
C	0.641575	1.097912	-0.000061
C	-1.784640	1.765483	-0.000013
N	-2.520822	2.669071	0.000015
C	1.738480	0.006395	0.000001
H	0.783986	1.743096	-0.876669
H	0.784000	1.743222	0.876450

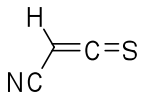
C	1.658866	-0.865744	1.267790
H	2.488269	-1.580585	1.288986
H	1.725815	-0.250846	2.172046
H	0.730789	-1.440698	1.323817
C	1.658893	-0.865853	-1.267711
H	2.488310	-1.580680	-1.288849
H	0.730834	-1.440842	-1.323688
H	1.725827	-0.251041	-2.172027
C	3.091830	0.749964	-0.000013
H	3.920699	0.034711	0.000059
H	3.199103	1.385364	-0.886015
H	3.199049	1.385491	0.885901

Vibrational frequencies (cm^{-1}) (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	25.6	1.9	1
2	A	89.1	0.6	0
3	A	95.8	0.7	0
4	A	113.4	3.9	1
5	A	185.8	0.4	0
6	A	203.4	0.2	0
7	A	219.5	0.2	0
8	A	244.5	0.0	0
9	A	261.3	0.0	0
10	A	305.7	0.0	0
11	A	317.3	0.1	0
12	A	371.7	0.1	0
13	A	387.0	1.6	0
14	A	394.5	0.5	0
15	A	414.7	1.6	0
16	A	503.8	0.3	0
17	A	539.8	4.4	1
18	A	560.3	0.7	0
19	A	660.4	8.3	2
20	A	730.2	0.6	0
21	A	853.6	0.2	0
22	A	885.9	4.3	1
23	A	909.0	0.2	0
24	A	910.3	0.3	0
25	A	929.3	0.0	0
26	A	1003.5	1.3	0
27	A	1022.5	0.1	0
28	A	1065.8	21.1	6
29	A	1089.3	7.7	2
30	A	1148.5	0.9	0
31	A	1186.1	23.0	7
32	A	1231.7	10.4	3
33	A	1270.9	2.4	1
34	A	1306.8	40.3	12
35	A	1361.1	4.2	1
36	A	1365.4	8.5	2
37	A	1392.1	8.5	2
38	A	1423.2	1.9	1
39	A	1439.5	0.5	0
40	A	1442.1	0.1	0
41	A	1442.8	0.1	0
42	A	1464.2	4.0	1
43	A	1465.1	5.0	1
44	A	1472.1	7.7	2

45	A	1748.6	344.2	100
46	A	2234.1	47.6	14
47	A	2911.2	9.8	3
48	A	2919.2	28.6	8
49	A	2925.6	31.0	9
50	A	2932.0	8.9	3
51	A	2947.8	10.7	3
52	A	2986.9	5.5	2
53	A	2989.2	1.9	1
54	A	2991.1	37.0	11
55	A	2996.2	56.9	17
56	A	3007.1	2.4	1
57	A	3011.0	56.5	16

Cyanothioketene



Point group: CS; State = 1-A’
HF = -567.7942652 Hartree
Zero-point correction= 0.029782 (Hartree/Particle)

Atom type	Coordinates (angstroms): X	Y	Z
C	-1.043961	-0.178405	0.000000
C	0.000000	0.640525	0.000000
C	-0.903555	-1.591882	0.000000
N	-0.807446	-2.752686	0.000000
H	-2.044185	0.250785	0.000000
S	1.211337	1.612287	0.000000

Vibrational frequencies (cm^{-1}) (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A'	113.0	3.9	1
2	A'	367.6	1.7	0
3	A"	370.7	4.1	1
4	A"	406.6	0.6	0
5	A'	545.5	2.5	1
6	A"	642.0	34.7	8
7	A'	826.0	10.9	2
8	A'	1012.8	5.6	1
9	A'	1233.1	12.3	3
10	A'	1751.9	446.2	100
11	A'	2250.0	52.5	12
12	A'	3047.7	24.1	5