fore upon its physical state. The discussion is further complicated by our lack of knowledge of the partial specific volume of the lattice water. The calculations made here, of the changes in partial specific volume of the protein, depend upon the assumption that the partial specific volume of the water remains unchanged. Perutz[19] and his co-workers have adopted the alternative assumption that the partial specific volume of the protein remains constant in the crystal at all stages of drying and that the partial specific volume of the liquid of crystallization changes. Both assumptions are probably equally inadequate since the intermolecular binding between the molecules of protein and of water presumably leads to changes in the specific volume of both components of the crystals.

The formula of Adair and Adair cannot be used with accuracy for calculations on "air-dried" crystals since it is based on the assumption that values for the partial specific volume of both protein and water remain constant on drying the crystal. It does, however, appear to be applicable to the calculation of the weight fractions of protein in "wet" crystals and thus the protein molecular weights, where composition measurements are not available.

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[CONTRIBUTION FROM DEPARTMENT OF CHEMISTRY, OREGON STATE COLLEGE]

Quinazolines. XIII. A Study of the Infrared Spectra of Certain Quinazoline Derivatives[1]

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The infrared spectra of twenty quinazoline, quinazolone and quinazolinedione derivatives were obtained as a preliminary to the investigation of the structures of some anomalous quinazoline compounds. The ten compounds representing the quinazoline series are found to give rise to three bands in the "double bond" region: 1478 to 1517 cm.$^{-1}$, 1566 to 1581 cm.$^{-1}$, and 1612 to 1628 cm.$^{-1}$. These bands are designated "Quinazoline I, II and III," respectively. However, it was observed that 4-mercaptoquinazoline has an anomalous absorption in this region which indicated the possibility of a thione structure. The infrared spectra of 4-mercaptoquinazoline and 2-methyl-4-mercaptoquinazoline were obtained in the region 2500 to 3500 cm.$^{-1}$, using a lithium fluoride prism. It was found that both compounds possess a band in the N–H region but no band in the S–H region which proves the thione structure. The six compounds representing the quinazalone series were investigated and the carbonyl band was found to give rise to an absorption in the region 1637 to 1704 cm.$^{-1}$. The C═N band was more difficult to identify as conjugation and substitution effects are more pronounced. No bands which could be identified with the quinazalone ring system were observed. The quinazolinedione series was found to possess two carbonyl frequencies in agreement with other diacylimides. Two other bands found in the "double bond" region are apparently associated with the quinazolinedione ring system.

There have been few systematic investigations of ring systems to find characteristic bands which would help identify the rings. The phenyl group, of course, has been extensively investigated and three or four characteristic bands establish the presence of this group readily.[2] Randall, *et al.*,[2] have also assigned a pair of characteristic absorption bands both to the thiazole and benzthiazole rings. The lack of assigned bands for most ring systems makes it necessary to obtain a large number of spectra when undertaking a structural investigation involving some specific ring. This was the case when it was necessary in this Laboratory to use the infrared spectra as an aid in investigating the structures of certain quinazoline compounds.[3,4]

The only systematic study of absorption spectra of quinazoline derivatives published thus far is that of Elderfield, *et al.*,[5] who recorded the ultraviolet absorption spectra of quinazoline, dihydroquinazoline and related derivatives. A few isolated quinazalone compounds have had their spectra recorded in the ultraviolet but the use of ultraviolet spectra in the investigation of structures is limited by solvent effects and lack of resolution of the vibrational spectra. Since the vibrational spectrum furnishes the most information with regard to functional groups in any complex organic molecule, the decision was made to study the absorption of quinazoline compounds in the infrared. During the course of the present work the spectra of several quinazolines, quinazalones and quinazolinediones were obtained. From these data it is apparent that certain characteristic absorption bands are associated with the quinazoline ring.

Experimental

Preparation of Compounds.—The compounds used in this investigation are given in Table I. The references cited refer to the method of preparation.

Preparation of Samples for Infrared Absorption.—Two compounds of this series (4-methylquinazoline and 2,4-dimethylquinazoline) were liquids at room temperature and were observed as capillary films between rock salt windows. Samples of the low melting solids (m.p. less than 150°)

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(2) H. N. Randall, *et al.*, "Infrared Determination of Organic Structures," D. Van Nostrand Co., Inc., New York, N. Y., 1949.

(3) A. Tomisek and B. E. Christensen, THIS JOURNAL, **70**, 2423 (1948).

(4) C. H. Wang, T. C. Feng and B. E. Christensen, *ibid.*, **72**, 4887 (1950).

(5) R. C. Elderfield, *et al.*, *J. Org. Chem.*, **12**, 405 (1947).

TABLE I

	M.p., °C.		M.p., °C.
QUINAZOLINES			
Quinazoline[5]	48	6-Acetyl-2,4-dimethylquinazoline[10]	92
2-Methoxyquinazoline[6]	58	2,4-Dimethoxyquinazoline[12]	69
4-Methoxyquinazoline[7]	33	4-Mercaptoquinazoline[13]	329 dec.
2-Methylquinazoline[8]	...	2-Methyl-4-mercaptoquinazoline[14]	...
4-Methylquinazoline[9]	...	2,4-Dimethylquinazoline[11]	...
QUINAZOLONES			
4-Quinazolone[15]	220	2,3-Dimethyl-4-quinazolone[16]	111
2-Methyl-4-quinazolone[16]	240	1,2-Dimethyl-4-quinazolone[18]	206
3-Methyl-4-quinazolone[17]	104-106	2-Quinazolone[19]	250
QUINAZOLINEDIONES			
2,4-Quinazolinedione[20]	above 350	3-Methyl-2,4-quinazolinedione[22]	240
1-Methyl-2,4-quinazolinedione[21]	265	1,3-Dimethyl-2,4-quinazolinedione[12]	170

were prepared by heating approximately 10 mg. of sample between rock salt windows until a clear capillary film was obtained, which was then allowed to solidify. The high melting solids were prepared in the form of emulsions in a paraffin oil (sold under the trade name of "Nujol") as described by Randall, *et al.*[2] The strong bands due to this material which appear at about 2915, 1460 and 1375 cm.$^{-1}$ are designated with a footnote in Tables II and III.

Infrared Spectrometer.—The instrument employed consisted of the source, monochromator, and detector of the Perkin–Elmer Model 12C instrument together with a light-chopper, amplifier and recording unit designed after the double-beam modification described by Savitzky and Halford.[23] The present data were, however, obtained by the single-beam method, *i.e.*, by recording the absorption of a suitable blank, followed by that of the sample; the transmission curves of Fig. 1 through 6 were plotted by determining I/I_0 point-by-point.

A sodium chloride prism was ordinarily employed between 3500 and 700 cm.$^{-1}$, but was occasionally replaced by a lithium fluoride prism for better resolution in the range 3500–2500 cm.$^{-1}$. Relatively large slit settings were used, namely, 0.045 mm. starting at 3500 cm.$^{-1}$, 0.090 mm. at 2000 cm.$^{-1}$, 0.225 mm. at 1200 cm.$^{-1}$, and 0.500 mm. at 700 cm.$^{-1}$.

Results

The transmission curves for the quinazoline and quinazolone series are given in Figs. 1 through 6. The frequencies of the band maxima are summarized in Tables II, III and IV; in the tables, qualitative estimates of the relative intensities are given, but these estimates are, of course, not very accurate for some peaks whose apparent strength may be due to superposition upon a strong and relatively broad band.

Discussion

Quinazolines.—This group consists of the methyl, methoxy and mercapto derivatives of quinazoline (Table II, Figs. 1–4). The region of the spectra of these compounds which is of the greatest interest lies between 1500 and 1700 cm.$^{-1}$. This part of the spectrum is often called the "double bond" region and bands due to the C=O, C=N and C=C occur here; the N–H bending of amines, the phenyl group and various ring structures containing double bonds also give rise to absorption bands in this region.[2] In the case of quinazoline and its derivatives, three bands are found which occur between 1478 and 1517 cm.$^{-1}$, between 1566 and 1581 cm.$^{-1}$, and between 1612 and 1628 cm.$^{-1}$. These bands will hereafter be designated "Quinazoline I, II and III," respectively. These bands are generally sharp and quite strong, being of approximately the same intensity as an absorption due to a carbonyl group. A comparison of the strength of these bands can readily be made from the spectrum of 6-acetyl-2,4-dimethylquinazoline (Fig. 4) which contains a conjugated carbonyl group as well as the completely conjugated quinazoline ring.

It is difficult to attribute the individual absorption bands to specific groups in the molecule. At first glance it would appear that the absorption bands are those associated with a conjugated phenyl group which has bands at 1488–1500 cm.$^{-1}$, 1580–1587 cm.$^{-1}$ and 1605–1619 cm.$^{-1}$.[2] Another possibility is that the absorption bands "Quinazoline II and III" are caused by the C=N groups, of which there are two, present in the quinazoline ring. The remaining band, "Quinazoline I," could then be attributed to the conjugated phenyl group, the other bands of the phenyl group being systematically concealed by the C=N absorptions. However, even if this were the case, the assignment of a specific absorption band to a specific C=N group would be difficult. The simplest method of circumventing this difficulty is to consider the three bands as being due to the conjugated quinazoline ring system as a whole without designating the structural detail associated with each specific absorption band.

Of the ten compounds investigated containing a conjugated quinazoline ring system, only one, 4-mercaptoquinazoline, shows an anomalous band of considerable strength in the region 1500 to 1700

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TABLE II

INFRARED ABSORPTION SPECTRA IN CM.$^{-1}$ OF QUINAZOLINE SERIES

vw, very weak; w, weak; m, medium; s, strong; vs, very strong; 1, quinazoline (melt); 2, methylquinazoline (melt); 3, 4-methylquinazoline (capillary film); 4, 2,4-dimethylquinazoline (capillary film); 5, 2-methoxyquinazoline (melt); 6, 4-methoxyquinazoline (melt); 7, 2,4-dimethoxyquinazoline (melt); 8, 4-mercaptoquinazoline (Nujol); 9, 2-methyl-4-mercaptoquinazoline (Nujol); 10, 6-acetyl-2,4-dimethylquinazoline (Nujol).

1	2	3	4	5
3020w	3020w	3380m	3405vw	2915w
1622s	1622vs	3040w	2915vw	1668vw
1566vs	1574vs	1696s	1652vw	1621vs
1492s	1489s	1645m	1622w	1584vs
1408w	1408vs	1612s	1569vs	1475vs
1379vs	1381s	1566vs	1498m	1437m
1306m	1332w	1498s	1437m	1399vs
1238vw	1302vw	1451w	1401m	1351vs
1214w	1274w	1399s	1369w	1323s
1152m	1239m	1357m	1334m	1295m
1138m	1203m	1249m	1214w	1278m
1075m	1138w	1163m	1163vw	1244s
1017vw	1123vw	1108w	1126vw	1217s
964vw	1042w	1029w	1025w	1142m
943m	1012w	962w	988w	1121vw
926w	966w	884m	960vw	1049s
870w	942w	822vw	941vw	1016w
823w	869w	794w	866w	978m
796s	791s	765vs	789w	953w
779w	759vs	714vw	763vs	920vw
755vs	725w			867w
				798m
				764m
				727s

6	7	8	9	10
2945w	3000w	3130w	3130w	3380m
1684vw	2930w	2915s[a]	2915vs[a]	3150m
1622vs	1628vs	1684vw	1615m	2915vs[a]
1572vs	1581vs	1622m	1569vs	1680vs
1503vs	1517s	1595s	1512s	1615m
1449vs	1461s	1569m	1461vs[a]	1566vs
1381vs	1387s	1523w	1421w	1523m
1306m	1365s	1401vw	1379w[a]	1495m
1268vw	1328s	1338vw	1351vw	1459vs[a]
1199m	1282w	1308m	1321w	1444vs
1163m	1247m	1265m	1257w	1404s
1121w	1203m	1252vs	1241vs	1373vs[a]
1098vs	1135w	1204w	1218m	1334s
978s	1110m	1160w	1156w	1314m
886m	1073m	1118m	1123m	1260vs
876m	1025w	1031w	1042m	1211m
817vw	1003vw	955vw	1002m	1131m
802w	982w	909m	951w	1073m
772vs	956m	889w	870vw	1023m
747m	920vw	870vs	837vs	986w
	892vw	811m	763vs	960w
	795m	773s		943vw
	767vs	765vs		900w
	747vw			854vs
				820vw
				759vw
				721w

[a] Nujol absorption band.

TABLE III

INFRARED SPECTRA IN CM.$^{-1}$ OF QUINAZALONES

vw, very weak; w, weak; m, medium; s, strong; vs, very strong: 1, 4-quinazalone (Nujol); 2, 2-methyl-4-quinazalone (Nujol); 3, 3-methyl-4-quinazalone (melt); 4, 2,3-dimethyl-4-quinazalone (melt); 5, 1,2-dimethyl-4-quinazalone (Nujol); 6, 2-quinazalone (Nujol).

1	2	3	4	5	6
3132m	3132m	2965w	2915w	2915vs[a]	3150m
2915vs[a]	3040m	2915w	1672vs	1637vs	3040m
1704vs	2915s[a]	1855w	1593vs	1597vs	2915vs[a]
1664vs	1676vs	1732w	1566s	1534vs	1684vs
1608vs	1625vs	1676vs	1466s	1498s	1645s
1461m[a]	1478m	1612vs	1415m	1459s[a]	1608s
1391m	1421w	1557m	1381s	1406s	1500w
1330m	1343vw	1473s	1343s	1336w	1459s[a]
1310m	1319vw	1439s	1298m	1295vw	1417vs
1262m	1295m	1399m	1270m	1265w	1375w[a]
1238m	1255w	1342s	1234vw	1187m	1312m
1174m	1144m	1324s	1191vw	1160w	1273w
1152w	1041w	1298m	1153m	1112w	1224w
1125w	1029vw	1265m	1040m	1075w	1192vw
932m	1001w	1218w	1018m	1040vw	1133w
921s	988w	1190m	958vw	1025m	1083w
911m	888s	1156m	873m	902vw	1060m
884w	773vs	1108m	797vw	810vw	945vw
824w	763m	1071m	778s	775vs	919vw
802w		1027w	702m	706vw	885vw
777w		935s			821w
765vs		877m			795vw
		798m			746vs
		773vs			
		703s			

[a] Nujol absorption band.

TABLE IV

INFRARED SPECTRA IN CM.$^{-1}$ OF QUINAZOLINEDIONES

vw, very weak; w, weak; m, medium; s, strong; vs, very strong: 1, 2,4-quinazolinedione (Nujol); 2, 1-methyl-2,4-quinazolinedione (Nujol); 3, 3-methyl-2,4-quinazolinedione (Nujol); 4, 1,3-dimethyl-2,4-quinazolinedione (Nujol).

1	2	3	4
3150m	3150m	3150w	2915vs[a]
3040m	3040m	2915m[a]	1700vs
2915vs[a]	2915s[a]	1720vs	1656vs
1696vs	1700vs	1668vs	1612s
1684vs	1668vs	1594m	1495vs
1664vs	1601vs	1495m	1459s[a]
1615s	1489s	1459s[a]	1430s
1509m	1437m	1434m	1381m[a]
1440s	1399s	1389w	1351m
1406m	1332m	1343vw	1334m
1304m	1179w	1306m	1121w
1141m	1154w	1226vw	1105w
1040vw	1114vw	1174vw	1066w
858w	1076w	1043w	1040w
796w	1042w	1028w	1001w
776w	952vw	927vw	865w
759s	876w	873vw	755vs
	860w	837w	
	832w	763vs	
	759s	754w	
	726m	716w	

[a] Nujol absorption band.

cm.$^{-1}$. Some of the other compounds, notably 4-methyl and 2,4-dimethylquinazoline, show weak bands in the region 1680 to 1700 cm.$^{-1}$ which probably arise from impurities containing a carbonyl group.

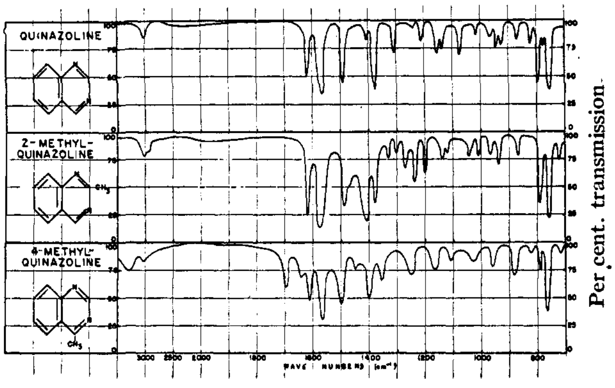


Figure 1.

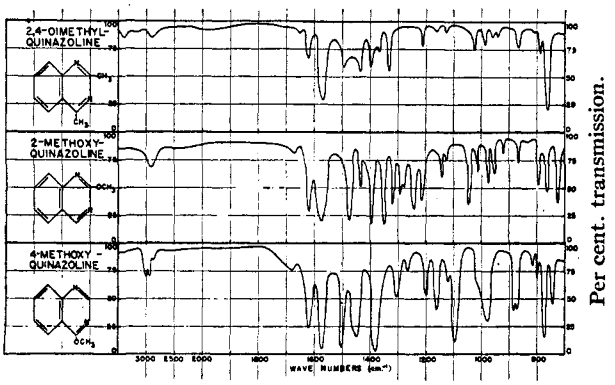


Figure 2.

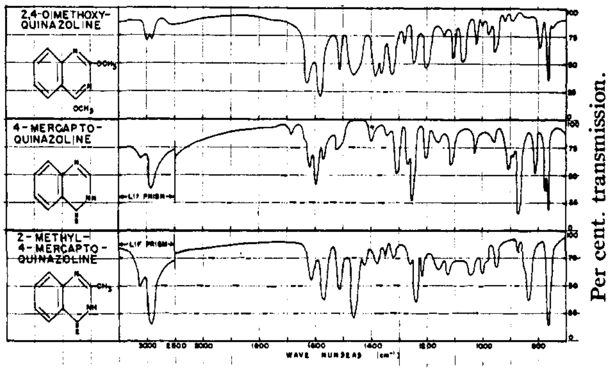


Figure 3.

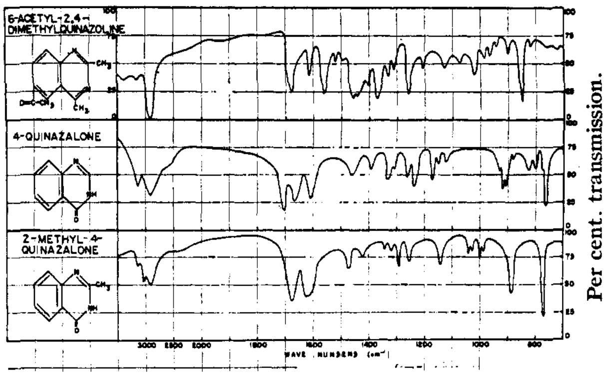


Figure 4.

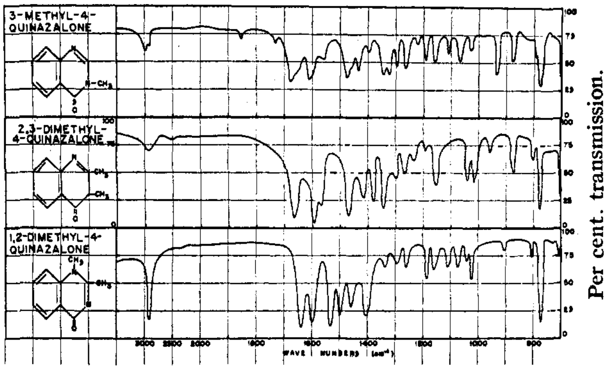


Figure 5.

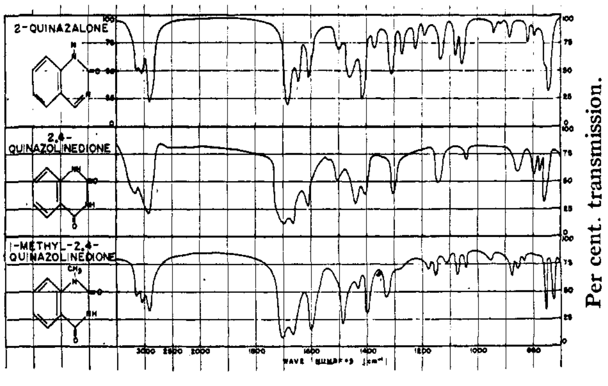
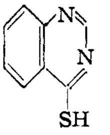
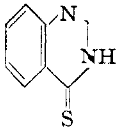


Figure 6.

For this reason 4-mercaptoquinazoline was again investigated to determine if the compound possibly had a thione structure rather than a thiol. The structures of the two forms are





There has been a considerable amount of work done recently on problems of a similar nature and complete agreement on the correct structure has not always been reached. Randall, *et al.*, in their book, present the spectra of many thioamides and discuss in detail the structure of the compound commonly called 2-mercaptothiazoline.[2] They concluded that this compound was actually a thione since it possessed absorptions at 3125 and 1512 cm.$^{-1}$ indicating the presence of a N–H group and a "thioureide" group, respectively. If the compound were a thiol the bands expected would be at 2500 cm.$^{-1}$, due to the S–H group, and in the vicinity of 1650 cm.$^{-1}$ for the C=N group.

In the investigation of the structure of 4-mercaptoquinazoline it was decided to include 2-methyl-4-mercaptoquinazoline due to their great similarity. It was the opinion that the spectrum from 2500 to 3300 cm.$^{-1}$ offered the greatest possibilities since the N–H and S–H stretching frequencies lie in this region. For this purpose a lithium fluoride prism was employed to increase the resolution. Both spectra when obtained under these conditions show bands at 3130 cm.$^{-1}$. These absorptions almost certainly arise from a N—H group and coupled with the absence of any absorption in the 2500 cm.$^{-1}$ region indicate the structures to be of the thione type. Two of the absorption bands in the 1500–1700 cm.$^{-1}$ region can be attributed to the C=N group (1615 cm.$^{-1}$) and the thioureide group (1500 cm.$^{-1}$). The other bands cannot be definitely attributed to any specific functional groups.

Quinazalones.—An examination of the spectra of the quinazalones (Table III and Figs. 4–6) shows two or three strong bands occurring in the "double bond" region from 1500 to 1700 cm.$^{-1}$. The strongest and most recognizable band in this region, the N-acyl carbonyl, lies between 1637 and 1704 cm.$^{-1}$ in all the compounds investigated. According to Randall, *et al.*, the normal position for this band is from 1630 to 1719 cm.$^{-1}$.[2] The methylation of the quinazalone ring in the 2 or 3 position or in both, has about the same effect in causing the carbonyl frequency to be lowered by 20 to 30 cm.$^{-1}$. Methylation in the 1,2-position, however, results in a lowering of the frequency by 67 cm.$^{-1}$. This large shift may be due to the fact that the carbonyl group of 1,2-dimethyl-4-quinazalone is directly conjugated with a N=C group, the structure being C_6H_4—C—N=C. The apparently greater conjugation effect produced by an adjacent C=N group over that produced by a phenyl ring is demonstrated to some extent by 2-quinazalone which has a carbonyl frequency 20 cm.$^{-1}$ lower than that of 4-quinazalone.

The absorption band caused by the presence of a C=N group can be clearly identified in only one case, that of 2-methyl-4-quinazalone where it occurs at 1625 cm.$^{-1}$. Other cases where it can be identified with a lesser degree of certainty are 3-methyl-4-quinazalone, 2,3-dimethyl-4-quinazalone and 1,2-dimethyl-4-quinazalone, the frequencies being 1612, 1593 and 1597 cm.$^{-1}$, respectively. The spectra of 4-quinazalone and 2-quinazalone are difficult to interpret with respect to the absorption band to be attributed to the C=N group. Both of these compounds have two absorption bands which fall within the region 1580 to 1762 cm.$^{-1}$ assigned to this group by Randall, *et al.*[2] The frequencies possibly in the case of 4-quinazalone are 1664 and 1608 cm.$^{-1}$ and for 2-quinazalone 1645 and 1608 cm.$^{-1}$. If it is assumed that the conjugation effects are the same in both compounds, the 1608 cm.$^{-1}$ frequency is the one preferred. This gives close agreement to the frequencies observed in the other compounds (1593 to 1625 cm.$^{-1}$). However, if the difference in carbonyl frequencies between 2-quinazalone and 4-quinazalone is to be ascribed to a difference in conjugation effects, the same difference would be expected to apply in the case of the C=N frequencies and make the absorption bands at 1645 and 1664 cm.$^{-1}$ more acceptable. This interpretation has much in its favor as the difference of 20 cm.$^{-1}$ observed in the carbonyl frequencies is matched by a difference of 19 cm.$^{-1}$ in the C=N frequencies. This close agreement of frequency shifts of two conjugated functional groups has been noted by Rasmussen and Brattain in their study of conjugation effects in esters.[24]

The possible origin of a third band in the 1500 to 1700 cm.$^{-1}$ region, found in most of the quinazalones, is difficult to ascertain. In some cases it may be one of the bands associated with the presence of a phenyl group. Another possibility, as has been pointed out by Randall, *et al.*,[2] is that a C–N frequency may invade this so-called "double bond" region. Whatever their origin, these absorption bands offer little help in any attempt to establish characteristic absorption frequencies for the quinazoline ring.

Quinazolinedione.—The quinazolinedione derivatives belong to that group of compounds generally designated as cyclic diacylimides. The diacylimides have been extensively studied by Randall, *et al.*,[2] and the carbonyl frequencies well characterized. In the present investigation, quinazolinedione and three methyl derivatives were studied (Table IV and Fig. 6). The two carbonyl frequencies were easily identified with one lying between 1696 and 1720 cm.$^{-1}$ and the other between 1656 and 1668 cm.$^{-1}$. The frequencies observed by Randall, *et al.*,[2] were 1720 to 1780 cm.$^{-1}$ for the 4-position carbonyl and 1655 to 1712 cm.$^{-1}$ for the 2-position carbonyl. The shift toward longer wave lengths observed in the case of the 4-position carbonyl of the quinazolinediones is readily explainable on the basis of conjugation with the phenyl ring. The 2-position carbonyl is not conjugated and the absorption band falls within the region observed by Randall, *et al.*[2]

In addition to the two carbonyl frequencies, there appear two additional absorption bands in the double bond region: one from 1489 to 1509 cm.$^{-1}$ and the other from 1594 to 1615 cm.$^{-1}$. These two bands are more than likely associated with the quinazolinedione ring system and may offer some help in identifying this type of ring. It is possible to interpret the two bands as being those associated with a conjugated phenyl group; however, the third band at 1575 to 1585 cm.$^{-1}$ found in conjugated phenyl rings is missing in all cases studied.

The investigation of the quinazalones and quinazolinediones was limited for the most part to the 1500–1700 cm.$^{-1}$ region in a search for characteristic ring frequencies. The 3000 cm.$^{-1}$ region was not neglected but since any absorption bands when found in this vicinity can be attributed to the presence of N–H or C–H groups, they are not discussed. However, at longer wave lengths, an absorption band characteristic of ortho substituted phenyl groups has been found between 746 and 778 cm.$^{-1}$. This is in agreement with the observations of Whiffen and Thompson[25] who give an approximate value of 750 cm.$^{-1}$. They attribute this band to a motion involving the deformation of C–H bonds out of the plane of the ring. In the spectra of the quinazolines, quinazalones and quinazolinediones, this band generally appears as the strongest band in the region 700–1000 cm.$^{-1}$ and is in most cases easily identified.

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