INFRARED CARBONYL FREQUENCIES OF THIOLACTONES AND LACTONES

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Abstract — Infrared carbonyl frequencies of thiolactones and the corresponding lactones are tabulated according to ring size, substituents, unsaturation, heteroatoms, and solvent effects.

For over thirty years the infrared carbonyl frequencies of lactones and thiolactones have been used to investigate ring size, substituent position, and location and degree of unsaturation. The localized, high intensity nature of the carbonyl stretching vibrations make them well-suited for deducing structural relationships, and useful generalizations have emerged from such studies. The principal books and reviews which summarized these findings, however, tended either to cite a few examples illustrating the observed ranges of commonly encountered lactone systems[11,30,31,193,194,287] or to focus on a particular ring system.[269,289] None of these treatments dealt primarily with thiolactones.[99a]

The theory of carbonyl absorptions is presented in a variety of textbooks on infrared spectroscopy. In this review an attempt has been made to collect an extensive (but not exhaustive) set of thiolactones for which the C=O frequencies have been reported. For almost all of the examples, data for the corresponding lactones were located. Thus the present summary affords an extended set of comparisons useful for structural correlations. From the vast number of thiolactones available in the literature, examples of simple alkyl and aryl groups were selected as representative substituents. In many cases the original article contained spectral information on additional derivatives.

The Tables are organized on the basis of ring size, number and relative position of heteroatoms, degree and relative position of unsaturation, and solvent affects. Nomenclature is omitted in favor of formulas. In those cases where the total number of substituents becomes cumbersome for only a single generic structure, several formulas are used to represent sub-groups of the same ring system. The symbol Z represents the S or O atom of the lactone moiety and is designated as position 1; the symbol Y is used for any other heteroatom. Solvents are identified by molecular formulas, mull refers to dispersion in mineral oil (Nujol), and a dash means that the phase was

unspecified. In cases where multiple bands were reported with some marked as weak or shoulders, only the value of the strong band is tabulated. Values of carbonyl frequencies are in wave numbers, cm^{-1}; $\nu^{S}_{C=O}$ refers to thiolactones, $\nu^{O}_{C=O}$ to lactones.

In general, the following trends are observed. For a given thiolactone the carbonyl frequency is ca. 60-80 cm^{-1} lower than the corresponding lactone. As saturated thiolactones change in size from three- to six-membered rings, there is a decrease of ca. 40-50 cm^{-1} for each increase of one methylene group; comparable decreases occur in the series of corresponding lactones. Endocyclic double bonds (including benzo derivatives) which are α,β to the carbonyl group cause a shift to lower frequencies; endocyclic double bonds (including benzo derivatives) which are α,β to the heteroatom cause a shift to higher frequencies. Fully-conjugated systems such as thiopyrones and pyrones exhibit shifts to lower frequencies; but comparable shifts in coumarins, isocoumarins, and their sulfur analogues are much less pronounced. Exocyclic double bonds α to the carbonyl group cause a shift to lower frequencies, whereas exocyclic double bonds α to the heteroatom cause a shift to higher frequencies. Alkyl substituents exert only a minor influence on observed frequencies. Phenyl substituents α to the carbonyl group cause a shift to lower frequencies, but the effect of the same substituent in other positions is less predictable. The incorporation of additional heteroatoms in the lactone ring results in a variety of effects, the most pronounced of which occurs when the second heteroatom is also adjacent to the carbonyl group. In such cyclic carbonates the dithio analogues are shifted by ca. 150 cm^{-1} to lower frequencies. Finally, solvent effects are not always consistent; but, in general, higher frequencies are observed when the phase is mineral oil, potassium bromide, or carbon tetrachloride while lower frequencies are exhibited by neat liquids or chloroform solutions.

Table I

Ring size: 3

Heteroatoms: 1-Z

Unsaturation: none

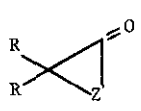
Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	R = t-Bu	-	1810,1785	314	CH_2Cl_2	1889	84

Table II

Ring size: 4

Heteroatoms: 1-Z

Unsaturation: none

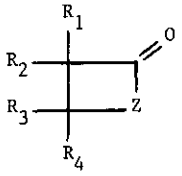
Compound				Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
									
R_1	R_2	R_3	R_4						
H	H	H	H	$HCCl_3$	1776	180	CCl_4	1852	32
iPr	H	H	H	neat	1760	122	neat	1820	122
Ph	H	H	H	neat	1750	122	neat	1820	122
Me	Me	H	H	CCl_4 CCl_4	1769 1740	179 199	neat	1828	83
Ph	Et	H	H	neat	1750	122	neat	1820	122
H	H	Me	Me	CCl_4	1772	180	neat	1821	83
Me	Me	Me	Me	-	1757,1721	130	neat	1821	83
Ph	Ph	Ph	Ph	KBr $DCCl_3$	1735 1742	198 198	KBr	1820	69

Table III

Ring size: 4

Heteroatoms: 1-Z

Unsaturation: benzo or exocyclic

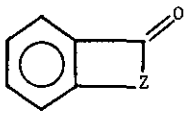
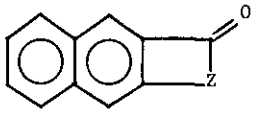
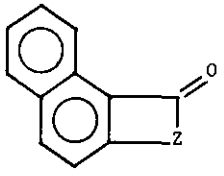
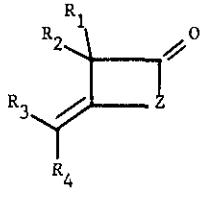
Compound	Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	gas	1800	376	gas	1930	376
	neat	1803	71	argon 8°K	1904	72
	-	1800	367	-	1893,1874	367
	-	1793	367			
						
R_1 R_2 R_3 R_4						
H H CF_3 CF_3	neat	1821	282	-	1953	110
Me H CF_3 CF_3	neat	1821	282	-	1923	110
Me Me Me Me	neat	1820,1785	129 130	neat	1876,1825	105

Table IV

Ring size: 5

Heteroatoms: 1-Z

Unsaturation: none

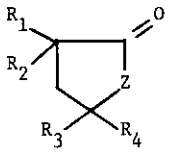
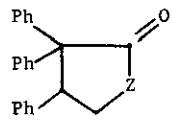
Compound					Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
										
R_1	R_2	R_3	R_4							
H	H	H	H		neat	1705	201	neat	1773	232
					$HCCl_3$	1695	344	$HCCl_3$	1773	343
					-	1710	297	-	1760	297
								CCl_4	1786	32
CH_2OH	H	H	H		neat	1675	217	-	1760	304
CPh_3	H	H	H		mull	1679	292			
CO_2Me	H	H	H		-	1735,1700	55	$HCCl_3$	1778,1740	281
CO_2Me	H	Me	H		-	1735,1700	55	neat	1780,1745	195
H	H	Me	H		-	1710	297	-	1765	297
								neat	1770	237,290
								neat	1763	170
								$HCCl_3$	1773	343
								CCl_4	1783	240
H	H	Me	Me		-	1700	297	-	1760	297
								neat	1770	170,237
								CCl_4	1780	346
Me	H	H	Me	trans	neat	1670	350a	neat	1760	350a
CH_2Ph	H	H	Me	trans	neat	1685	350a			
					-	1720	257			

Table IV (continued)

Ring Size: 5

Heteroatoms: 1-Z

Unsaturation: none

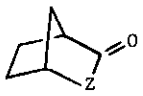
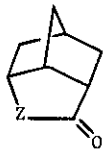
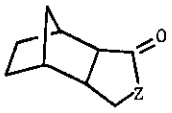
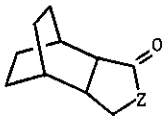
Compound	Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	CCl_4	1715	33	neat	1770	248
				-	1779	256
	mull	1695	156	KCl	1780	86
				$HCCl_3$	1776	343
				CCl_4	1790	86
				CCl_4	1785	365
	$HCCl_3$	1686	344	$HCCl_3$	1761	343
				$HCCl_3$	1767	89
	$HCCl_3$	1693	344	$HCCl_3$	1760	344

Table V

Ring size: 5

Heteroatoms: 1-Z

Unsaturation: endocyclic or exocyclic

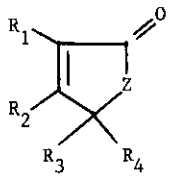
Compound				Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
									
R_1	R_2	R_3	R_4						
H	H	H	H	neat	1675	100	neat	1785,1750	119
							neat	1776,1742	214
				-	1682	176	$HCCl_3$	1783,1751	47
				-	1680	66	$HCCl_3$	1777,1745	214
				-	1670	141	CCl_4	1784,1742	186
Me	H	H	H	-	1675	66	neat	1760	174
							neat	1750	49,119
							CCl_4	1764	214
t-Bu	H	H	H	-	1685	66			
OH	H	H	H	KBr	1680	140	KBr	1750	246
OMe	H	H	H	KBr	1680	166	$HCCl_3$	1765	355
Br	H	H	H	CCl_4	1720	23	KBr	1761,1749	350
H	Me	H	H	CH_2Cl_2	1682	78	$HCCl_3$	1765	117
							neat	1780,1750	119
							neat	1779,1751	214
							neat	1785,1750	268
							CCl_4	1790,1755	225
							CCl_4	1780,1750	357
H	Ph	H	H	KBr	1655	306	-	1740	363

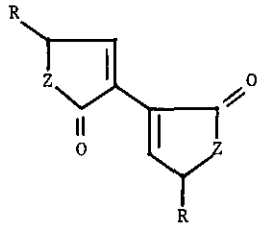
Table V (continued)

Ring size: 5

Heteroatoms: 1-Z

Unsaturation: endocyclic or exocyclic

Compound				Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
R_1	R_2	R_3	R_4						
H	H	Me	H	-	1687	176	-	1786,1770	102
				-	1678	141	CCl_4	1785,1766	121
							CCl_4	1782,1765	183
H	H	CH_2Ph	H	-	1690	176			
H	H	Cl	H	neat	1700	165	neat	1800	112
							CCl_4	1818	323
H	H	Br	H	-	1710	175			
H	H	SMe	H	-	1697	176			
H	H	OEt	H				neat	1780,1750	112
							neat	1800,1700	208
Me	H	Me	H	neat	1675	267	neat	1761	195
				-	1680	66	$HCCl_3$	1805,1745	157
							$HCCl_3$	1750	171
OH	H	Me	H	neat	1690	246	KBr	1750	246



R				
H	KBr	1675	265	
Me	KBr	1672	163	
t-Bu	KBr	1663	163	

Table V (continued)

Ring size: 5

Heteroatoms: 1-Z

Unsaturation: endocyclic or exocyclic

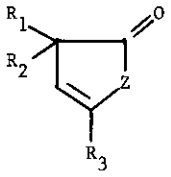
Compound			Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
								
R_1	R_2	R_3						
Me	H	H	CCl_4	1675,1668	92	-	1800	340
Me	Me	H	neat	1715	267	neat	1802	67
H	H	Me	-	1722	176	neat	1810	164
			-	1715	141	CCl_4	1815	121
						CCl_4	1806	183
						$HCCl_3$	1795,1729	157
						$HCCl_3$	1790	369
H	H	Et	neat	1700	153	$HCCl_3$	1795	184
H	H	Ph	KBr	1725	155	CCl_4	1816	121
						mull	1805,1790	178
H	H	CH_2Ph	-	1722	176			
H	H	SMe	-	1725	176			
Me	Me	Me	neat	1715	267			

Table V (continued)

Ring Size: 5

Heteroatoms: 1-Z

Unsaturation: endocyclic or exocyclic

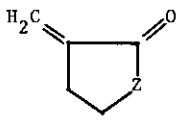
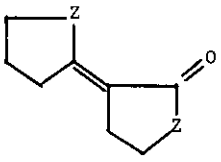
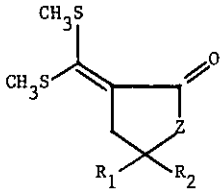
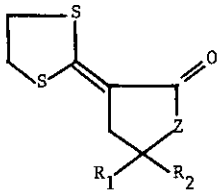
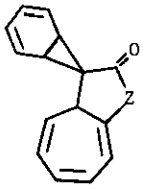
Compound			Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
			neat	1680	217	neat	1765	152,172
						$HCCl_3$	1765	136
						$HCCl_3$	1759	302
	Z		KBr	1645	278	mull	1740	239
	E		KBr	1630	278			
	R_1	R_2						
	H	H	-	1645	55,297	-	1675	297
	H	Me	-	1650	297	-	1680	297
			-	1655	55			
	Me	Me	-	1660	297	-	1710	297
	R_1	R_2						
	H	H	-	1620	297	-	1705	297
	H	Me	-	1620	297	-	1710	297
	H	Ph	-	1620	296			
	Me	Me	-	1630	297	-	1705	297
			KBr	1645	244	KBr	1785	16

Table VI

Ring size: 5

Heteroatoms: 1-Z

Unsaturation: endocyclic and exocyclic

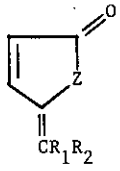
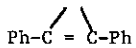
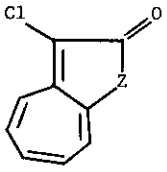
Compound			Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	R_1	R_2						
	H	Me	-	1688	176	CCl_4	1785,1740	184
	H	Ph	-	1683	176	$HCCl_3$	E 1763	373
						$HCCl_3$	Z 1765	373
	Me	Me	-	1677	176			
	Ph	Ph	CS_2	1675	39			
	$-(CH_2)_4-$		-	1675	176			
	$-(CH_2)_5-$		KBr	1660,1652	349			
	$-(CH=CH)_3-$		KBr	1640,1623	349			
			$HCCl_3$	1658,1650	349			
			KBr	1852	348			
			KBr	1750,1655	63	$HCCl_3$	1780,1755	76

Table VI (continued)

Ring size: 5

Heteroatoms: 1-Z

Unsaturation: endocyclic and exocyclic

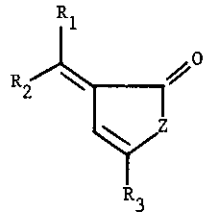
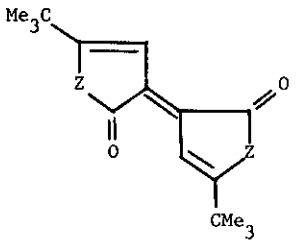
Compound			Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
								
R_1	R_2	R_3						
H	Ph	H	KBr	1670	266			
H	Ph	Ph				-	1785	115
H	Ph	p-tolyl	mull	1680	154			
Me	Me	H	KBr	1690	266			
Et	Me	H	neat	1660	266			
Et	Ph	H	neat	1665	266			
Ph	Ph	H	KBr	1680	266			
			KBr	1670	163			

Table VII

Ring size: 5

Heteroatoms: 1-Z

Unsaturation: benzo derivatives and exocyclic

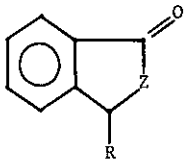
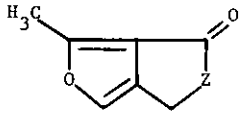
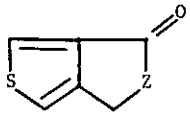
Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	R						
	H	KBr	1685	228	mull	1750	143,144
		CCl_4	1686	277	CCl_4	1761	277
		CCl_4	1690	218	CCl_4	1778	186
		$HCCl_3$	1684	344	$HCCl_3$	1778	343
		$HCCl_3$	1680	100	$HCCl_3$	1761	269,186
	Ph	CCl_4	1700	6	CCl_4	1761	277
					$HCCl_3$	1755	364
					KBr	1758	7
					mull	1755	37
					-	1750	74
		$HCCl_3$	1730	303			
					-	1820	280

Table VII (continued)

Ring size: 5

Heteroatoms: 1-Z

Unsaturation: benzo derivatives and exocyclic

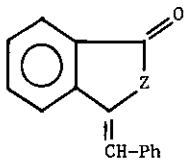
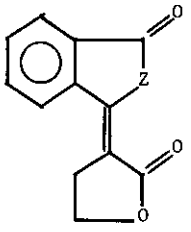
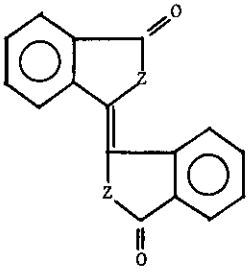
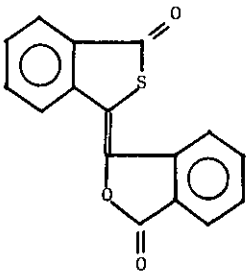
Compound	Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	mull	1680	43	mull	1770	43
	mull	1720,1680	239	mull	1775,1745	239
	KBr	1700	222	KBr	1786	222
				KBr	1789	335
	mull	1700	43	KBr	1785	241
				KBr	1780	27,147
				KBr	1779	65
				mull	1780	43,286
				mull	1787	276
	KBr	1701	42,222	KBr	1792	43,222
	mull	1690	276	mull	1782	276

Table VII (continued)

Ring size: 5

Heteroatoms: 1-Z

Unsaturation: benzo derivatives and exocyclic

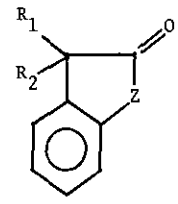
Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
							
R_1	R_2						
H	H	$HCCl_3$	1750	202	$HCCl_3$	1805	202
		CCl_4	1723	219	CCl_4	1802	277
		KBr	1745	125	mull	1820	21
		KBr	1710	96			
H	Me	neat	1717	81	neat	1808	106
		$HCCl_3$	1705	361	CCl_4	1805	247
		-	1705	96			
H	Ph				KBr	1795	247
					$HCCl_3$	1812	262
					$HCCl_3$	1810	8
H	OMe	KBr	1640	362			
Me	Me	$HCCl_3$	1725	361	neat	1805	106
					neat	1800	259
Ph	Ph	KBr	1720	255			

Table VII (continued)

Ring size: 5

Heteroatoms: 1-Z

Unsaturation: benzo derivatives and exocyclic

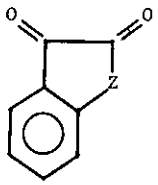
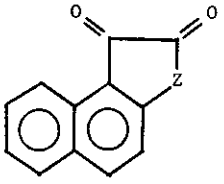
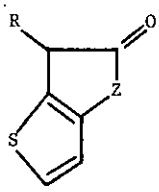
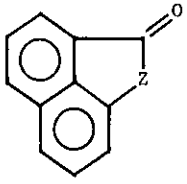
Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
		KBr	1735,1712	98	mull	1833,1740	142
		KBr	1730,1712	40	-	1832,1739	321
		CCl_4	1740,1724	40			
		KBr	1730,1690	366			
	R						
	H	CCl_4	1725	223			
	Me	CCl_4	1725	223			
	Ph	CCl_4	1730	223			
		CCl_4	1701	336	CCl_4	1802,1792	291 336
		KBr	1690	252			

Table VIII

Ring size: 6

Heteroatoms: 1-Z

Unsaturation: none; endocyclic or exocyclic

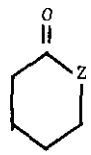
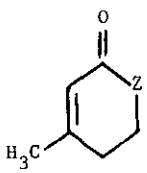
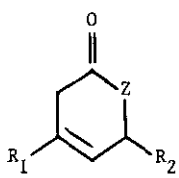
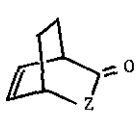
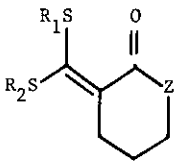
Compound	Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	-	1655	297	-	1720	297
	neat	1664	201	neat	1739	290
				CCl_4	1739	32
				$HCCl_3$	1732	186
				CS_2	1750	186
	neat	1645	44	neat	1725	243,308
				$HCCl_3$	1725	229
				CCl_4	1738	120
				CCl_4	1720	146
						
R_1 R_2						
H H	neat	1670	44	neat	1757	48
Me H	*neat*	1665	44	neat	1736	48
				neat	1749	243
H Me	neat	1670	44			
	CCl_4	1680	293	neat	1751	48

Table VIII (continued)

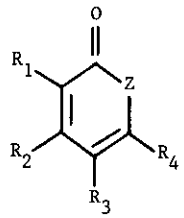
Ring size: 6

Heteroatoms: 1-Z

Unsaturation: none; endocyclic or exocyclic



R_1	R_2	Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
Me	Me	-	1610	297	-	1685	297
$-CH_2CH_2-$		-	1580	297	-	1660	297



R_1	R_2	R_3	R_4	Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
H	H	H	H	$HCCl_3$	1636	322	$HCCl_3$	1738,1722	322
							$HCCl_3$	1739,1721	186
							CCl_4	1752,1716	186
Ph	H	Ph	H	CH_2Cl_2	1630	231			
H	Ph	H	Ph	KBr	1631	108	KBr	1700	29,339
				mull	1635	211			
				CH_2Cl_2	1632	231			
Ph	H	H	Ph	KBr	1627	191			
				mull	1630	181			
				$HCCl_3$	1635	181			
				CH_2Cl_2	1634	231			
H	Ph	Ph	Ph	KBr	1625	107	KBr	1721	109

Table VIII (continued)

Ring size: 6

Heteroatoms: 1-Z

Unsaturation: none; endocyclic or exocyclic

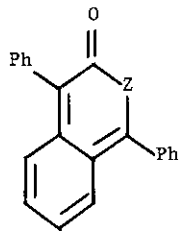
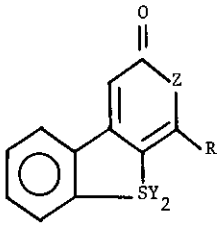
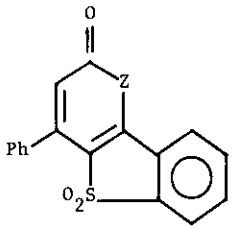
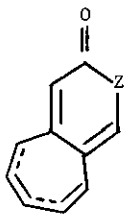
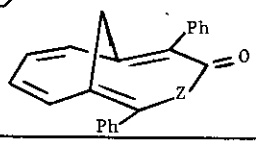
Compound	Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	mull	1600	181	mull	1693	162
						
R Y						
Ph –	KBr	1620	59	KBr	1710	59
H O	KBr	1625	59	KBr	1720	59
	KBr	1620	59	KBr	1740	59
	–	1595	192			
	–	1635	192			

Table IX

Ring size: 6

Heteroatoms: 1-Z

Unsaturation: benzo derivatives

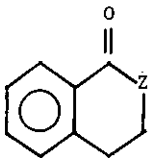
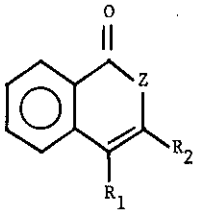
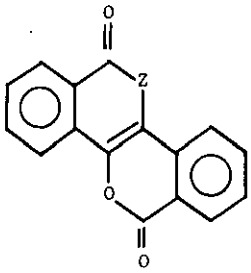
Compound	Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	CCl_4	1655	219	$HCCl_3$	1714	218
						
R_1 R_2						
H H	$HCCl_3$	1640	97	$HCCl_3$	1745	200
	C_2Cl_4	1650	91	CCl_4	1736	277
				mull	1750,1730	253
H . Ph	KBr	1634	212	KBr	1716	212
				$HCCl_3$	1749	58
				$HCCl_3$	1740	295
				CCl_4	1745	73,277
				-	1720	133
Ph Ph	KBr	1632	212	KBr	1710	212
				mull	1736,1724	226
	KBr	1748,1656	42 222	KBr	1745	65
	mull	1745,1660	43	mull	1745	43
				mull	1752	57
				mull	1720	286

Table IX (continued)

Ring size: 6

Heteroatoms: 1-Z

Unsaturation: benzo derivatives

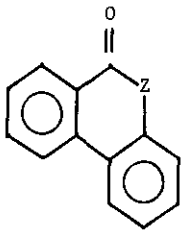
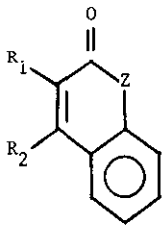
Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
		mull	1625	231	KBr	1724	137
					-	1735	242
							
R_1	R_2						
H	H	KBr	1640	300	KBr	1750	300
		KBr	1637	270	KBr	1725	270
		mull	1668	235	mull	1720	221
					mull	1705	26
		CCl_4	1683	277	CCl_4	1730	277
		CCl_4	1659	300	CCl_4	1759	300
		CCl_4	1658	270	CCl_4	1738	270
		$HCCl_3$	1640	300	$HCCl_3$	1734	300
					$HCCl_3$	1724	290
Me	H	KBr	1620	216,270	KBr	1707	270
		KBr	1612	300			
		mull	1632	231	mull	1705	26
		CCl_4	1636	300	CCl_4	1736	300
		CCl_4	1629	270	CCl_4	1730	270
		$HCCl_3$	1627	300	$HCCl_3$	1712	333
					$HCCl_3$	1711	270
Ph	H	mull	1630	235	KBr	1720	94
		CCl_4	1643	300	$HCCl_3$	1724	333
					$HCCl_3$	1710	288
3-thienyl	H	mull	1625	235			

Table IX (continued)

Ring size: 6

Heteroatoms: 1-Z

Unsaturation: benzo derivatives

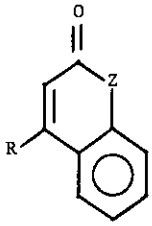
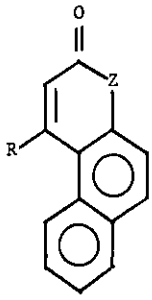
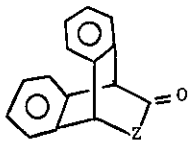
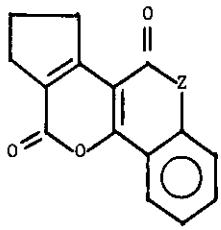
Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	R						
	Me	CCl_4	1648	300	CCl_4	1744	300
		$HCCl_3$	1633	300	mull	1725	221
	Ph	CCl_4	1650	353	-	1729	263
							
	H	mull	1645	231	mull	1720	88,254
					$HCCl_3$	1724	17
	Ph	CCl_4	1660	353	-	1735	12
		CH_2Cl_2	1695	5			
		KBr	1720,1630	234	-	1750,1700	189

Table IX (continued)

Ring size: 6

Heteroatoms: 1-Z

Unsaturation: benzo derivatives

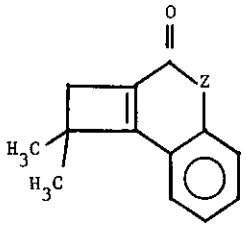
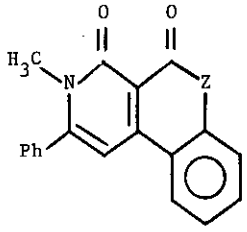
Compound	Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	KBr	1637	188			
	KBr	1679	360	KBr	1746	360
	$HCCl_3$	1680	360	$HCCl_3$	1749	360

Table X

Ring size: 4

Heteroatoms: 1-Z, 3-Y

Unsaturation: none

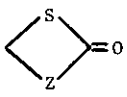
Compound	Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	mull	1800, 1750	123			

Table XI

Ring size: 5

Heteroatoms: 1-Z, 2-Y

Unsaturation: none; endocyclic; benzo derivatives

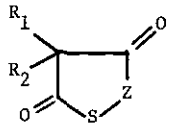
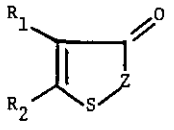
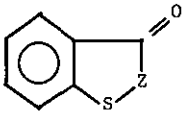
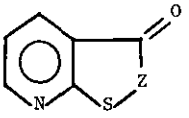
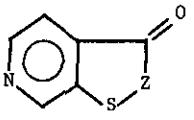
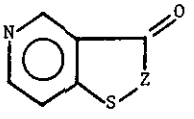
Compound			Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	R_1	R_2						
	Et	Et	neat	1720,1680	313			
	n-Bu	n-Bu				CCl_4	1783	3
	$-(CH_2)_3-$		neat	1760,1670	313	$HCCl_3$	1803	224
	R_1	R_2						
	Ph	H	KBr	1625	45			
	H	Ph	KBr	1650,1640	45			
	Ph	Ph	KBr	1650	45			
	$-(CH_2)_3-$		KBr	1650,1640	45			
			KBr	1670,1650	45			
			CCl_4	1680	298			
			KBr	1670	22			
			KBr	1640	22			
			KBr	1650	22			

Table XI (continued)

Ring size: 5

Heteroatoms: 1-Z, 2-Y

Unsaturation: none

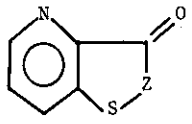
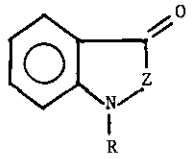
Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
		KBr	1650	22			
	R						
	H	$HCCl_3$	1662	52	$HCCl_3$	1773,1751	80
		KBr	1605	52			
	Me	KBr	1645,1600	4			

Table XII

Ring size: 5

Heteroatoms: 1-Z, 3-Y

Unsaturation: none; exocyclic

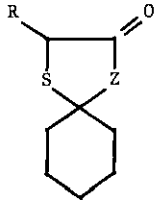
Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	R						
	H	-	1680	316	CCl_4	1765	210
	Me	-	1680	316	NaCl	1760	64

Table XII (continued)

Ring size: 5

Heteroatoms: 1-Z, 3-Y

Unsaturation: none; exocyclic

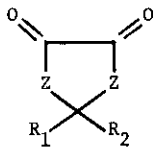
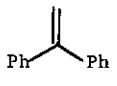
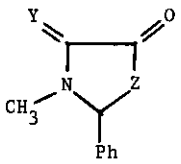
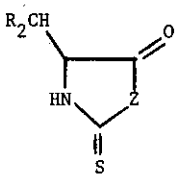
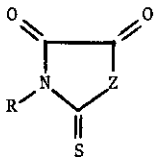
Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	R_1 R_2						
	H H	KBr	1658	312	KBr	1845,1792	327
	$-(CH_2)_5-$	$HCCl_3$	1689	61			
		CCl_4	1682	275			
	Y						
	O	mull	1720,1710	329			
	S				KBr	1795	196
	R						
	Ph	-	1735	250			
	Me				-	1848	203
	R						
	H	-	1742	148			
	Me	-	1740,1715	149			
	Ph	-	1755,1725	149			

Table XII (continued)

Ring size: 5

Heteroatoms: 1-Z, 3-Y

Unsaturation: endocyclic and exocyclic

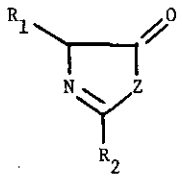
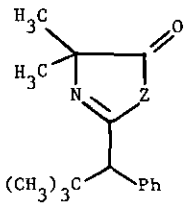
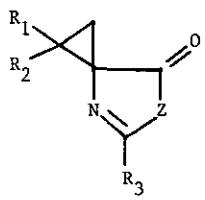
Compound			Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	R_1	R_2						
	H	Ph	$HCCl_3$	1730	20	$HCCl_3$	1821	356
						CH_2Cl_2	1825	168
						KBr	1810	352
						MeCN	1835	372
	Me	Ph	$HCCl_3$	1725	342	$HCCl_3$	1835	324
						neat	1840	261
						KBr	1830	131
	iPr	Ph	$HCCl_3$	1724	20	-	1830	95
	Ph_2CH	Ph	$HCCl_3$	1705	117	mull	1810	116
	Ph_2CH	OCH_2Ph	neat	1720	330			
	iPr	OCH_2Ph				neat	1845	34
			neat	1720	315			
								
R_1	R_2	R_3						
H	Ph	Me	KBr	1690	15	KBr	1795	14
Ph	H	Me	KBr	1690	15	KBr	1795	14
Me	Ph	Me	KBr	1720	15	KBr	1810	14

Table XII (continued)

Ring size: 5

Heteroatoms: 1-Z, 3-Y

Unsaturation: endocyclic and exocyclic

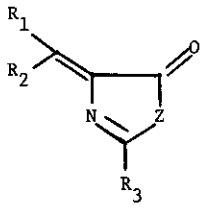
Compound			Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
R_1	R_2	R_3						
H	Ph	Ph	KBr	1700	15	KBr	1800	14
H	Ph	OCH_2Ph	KBr	1720	15			
H	Ph	SCH_2Ph	KBr	1710	15			
								
R_1	R_2	R_3						
H	Ph	Me	KBr	1699,1678	36	$HCCl_3$	1810,1780	279
						mull	1800,1770	207
H	Ph	Ph	$HCCl_3$	1684	117	$HCCl_3$	1780,1760	279
						mull	1800,1774	215
						mull	1790,1770	207
Me	Me	Ph	$HCCl_3$	1686	20	CCl_4	1802	351
Me	Ph	Me	KBr	1680,1660	15	KBr	1790,1760	14
$-(CH_2)_5-$		Ph	-	1676	197	-	1770,1750	197
						mull	1780,1750	207
H	Ph	OCH_2Ph	KBr	1723,1697	36	-	1820,1795	185

Table XIII

Ring size: 5

Heteroatoms: 1-Z, 4-Y

Unsaturation: none

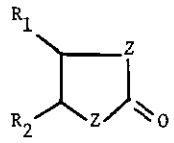
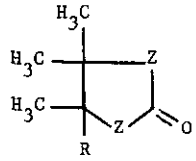
Compound			Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	R_1	R_2						
	H	H	neat	1638	232	neat	1798	232
						neat	1800	227
			$HCCl_3$	1672,1637	182	$HCCl_3$	1808	182
			$HCCl_3$	1666,1633	311	$HCCl_3$	1812	10,62
						$HCCl_3$	1795	25
						CCl_4	1831	62
						CCl_4	1825	10
						CCl_4	1820	32
						CCl_4	1818	240
	H	Ph	-	1633	233	CS_2	1816	150
						KCl	1770	150
	Br	Br	KBr	1745,1685	311			
cis	Me	Me	$HCCl_3$	1630	190			
trans	Me	Me	$HCCl_3$	1640	190			
trans	$-(CH_2)_3-$		$HCCl_3$	1685,1645	190			
cis	$-(CH_2)_4-$		neat	1716	118			
trans	$-(CH_2)_4-$		$HCCl_3$	1650,1610	190			
trans	$-(CH_2)_5-$		$HCCl_3$	1630	190			
	R							
	H		$HCCl_3$	1640	190			
	Me					-	1782,1754	305

Table XIII (continued)

Ring size: 5

Heteroatoms: 1-Z, 4-Y

Unsaturation: none

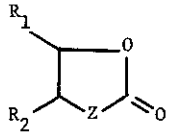
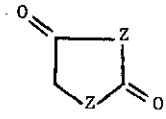
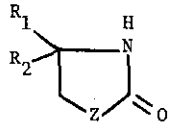
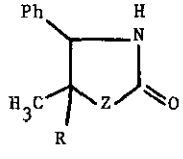
Compound			Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	R_1	R_2						
	H	H	neat	1724	209			
			$HCCl_3$	1739	182			
cis	Me	Me	neat	1730	118			
trans	Me	Me	neat	1723	118			
			-	1689,1637	202			
	R_1	R_2						
	H	H	KBr	1665	85	KBr	1725	85
						KBr	1724	232
						KBr	1730	151
			CCl_4	1710	85	CCl_4	1782	85
						CCl_4	1783	151
						$HCCl_3$	1760	274
						mull	1720	331
						mull	1710	151
	H	Ph	$HCCl_3$	1690	370	$HCCl_3$	1760	173
	Me	Ph	$HCCl_3$	1673	370	KBr	1740	124
	R							
	H		$HCCl_3$	1690	370			
	Me					KBr	1740	159

Table XIII (continued)

Ring size: 5

Heteroatoms: 1-Z, 4-Y

Unsaturation: none; exocyclic

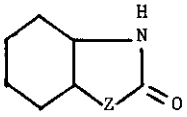
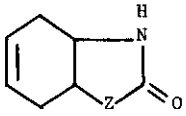
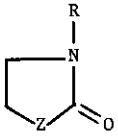
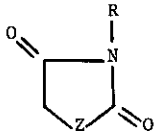
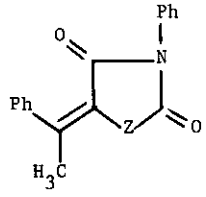
Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
		$HCCl_3$	1677	371			
					KBr	1730,1710	320
	R						
	Me	-	1670	77	$HCCl_3$	1746	274
		-	1665	358			
	Ph	-	1670	332	$HCCl_3$	1753	274
	R						
	Me	-	1690,1630	334			
	Ph	-	1760,1680	334			
		-	1681	249			

Table XIV

Ring size: 5
Heteroatoms: 1-Z, 4-Y
Unsaturation: endocyclic

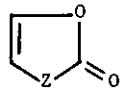
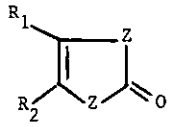
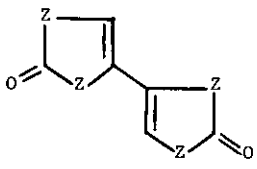
Compound			Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
			neat	1736	209	neat	1825	209
						neat	1830	150
						CCl_4	1833	150
						CS_2	1832	135
	R_1	R_2						
	H	Me	$HCCl_3$	1725,1685	38	$HCCl_3$	1832,1808	54
						CCl_4	1838,1792	54
	H	Ph	KBr	1660	28	KBr	1802	341
			$HCCl_3$	1733,1690	38	-	1805	245
	H	Br	-	1710,1670	311	CCl_4	1865	311
	Me	Et	$HCCl_3$	1642	38			
	Ph	Ph	$HCCl_3$	1690	38	CCl_4	1870,1820	328
						KBr	1820	158,341
	CN	CN	KBr	1680	46			
	$-CH_2-\underset{\underset{Me}{\vert}}{CH}-CH_2-$		neat	1720,1678	111			
	$-\underset{\underset{Me}{\vert}}{CH}-(CH)_2-$		neat	1718,1672	111			
	$-(CH_2)_4-$		$HCCl_3$	1738,1670	38	neat	1820,1750	158
			KBr	1640	9			

Table XIV (continued)

Ring size: 5

Heteroatoms: 1-Z, 4-Y

Unsaturation: endocyclic

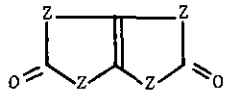
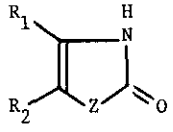
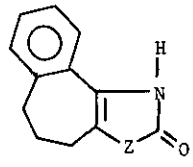
Compound			Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
			KBr	1678	325			
			KBr	1654	206			
	R_1	R_2						
	H	H	CCl_4	1693,1661	82	CH_2Cl_2	1765,1740	319
			THF	1692	375	KBr	1785,1760	318
	Me	H	CCl_4	1692,1660	82			
			THF	1692	375			
	t-Bu	H	CCl_4	1691,1660	82			
	Ph	H	CCl_4	1698,1661	82			
	H	Me	CCl_4	1695,1662	82			
	Me	CO_2Me	KBr	1680	139			
			mull	1659,1647	374			

Table XIV (continued)

Ring size: 5

Heteroatoms: 1-Z, 4-Y

Unsaturation: endocyclic

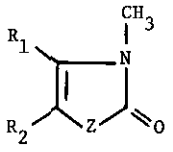
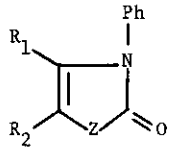
Compound			Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	R_1	R_2						
	H	H	KBr	1649	377	KBr	1740	319
			CCl_4	1676	82			
			CCl_4	1665	377			
			THF	1676	375			
	Me	H	CCl_4	1677	82			
			THF	1676	375			
	t-Bu	H	CCl_4	1685,1670	82			
	Ph	H	CCl_4	1677	82			
	H	Me	CCl_4	1678	82			
	H	CO_2Me	-	1700,1630	145			
	Me	CO_2Me	KBr	1670	139			
	CO_2Me	CO_2Me	-	1730,1675	145			
	Ph	Ph				KBr	1749	128
	SMe	Ph	-	1620	56			

Table XIV (continued)

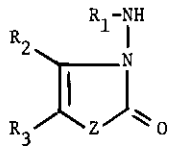
Ring size: 5

Heteroatoms: 1-Z, 4-Y

Unsaturation: endocyclic



R_1	R_2	Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
Ph	H	CH_2Cl_2	1663	285	mull	1757	301
H	CO_2Me	-	1705,1650	145			
Me	CO_2Me	KBr	1680,1670	139			
Ph	CO_2Et	-	1675,1655	145			
CO_2Me	CO_2Me	-	1725,1690	145			



R_1	R_2	R_3					
H	Ph	H	KBr	1695	104		
Me	Ph	H	KBr	1640	104		
Ph	Ph	H	KBr	1630	104		
Ph	Me	Me	KBr	1665	104		

Table XV

Ring size: 5

Heteroatoms: 1-Z, 4-Y

Unsaturation: benzo derivatives

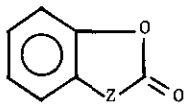
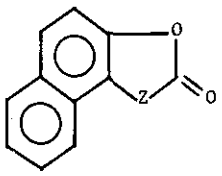
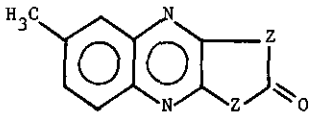
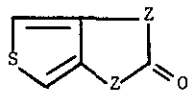
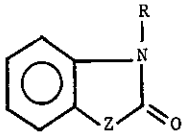
Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
		neat	1760	99	-	1855	233
					-	1835	90
					-	1820	354
		KBr	1753,1731	377			
		CCl_4	1776,1765	377			
		KBr	1733	134			
		KBr	1635	74a			
	R						
	H	mull	1655	338	KBr	1767,1726	258
					KBr	1740	251
					-	1769,1740	127
	Me	KBr	1681	377	KBr	1765	87
		-	1695	233	-	1769,1740	127
		-	1680	198			
		mull	1693	338			
		CCl_4	1686	377			
	$SiMe_3$	KBr	1650	204			

Table XVI

Ring size: 5
Heteroatoms: 1-Z, 2-Y, 4-Y and 1-Z, 3-Y, 4-Y
Unsaturation: endocyclic

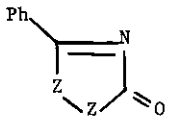
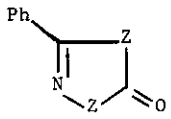
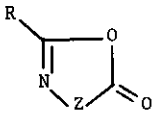
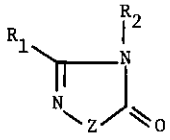
Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
		-	1683	93	$HCCl_3$	1815	160
		mull	1690	264	$HCCl_3$	1866,1834	310
		KBr	1680	28	-	1855,1828	101
	R						
	Me	neat	1760	167,264			
	Ph	mull	1740	167,264			
		CCl_4	1780,1750	326			
	CO_2Et	$HCCl_3$	1816,1750	167			
	R_1 R_2						
	Me Me	KBr	1680	347	KBr	1786	359
	Ph Me	KBr	1680	347	$HCCl_3$	1780	127
	Ph Ph	KBr	1673	347	$HCCl_3$	1776	310
	$-S-CH_2-CH_2-$	mull	1676	24			
	-S-CH = CH -	mull	1660	24			
	-N=CH-CH=CH-	mull	1677	24			

Table XVI (continued)

Ring size: 5

Heteroatoms: 1-Z, 2-Y, 4-Y and 1-Z, 3-Y, 4-Y

Unsaturation: endocyclic

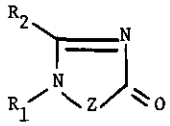
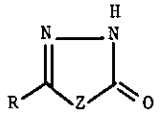
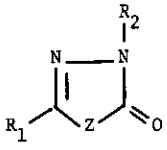
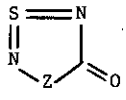
Compound			Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
								
R_1	R_2							
-CH=CH-S-			KBr	1735	272			
-CH=CCl-S-			CH_2Cl_2	1720,1690	273			
-N=CCl-CH=CH-			KBr	1720	272			
		R						
		H	CH_2Cl_2	1695	368			
		Me	CH_2Cl_2	1694	368	-	1770	205
		iPr	CH_2Cl_2	1692	368			
		c-C_6H_{11}				neat	1780	35
		c-C_3H_5	CH_2Cl_2	1694	368			
		t-Bu	CH_2Cl_2	1692	368	KBr	1770	205
		Ph	CH_2Cl_2	1696	368	CH_2Cl_2	1793	132
						KBr	1770	205
		R_1	R_2					
		H	Me	CH_2Cl_2	1678	368		
		Me	Me	CH_2Cl_2	1678	368		
		Et	Ph			mull	1796	187
		OMe	Ph	-	1686	203		
		NH_2	Ph	-	1675	307		
				-	1727	299		

Table XVII

Ring size: 6

Heteroatoms: 1-Z, 3-Z

Unsaturation: none; exocyclic

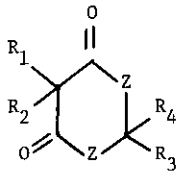
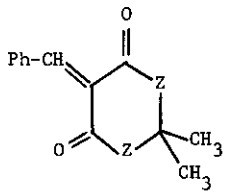
Compound				Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
									
R_1	R_2	R_3	R_4						
H	H	H	H	KBr	1661	312			
H	Me	H	H	KBr	1692,1667	312			
Me	Me	H	H	KBr	1672,1653	312			
H	H	H	Me	KBr	1669	312			
H	H	Me	Me	KBr	1658	312	KBr	1789,1745	41
							mull	1785,1753	1
							CCl_4	1794,1770	41
							$HCCl_3$	1787,1760	337
							$HCCl_3$	1778,1749	1
H	Me	Me	Me	KBr	1692,1664	312	$HCCl_3$	1790,1775	19
Me	Me	Me	Me	neat	1681,1658	312	mull	1780,1745	1
							CCl_4	1787,1749	1
							CCl_4	1782,1742	41
							$HCCl_3$	1770,1735	1
				KBr	1667,1647	312	KBr	1752,1720	41

Table XVIII

Ring size: 6

Heteroatoms: 1-Z, 3-Y

Unsaturation: endocyclic; benzo derivatives

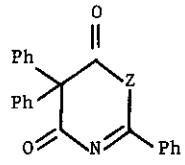
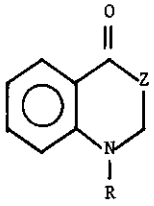
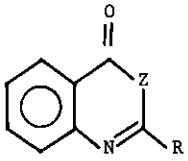
Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
		$HCCl_3$	1722,1690	126			
	R						
	Me	KBr	1615	213	KBr	1717	213
	Ph	KBr	1632	213	KBr	1712	213
	R						
	Me	KBr	1669	212	KBr	1760	283
	Ph	KBr	1651	212	KBr	1770	283
					KBr	1760	212
		$\underline{c}$-C_6H_{12}	1657	212	$\underline{c}$-C_6H_{12}	1768	212
					$HCCl_3$	1773	317
					$HCCl_3$	1755	345

Table XIX

Ring size: 6

Heteroatoms: 1-Z, 4-Y

Unsaturation: none; endocyclic and benzo derivatives

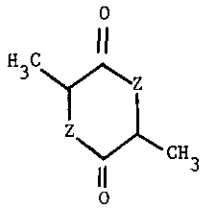
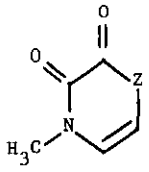
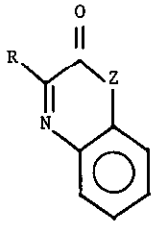
Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
		KBr	1680	60	mull	1750	238
		KBr	1665	161			
	R						
	Ph	-	1625	284	$HCCl_3$	1740	75,294
	NH_2	KBr	1695	18	mull	1790	230
		$HCBr_3$	1695	18			

Table XX

Ring size: 6

Heteroatoms: 1-Z, 5-Y; 1-Z, 2-Y, 3-Y; 1-Z, 4-Y, 5-Y

Unsaturation: benzo derivatives, endocyclic

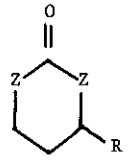
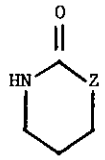
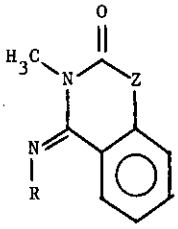
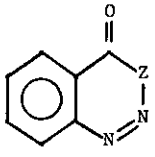
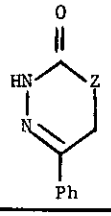
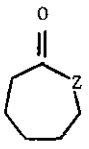
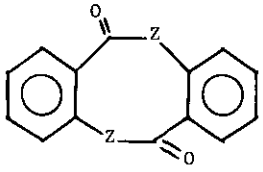
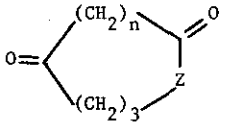
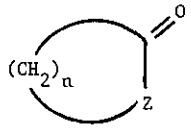
Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
	R						
	H	-	1600	2	neat	1747	151
		KBr	1590	309	CCl_4	1777	151
					CCl_4	1776,1768	62
					$HCCl_3$	1779,1753	62
					$HCCl_3$	1751	271
	Me	$HCCl_3$	1600	190	-	1733-1724	305
		KBr	1620	138	neat	1692	68
	R						
	Me	KBr	1672,1640	53			
	Ph	KBr	1655,1620	53			
		KBr	1670	113,114			
		KBr	1640	103			

Table XXI

Ring size: 7, 8, 12, 16

Heteroatoms: 1-Z

Unsaturation: none; benzo derivative

Compound		Phase	$\nu^{S}_{C=O}$	Ref.	Phase	$\nu^{O}_{C=O}$	Ref.
		-	1665	260	CCl_4	1739	32
					CCl_4	1730	79
		gas	1750,1740	376	gas	1760,1750	376
		-	1700	70			
		$HCCl_3$	1690,1675	298			
	n						
	6	KBr	1706,1678	13	CH_2Cl_2	1730,1710	51
	10	KBr	1704,1689	13	KBr	1733,1712	220
					neat	1735,1715	50
	n						
	14	KBr	1692	220	KBr	1733	220

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