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Accessory Publication

Pyrido[1,2-*a*]pyrimidinones and Thiazolo[3,2-*a*]pyrimidinones: Precursors for Pyridyl- and Thiazolyliminoprodadienones, R-N=C=C=C=O.

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Table S4: Observed and calculated IR data for the *s-Z* and *s-E* conformers of 2-thiazolyliminopropadienone **28** together with methyl *N*-(2-thiazolyl)ketenimine-1-thiocarboxylate **29**.

All calculations were performed at the B3LYP/6-31G** level using GAUSSIAN 98,[1] and all wavenumbers were scaled by a factor 0.9613.[2]

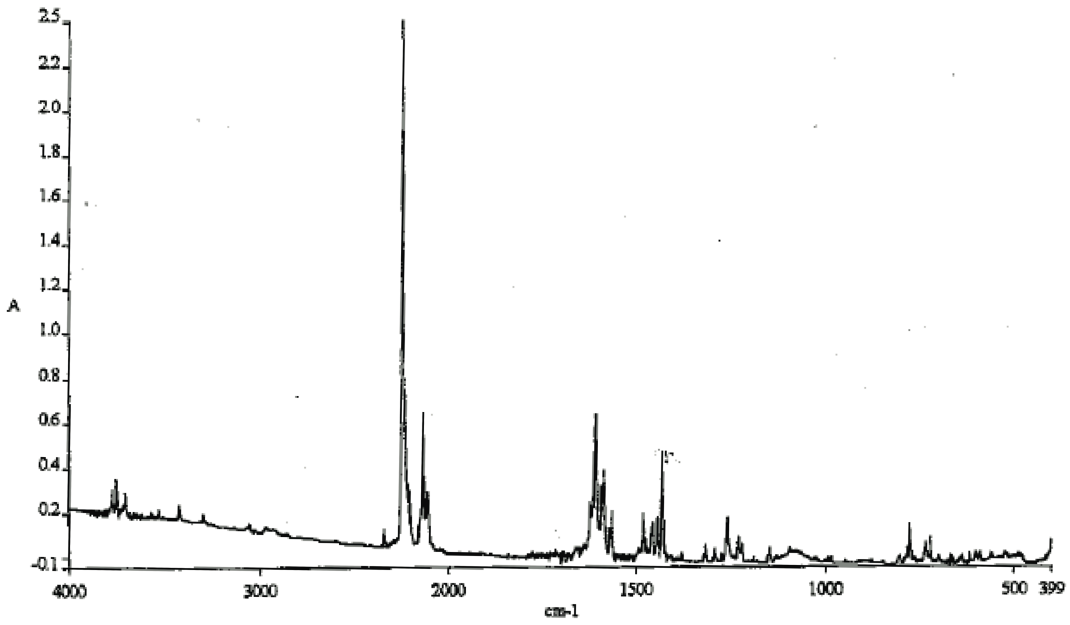

Figure S1. Ar matrix IR spectrum (7 K) of 2-pyridyliminopropadienone **6** from FVT of **16a** at 980 ^{o}C.

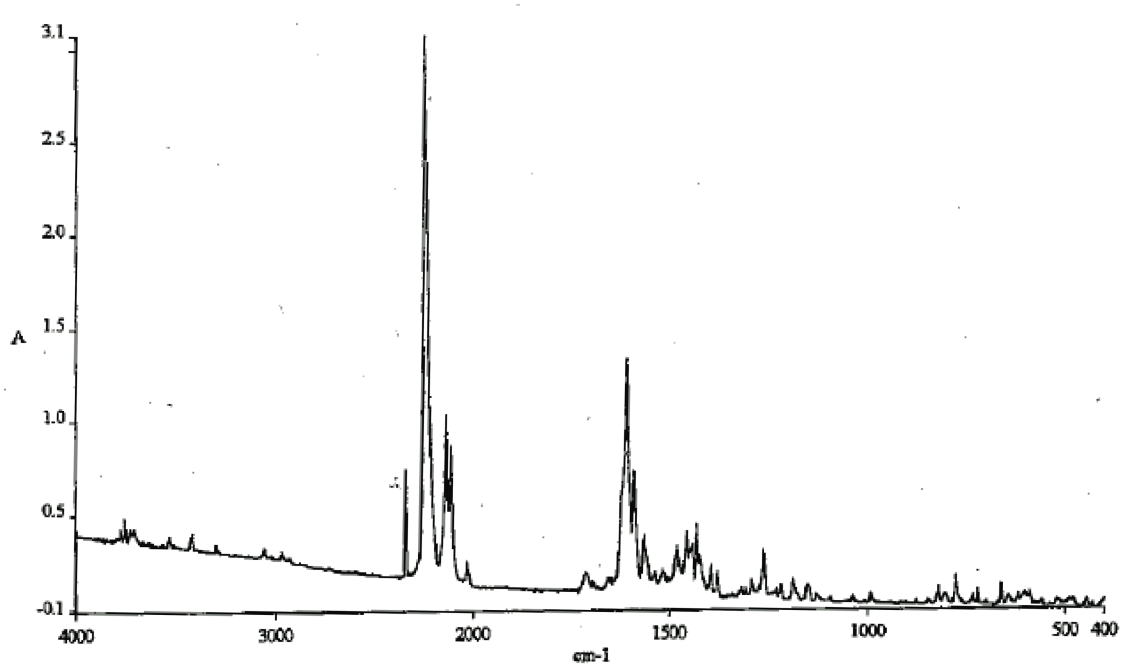

Figure S2. Ar matrix IR spectrum (7 K) of 2-pyridyliminopropadienone **6** and 2-(4-picolinyl)iminopropadienone **19b** from FVT of **16b** at 860 ^{o}C.

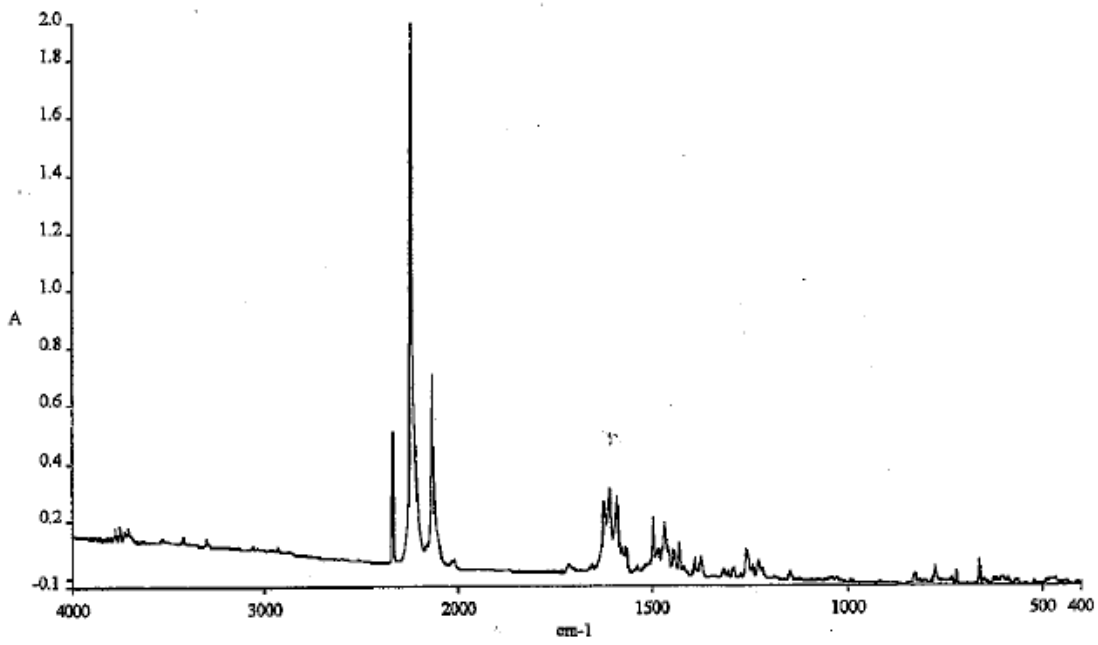

Figure S3: Ar matrix IR spectrum (7 K) of 2-pyridyliminopropadienone **6** and 2-(5-picolinyl)iminopropadienone **19c** from FVT of **16c** at 860 ^{o}C.

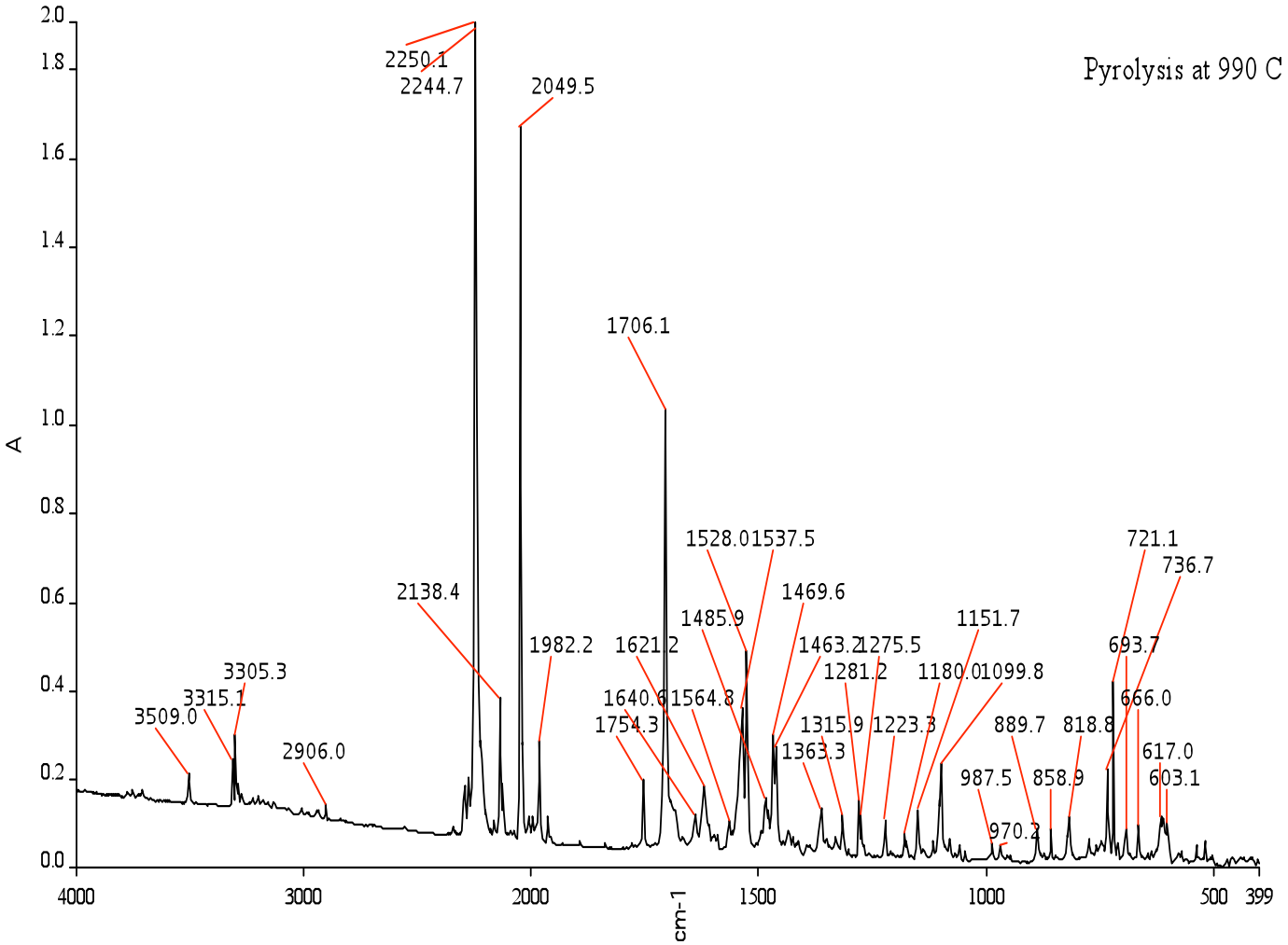

Figure S4: Ar matrix IR spectrum of the products of FVT of thiazolopyrimidinone **24** at 990 ^{o}C. Note that small amounts of HNCS (1982, 3509 cm^{-1}) and HCCH 3305, 737 cm^{-1}) are also formed.

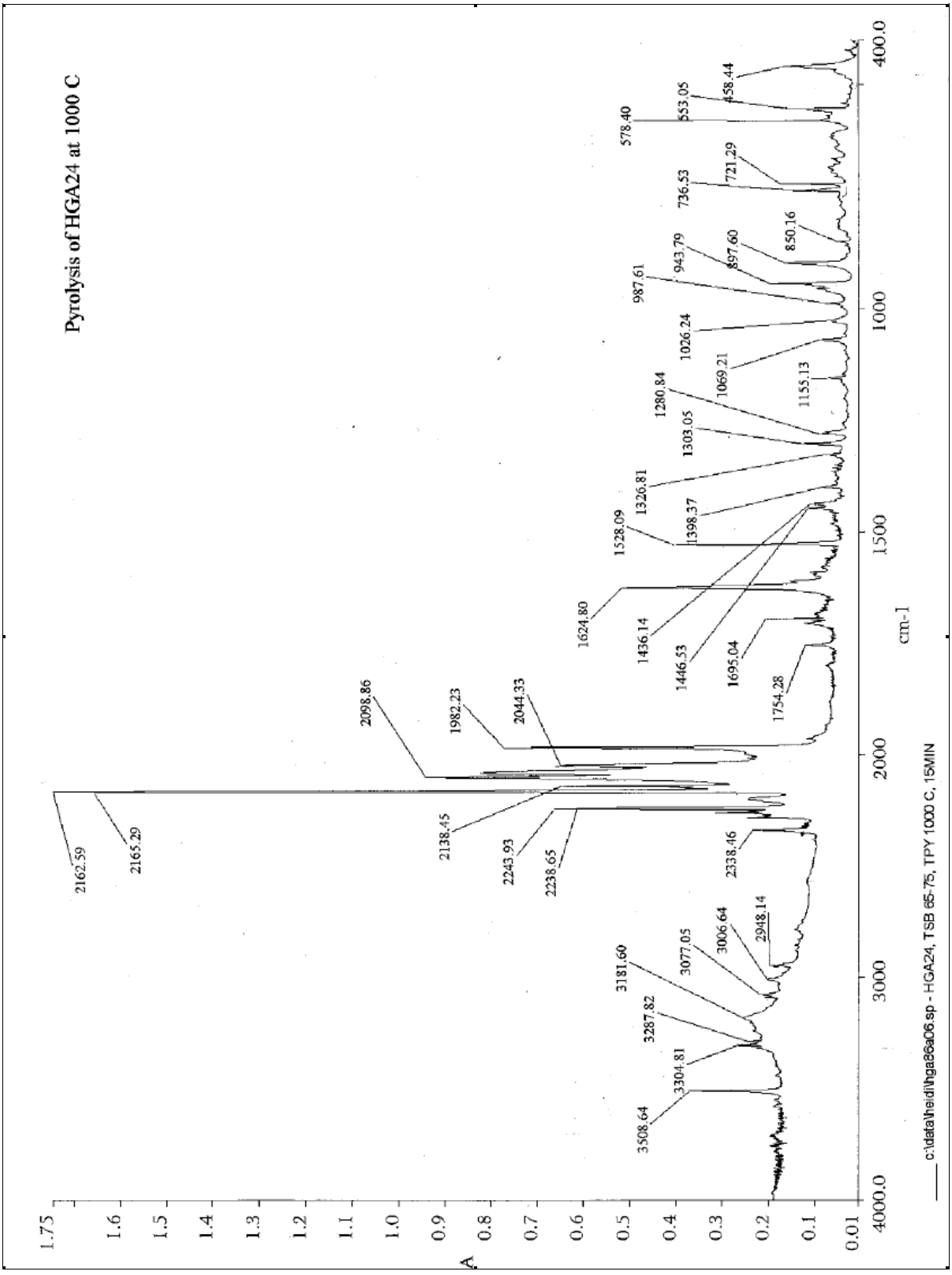

Figure S5: Ar matrix IR spectrum of the products of FVT of dihydrothiazolopyrimidinone **31** at 1000 ^{o}C. Peaks at 3304, 3288, 1327 and 737 cm^{-1} and due to acetylene, HCCH. Peaks at 3509 and 1982 cm^{-1} are due to isothiocyanic acid, HNCS. The peak at 1695 cm^{-1} is the

strongest peak in the starting material **31** and remains the strongest band in the IR spectrum of the products of FVT at 850 ^{o}C.

Table S1. IR spectroscopic data for *s-Z* and *s-E*-(2-pyridyl)iminopropadienone **6**.

Observed, Argon, 7K	DFT (B3LYP/6-31g**)			
	s-Z-6		***s-E-6***	
ν^{a}	$\nu^{a,b}$	I^{c}	$\nu^{a,b}$	I^{c}
2250 vs	2282	100	2285	100
2128 m	2140	5	2162	3
1611 m	1616	11	1630	8
1587 m	1575	4	1570	3
1567 w	1556	1	1554	2
1459 w	1440	2	1447	3
1433 m	1413	3	1406	1
1293 w	1278	0	1280	0
1261 w	1265	1	1263	0
1220 w	1211	2	1216	2
776 w	763	1	759	1

[a]The frequencies are in cm^{-1}; [b] calculated frequencies are scaled by a factor of 0.9613;
[c] relative intensities scaled up to the most intense peak as 100%.

Table S2. IR spectroscopic data for the products from FVT of **16b**

Observed, Argon 7K	Argon 23K		DFT (B3LYP/6-31g**)			
	15a	**15b**	***s-Z*-6**		***s-Z*-19b**	
ν^{a}	ν^{a}	ν^{a}	$\nu^{a,b}$	I^{c}	$\nu^{a,b}$	I^{c}
3535 w	3535 m	3535 m				
3429 w	3429 m	3429 m				
2249 vs			2282	100	2284	100
2149 m					2163	3
2128 m			2140	5		
1624 m		1624 vs			1630	8
		1617 vs				
1610 m	1611 vs		1616	11		
	1608 vs					
1593 m		1594 s			1580	2
1587 m	1586 w		1575	4		
1567 w	1575 m	1570 m	1556	1		
1562 w					1546	5
1483 w	1484 s	1491 m				
1477 w					1459	2
1459 w		1463 s	1440	2	1444	1
1445 w	1445 s					
1433 w			1413	3		
1424 w		1425 s				
1397 w					1372	0
1381 w		1379 w			1367	1
1317 w	1317 m					
1307 w		1307 m				
1293 w			1278	0		
1261 w		1265 w	1265	1	1267	1
1231 w					1242	1
1220 w			1211	2		
1189 w		1178 w			1146	1
1151 w	1149 w					
823 w					811	1
806 w		806 m				
777 w			763	1		

[a]The frequencies are in cm^{-1}; [b] calculated frequencies are scaled by a factor of 0.9613;

[c] relative intensities scaled up to the most intense peak as 100%.

Table S3. IR spectroscopic data for the products from F VT of **16c**.

Observed, Argon 7K	Argon, 23K		DFT (B3LYP/6-31g**)			
	15a	**15c**	***s-Z*-6**		***s-Z*-19c**	
ν^{a}	ν^{a}	ν^{a}	$\nu^{a,b}$	I.[c]	$\nu^{a,b}$	I.[c]
3535 w	3535 m	3526 w				
3429 w	3429 m	3424 w				
2935 w		2935 w				
2249 vs			2282	100	2281	100
2128 m			2140	5	2139	4
1624 m		1622 s				
1611 m	1611 vs		1616	11	1615	10
	1608 vs					
1591 m		1594 w			1585	3
1587 m	1586 w		1575	4		
1577 w	1575 m	1577 w				
1567 w			1556	1		
1540 w					1548	0
1500 m		1501 vs				
1484 w	1484 s					
1470 m					1452	4
1459 w			1440	2		
1446 w	1445 s					
1433 w			1413	3		
1394 w		1394 s				
1375 w					1366	2
1317 w	1317 m					
1293 w			1278	0		
1260 w		1264 w	1265	1	1262	1
1228 w					1212	2
1220 w			1211	2		
1149 w	1149 w	1140 w				
833 w					817	1
777 w			763	1		

[a]The frequencies are in cm^{-1}; [b] calculated frequencies are scaled by a factor of 0.9613;

[c] relative intensities scaled up to the most intense peak as 100%.

Table S4. IR spectroscopic data for FVT of **25**

Observed, Argon 7K	DFT (B3LYP/6-31**)					
	***s-Z*-28**		***s-E*-28**		**29**	
ν^{a}	$\nu^{a,b}$	I^{c}	$\nu^{a,b}$	I^{c}	$\nu^{a,b}$	I^{c}
2250 vs	2283	100				
2245 vs			2282	100		
2164 w	2156	2				
2127 w			2138	4		
2050 vs					2029	100
1706 s					1688	53
1641 w	1647	9				
1621 m			1629	10		
1486 w	1489	2			1487	4
1480 w			1475	1		
1426 w					1429	2
1413 w	1418	1			1416	1
					1410	1
1396 w			1396	1		
1363 w					1360	6
1281 w					1308	1
1276 w	1303	0	1303	0		
1223 w			1211	1		
1212 w	1206	0			1203	3
1152 w					1145	4
1118 w			1128	3		
1105 m	1106	2			1095	57
1100 m						
1060 w	1047	0	1048	1	1050	4
1049 w					1023	7
970 w					953	1
859 w					854	1
818 w	820	1	806	2		
737 m					733	3
721 m					724	5
					722	11
714 w					710	3
694 w	696	1	698	1	692	1
666 w			668	1		
603 w	601	0			591	9

[a]The frequencies are in cm^{-1}; [b] calculated frequencies are scaled by a factor of 0.9613; [c] relative intensities scaled up to the most intense peak as 100%.

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[1] Frisch, M. J.; Truchs, G. W.; Schlegel, H. B.; Gill, P. M. W.; Johnson, B. G.; Robb, M. A.; Cheeseman, J. R.; Keith, T.; Petersson, G. A.; Montgomery, J. A.; Raghavachari, K.; Al-Laham, M. A.; Zakrzewski, V. G.; Ortiz, J. V.; Foresman, J. B.; Cioslowski, J.; Stefanov, B. B.; Nanayakkara, A.; Challacombe, M.; Peng, C. Y.; Ayala, P. Y.; Chen, W.; Wong, M. W.; Andres, J. L.; Replogle, E. S.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Binkley, J. S.; Defrees, D. J.; Baker, J.; Stewart, J. P.; Head-Gordon, M.; Gonzalez, C.; Pople, J. A. *Gaussian 98*; Gaussian, Inc.: Pittsburgh PA, 1998; Vol. Revision A.6.

[2] M. W. Wong, *Chem. Phys. Lett.* **1996**, *256*, 391.