10.1071/CH08252_ AC

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Supplementary Information

1*H*-1,3-Diazepines and Ketenimines from Cyanotetrazolopyridines

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Content page

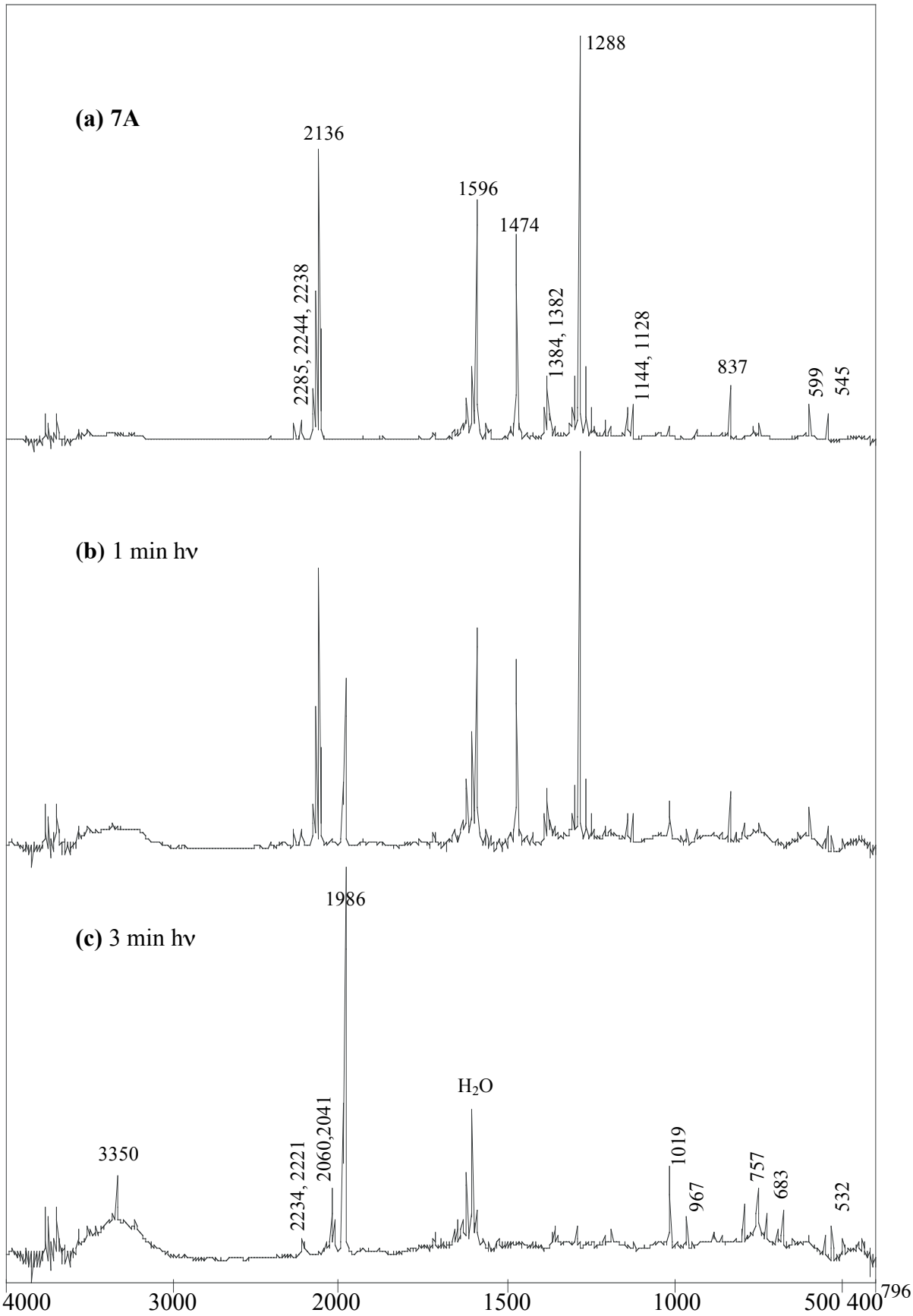
(a) 7A
2136
1288
1596
1474
2285, 2244, 2238
1384, 1382
1144, 1128
837
599
545
(b) 1 min hν
1986
(c) 3 min hν
H2O
3350
2234, 2221
2060,2041
1019
967
757
683
532
4000
3000
2000
1500
1000
500 400
796

Figure S1. IR spectra in Ar matrix at 7 K of (a) **8A,** (b) after 1 min and (c) after **3** min of UV irradiation.

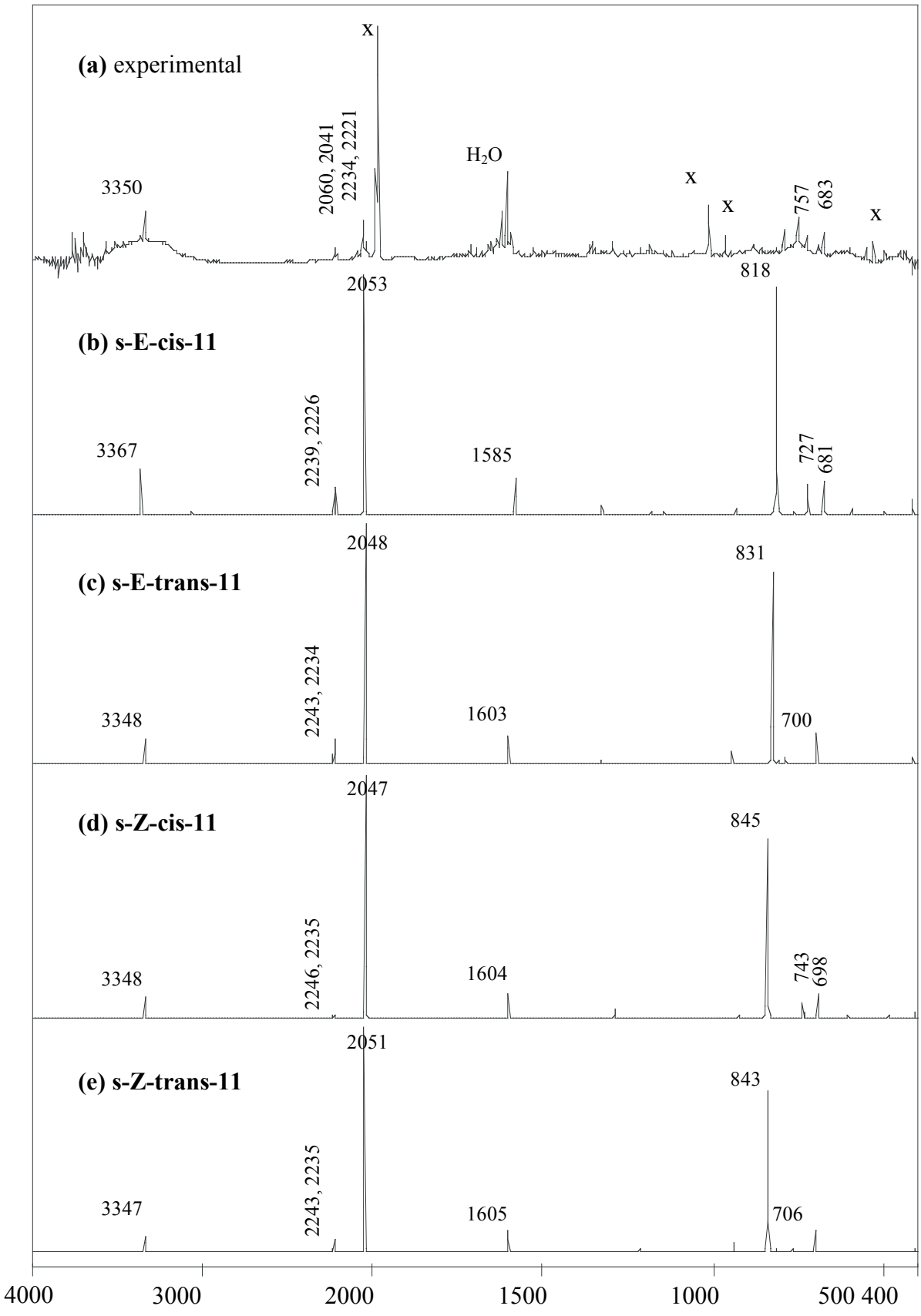

Figure S2. (a) IR spectrum obtained after 3 min UV irradiation of **8A** (x = **10**). Calculated IR spectra of (b) **s-E-cis-11**, (c) **s-E-trans-11**, (d) **s-Z-cis-11** and (e) **s-Z-trans-11** at the B3LYP/6-31+G* level (wavenumbers scaled by 0.9613).

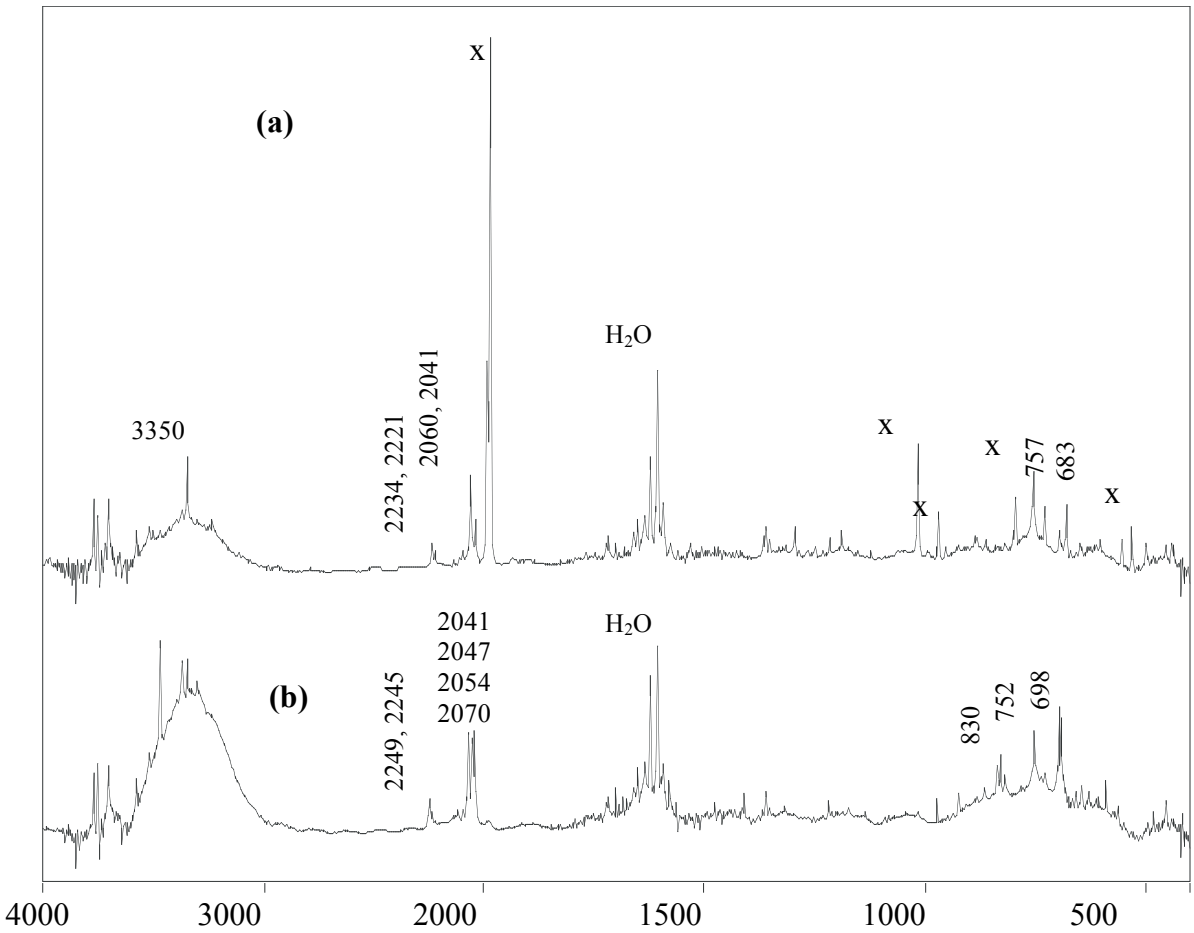

Figure S3. IR spectra in Ar matrix at 7 K after (a) 3 min (x = **10**) and (b) 60 min of UV irradiation of **8A**. The spectra are shown with the same absorbance scale.

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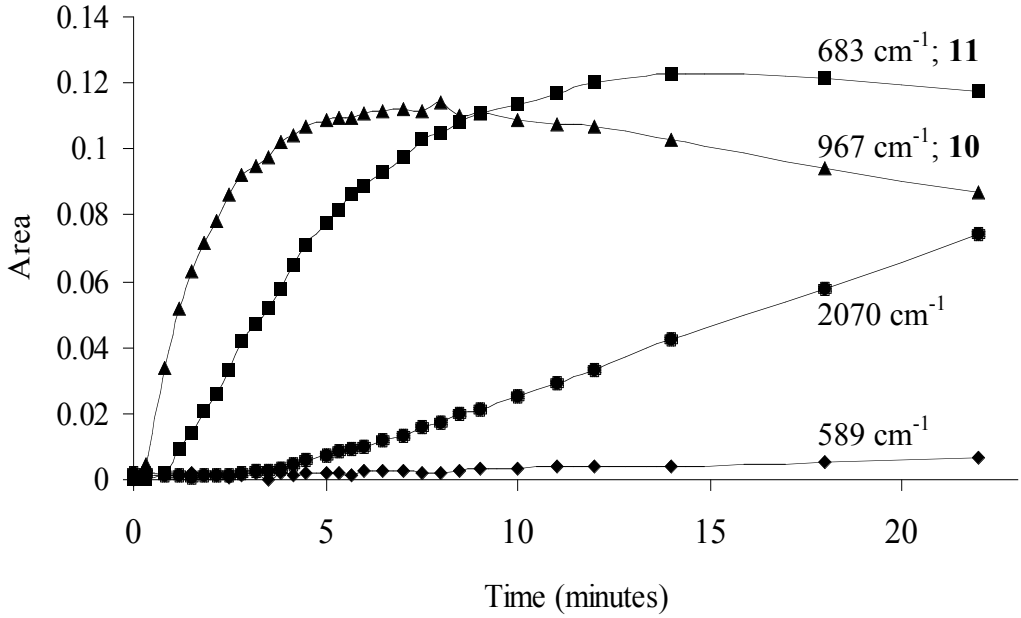


Figure S4. Representative area versus time profiles of the four groups of bands identified during photolysis of **8A**. Δ = 967 cm^{-1} of **10**; □ = 683 cm^{-1} of **11**; • = 2070 cm^{-1}; ♦ = 589 cm^{-1}.

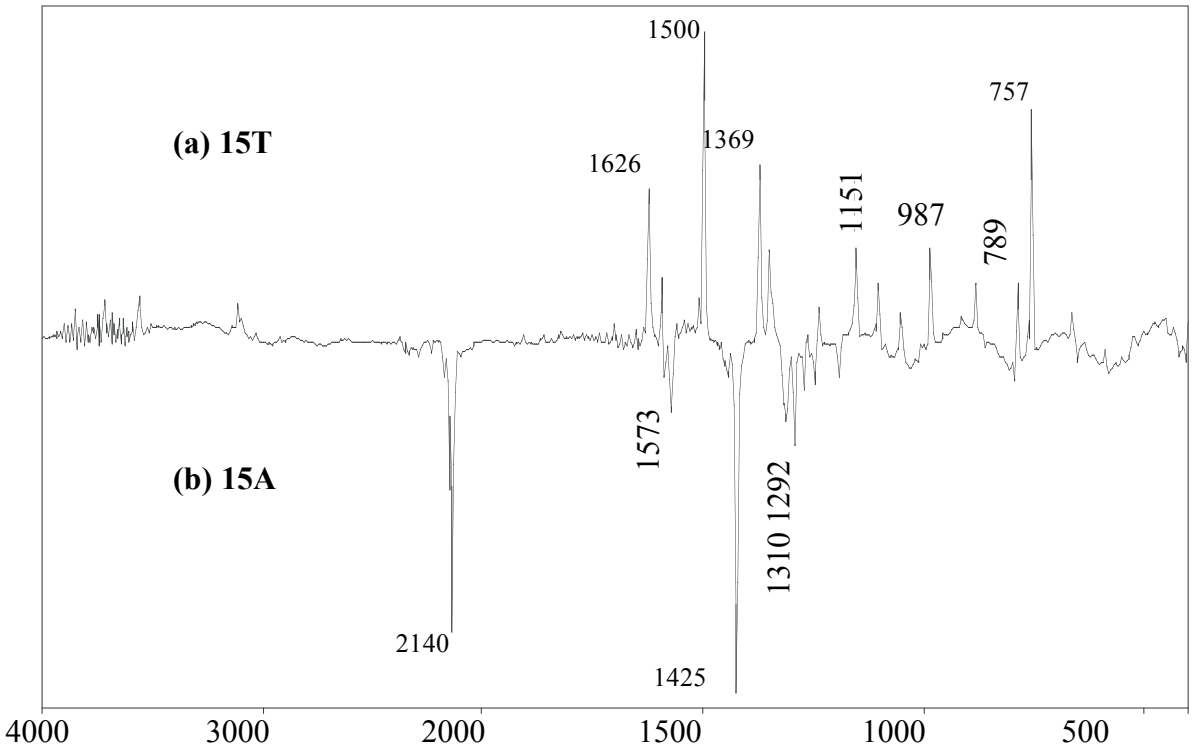


Figure S5. Difference IR spectrum showing (a) **15T** and (b) **15A** in Ar at 10 K, obtained by photolysis of a matrix containing both **15T** (unreactive) and **15A** (photo-reactive). The matrix

was produced by sublimation of **15T** through an FVT tube at 100 ^{o}C and depositing the material with Ar at 25 K.

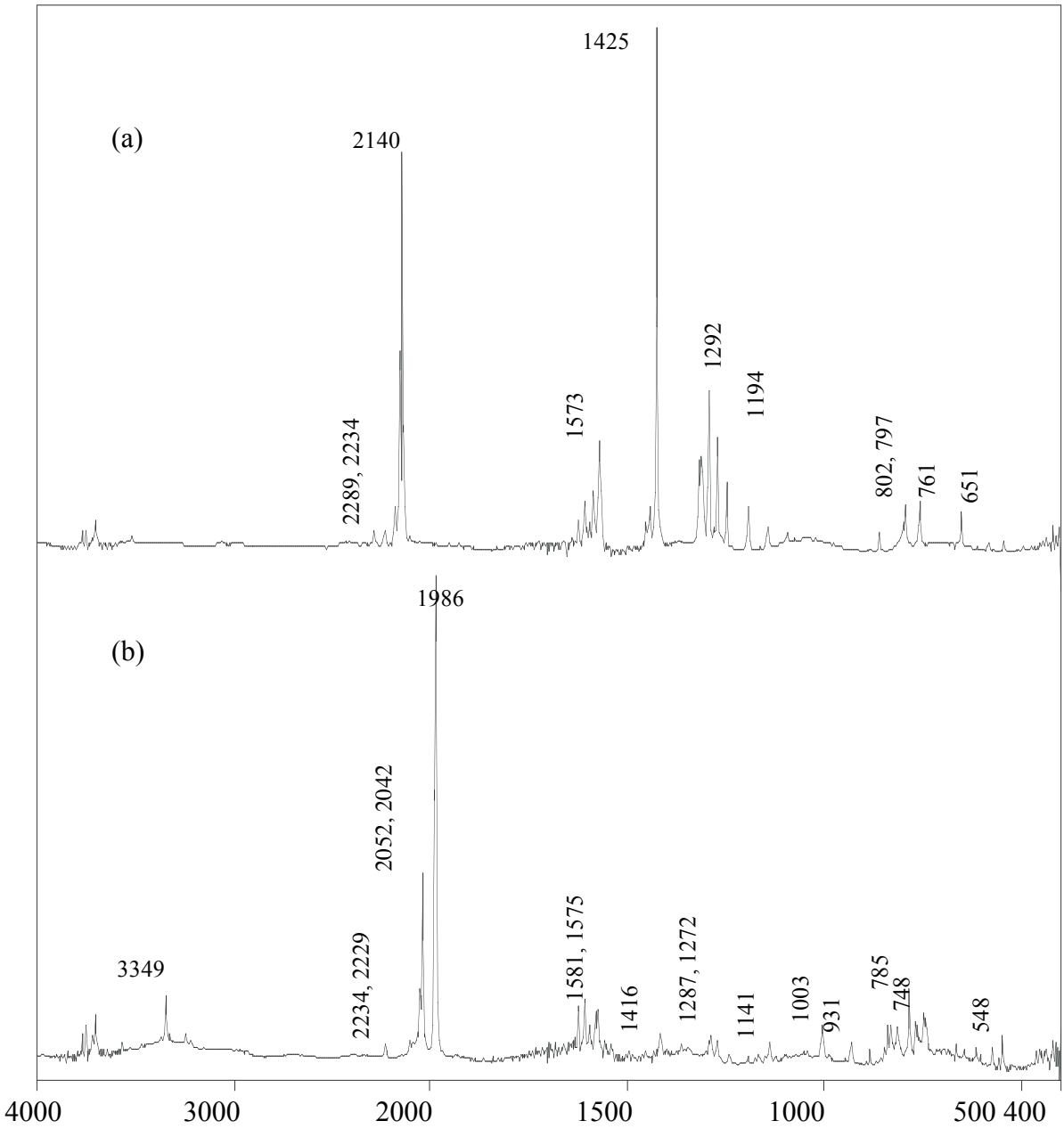


Figure S6. IR spectra in Ar matrix at 7 K of (a) **15A**, and (b) after 7.5 min of UV irradiation.

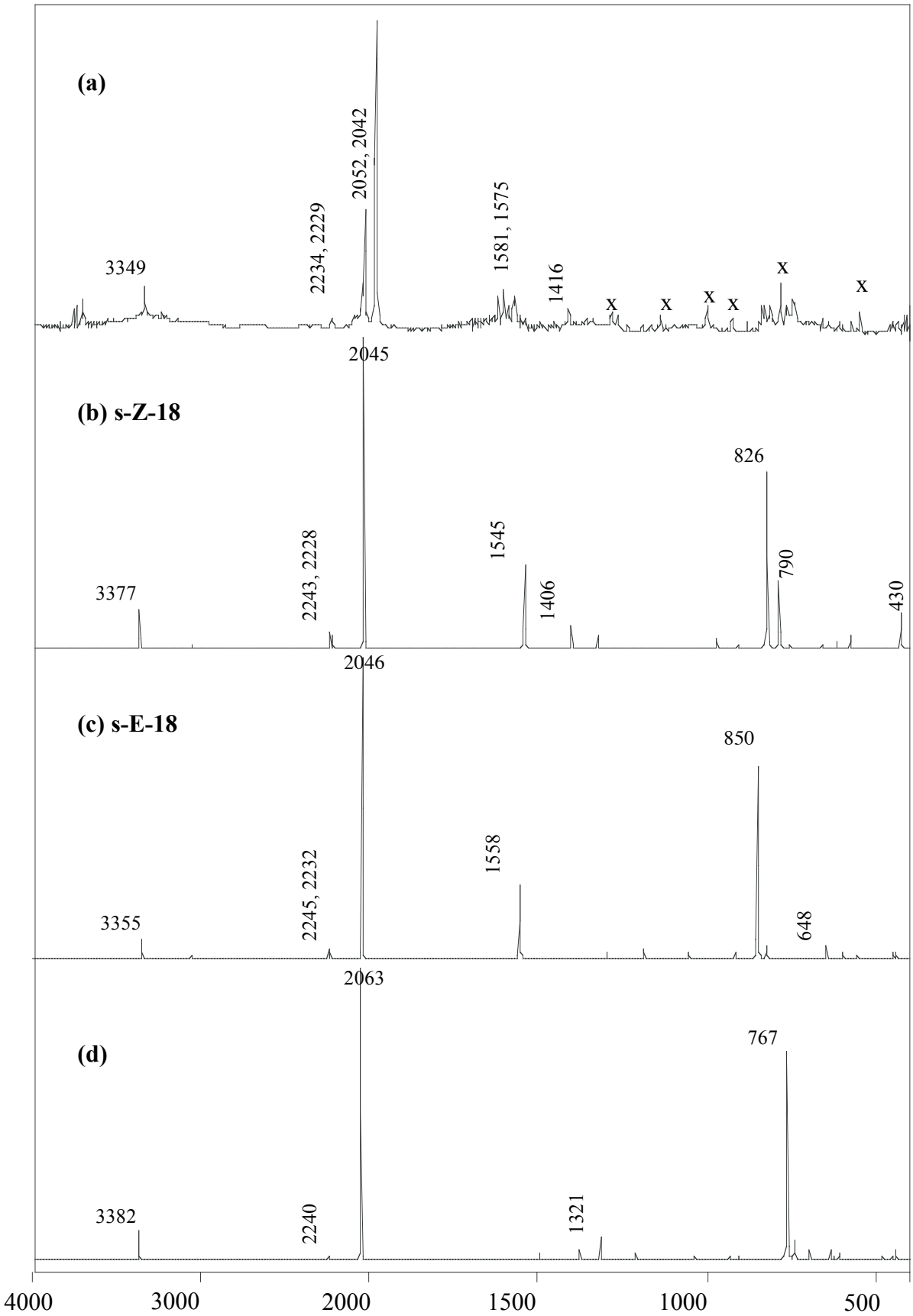
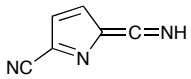


Figure S7. **(a)** IR spectrum obtained after 7.5 min of UV irradiation of **15A** (x **=** 17). Calculated IR spectra of **s-Z-18** (b) and **s-E-18** (c) at the B3LYP/6-31+G* level

(wavenumbers caled by 0.9613). (d) Ketenimines such as **22** have been postulated but dismissed as potential intermediates in the FVT reactions of 2-pyridylnitrenes (Harder, R.; Wentrup, C. *J. Am. Chem. Soc*. **1976**, *98*, 1259). The calculated IR spectrum of **22** is shown for comparison. Dicyanopyrroles were not formed in these photolyses.



22

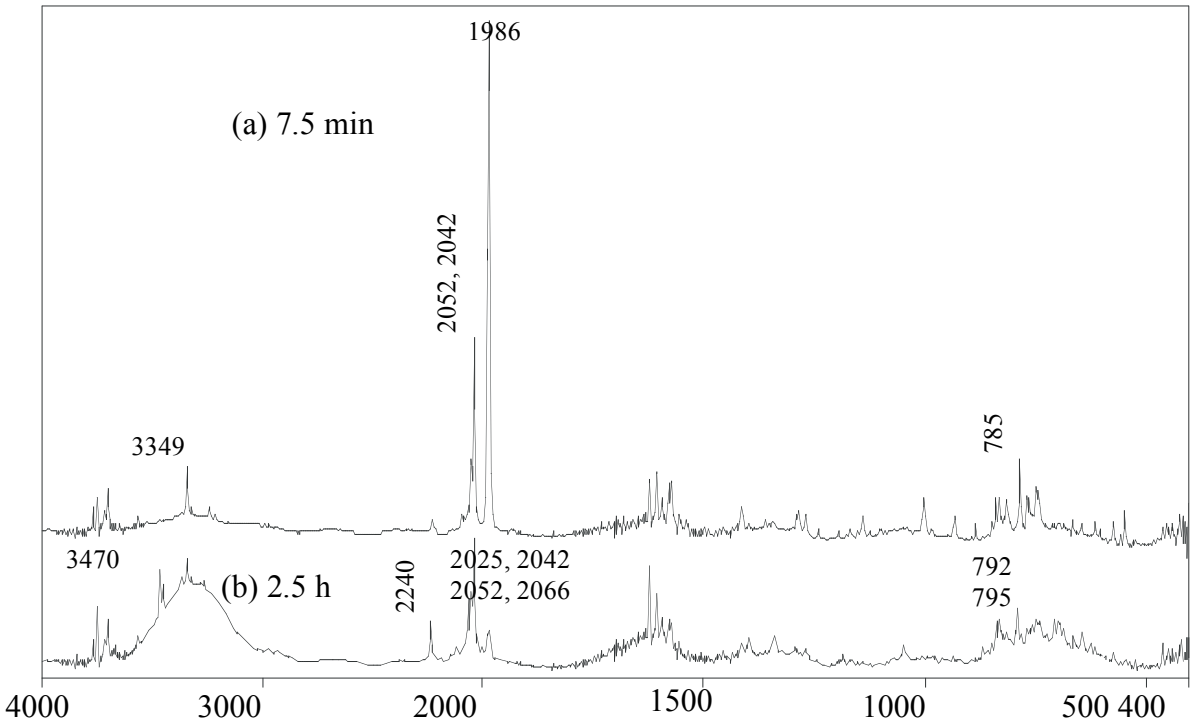


Figure S8. Disappearance of carbodiimide **17** after (a) 7.5 min, and (b) 2.5 h of UV irradiation.

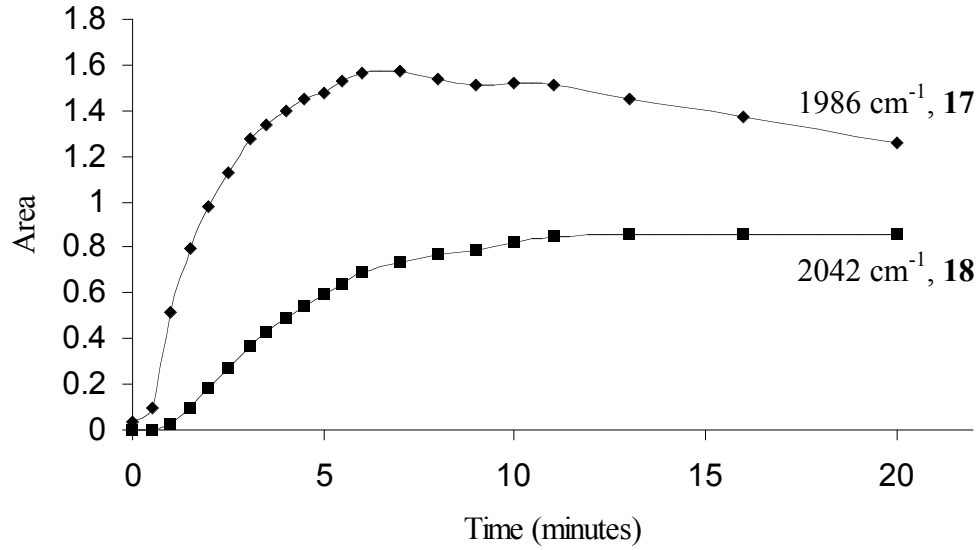
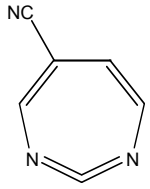


Figure S9. Representative area versus time profiles of the two groups of bands identified during photolysis of **15A**. ♦ = 1986 cm^{-1} of **17**, ■ = 2042 cm^{-1} of **18**.

Computational data

5-Cyano-1,3-diazacyclohepta-1,2,4,6-tetraene 10



GAUSSIAN 98; B3LYP/6-31+G*; POINT GROUP C_1

ZERO POINT VIBRATIONAL ENERGY = 49.43124 kcal/mol

ELECTRONIC ENERGY = -394.5908683 H

ZERO POINT CORRECTION = 0.078774 H

SUM OF ELECTRONIC AND ZERO POINT ENERGIES = -394.512095 H

STANDARD ORIENTATION

centre no.	**atom type**			**coordinates [Å]**
		x	**y**	**z**
1	C	-1.5512402841	0.0715939419	-1.1631101709
2	N	-0.8984108539	1.2858514698	-1.6163766624
3	C	0.3062228706	1.0120772996	-1.5629895634
4	N	1.4231509129	0.5542466478	-1.2616246980
5	C	1.3319025441	0.1890473965	0.1133283186
6	C	0.1927713658	-0.3695842715	0.6235386627
7	C	-1.0596001276	-0.6445118952	-0.1280971622
8	N	0.2224582169	-1.1759870565	3.0943018938
9	C	0.2223706873	-0.8081175337	1.9897957241
10	H	-2.4647818184	-0.1938889168	-1.6852515622
11	H	2.2273103719	0.3293780464	0.7108945087
12	H	-1.6474788211	-1.4872961830	0.2254584659

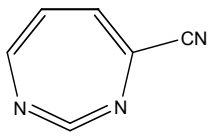
INFRARED SPECTRUM

mode no.	**unscaled frequency**	**absolute intensity**	**relative intensity#**	**scaled frequency*#**
1	125.8437	4.8524	1	120
2	162.525	8.7733	2	156
3	291.0188	12.9933	2	279
4	307.4052	1.9608	0	295
5	357.9577	12.9492	2	344
6	450.8844	6.708	1	433
7	514.1112	4.929	1	494

8	529.0177	22.7857	5	508
9	562.0447	7.7219	1	540
10	634.223	1.2493	0	609
11	658.501	3.8473	0	633
12	706.0941	7.2285	1	678
13	816.6704	32.5229	7	785
14	881.1282	2.4815	0	847
15	916.5956	7.7754	1	881
16	954.9828	5.8096	1	918
17	992.4395	28.184	6	954
18	1051.38	73.8327	16	1010
19	1160.488	1.3785	0	1115
20	1222.474	4.6145	1	1175
21	1297.072	13.6564	3	1246
22	1338.614	13.5283	3	1286
23	1402.476	5.1693	1	1348
24	1568.465	20.744	4	1507
25	1628.088	0.8892	0	1565
26	2055.486	436.2217	100	1975
27	2331.486	30.2712	6	2241
28	3201.876	0.3814	0	3077
29	3226.484	3.1197	0	3101
30	3231.822	5.4614	1	3106

[*] scaled by 0.9613. - [#] normalized to most prominent peak (=100)

4-Cyano-1,3-diazacyclohepta-1,2,4,6-tetraene 17



GAUSSIAN 98; B3LYP/6-31+G*; POINT GROUP C_1

ZERO POINT VIBRATIONAL ENERGY = 49.37817 kcal/mol

ELECTRONIC ENERGY = -394.5895189 H

ZERO POINT CORRECTION = 0.078689 H

SUM OF ELECTRONIC AND ZERO POINT ENERGIES = -394.51083 H

STANDARD ORIENTATION

centre no.	**atom type**			**coordinates [Å]**
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1	C	-2.0809472671	-0.2702323234	-0.9585189543
2	N	-1.3835153112	0.8764737913	-1.4838735785

3	C	-0.1808896895	0.6009729661	-1.3583733371
4	N	0.9094461433	0.1328406962	-0.9934622844
5	C	0.7361267448	-0.1031429461	0.4290596862
6	C	-0.4270007488	-0.6221368188	0.9165563935
7	C	-1.6396591313	-0.9212457799	0.1473565375
8	C	1.8594148301	0.1815845038	1.2678937425
9	N	2.7779072510	0.4074251334	1.9461596276
10	H	-3.0012245915	-0.5342784887	-1.4699918574
11	H	-0.4482878526	-0.8754966324	1.9735302806
12	H	-2.2796225673	-1.7021998357	0.5508508143

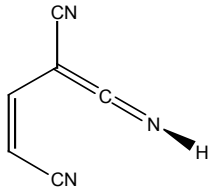
INFRARED SPECTRUM

mode no.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	104.449	0.6865	0	100
2	160.5069	3.291	0	154
3	298.84	2.7519	0	287
4	330.8769	13.4709	3	318
5	368.3068	12.1934	3	354
6	429.828	1.5609	0	413
7	534.6126	10.3922	3	513
8	549.9653	13.981	4	528
9	572.7507	1.12	0	550
10	616.0943	1.0983	0	592
11	681.2887	3.7818	1	654
12	758.2832	16.0318	4	728
13	805.1254	37.4346	10	773
14	857.3385	4.0833	1	824
15	912.8705	7.0599	2	877
16	959.2329	15.3471	4	922
17	963.0062	1.2644	0	925
18	1033.504	40.3152	11	993
19	1155.109	31.9889	9	1110
20	1215.709	3.931	1	1168
21	1281.819	5.5723	1	1232
22	1326.068	17.4621	5	1274
23	1403.15	6.2118	1	1348
24	1582.336	7.3971	2	1521
25	1634.482	2.0006	0	1571
26	2050.971	342.8047	100	1971
27	2333.395	17.0235	4	2243

28	3190.406	3.3266	0	3066
29	3201.916	0.6747	0	3078
30	3228.287	7.2305	2	3103

* scaled by 0.9613. - # normalized to most prominent peak (=100)

s-E-cis-2,4-dicyanovinylketenimine s-E-cis-11



GAUSSIAN 98; B3LYP/6-31+G*; POINT GROUP C_1

ZERO POINT VIBRATIONAL ENERGY = 47.69109 kcal/mol

ELECTRONIC ENERGY = -394.6104812 H

ZERO POINT CORRECTION = 0.076001 H

SUM OF ELECTRONIC AND ZERO POINT ENERGIES = -394.534481 H

STANDARD ORIENTATION

centre no.	**atom type**			**coordinates [Å]**
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1	C	0.6960533226	0.4709678251	0.0104242533
2	C	-0.4512261540	1.0108919137	-0.4429242379
3	C	0.9430499628	-0.9717514832	0.0469743688
4	C	0.0335630609	-1.9740968747	0.0358100102
5	C	-1.3762058660	-1.7717288775	0.0635977302
6	C	1.7182114762	1.3672437763	0.4560773910
7	N	-1.3931522837	1.4984763207	-1.0181445602
8	N	-2.5286597024	-1.6026551495	0.1123668253
9	N	2.5704314679	2.0719677911	0.8215476219
10	H	1.9937183193	-1.2450699219	0.0988416226
11	H	0.3734705753	-3.0054105554	0.0345052349
12	H	-2.2882000815	1.6868000634	-0.5634931594

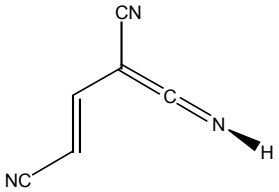
INFRARED SPECTRUM

mode no.	**unscaled frequency**	**absolute intensity**	**relative intensity#**	**scaled frequency*#**
1	42.2509	14.5708	3	40
2	106.5928	9.8661	2	102
3	134.1138	4.5581	0	128
4	160.899	1.5815	0	154

5	195.7213	3.9051	0	188
6	325.4775	2.9383	0	312
7	372.0194	0.1466	0	357
8	436.6075	32.0535	6	419
9	489.2507	0.6976	0	470
10	520.5797	6.9601	1	500
11	620.0458	9.6669	2	596
12	630.9069	2.6118	0	606
13	663.0052	1.6742	0	637
14	709.2343	71.9513	14	681
15	756.9863	59.5255	12	727
16	795.8518	3.4608	0	765
17	851.1007	451.8405	93	818
18	974.6121	10.7864	2	936
19	983.3824	0.6951	0	945
20	1193.669	3.7918	0	1147
21	1236.527	3.9283	0	1188
22	1380.528	23.1316	4	1327
23	1431.75	2.5875	0	1376
24	1649.414	73.1316	15	1585
25	2136.21	481.6192	100	2053
26	2316.16	51.7482	10	2226
27	2330.114	44.1541	9	2239
28	3198.696	2.8678	0	3074
29	3215.888	0.5069	0	3091
30	3502.807	92.6218	19	3367

* scaled by 0.9613. - # normalized to most prominent peak (=100)

s-E-trans-2,4-dicyanovinylketenimine s-E-trans-11



GAUSSIAN 98; B3LYP/6-31+G*; POINT GROUP C_1

ZERO POINT VIBRATIONAL ENERGY = 47.57859 kcal/mol

ELECTRONIC ENERGY = -394.6089184 H

ZERO POINT CORRECTION = 0.075821 H

SUM OF ELECTRONIC AND ZERO POINT ENERGIES = -394.533097 H

STANDARD ORIENTATION

centre no.	atom type			coordinates [Å]
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1	C	0.9031519361	-2.0586973846	0.2549208287
2	C	0.0102458833	-0.9562046076	0.0688921229
3	C	-1.2967731213	-1.2365665647	-0.0581861313
4	C	0.5433774228	0.4083238540	-0.0001598276
5	C	-0.1870920634	1.5394122084	-0.1094214205
6	C	0.4186061739	2.8268178908	-0.1729225082
7	N	-2.4882177710	-1.4473670720	-0.0220588420
8	N	1.6483682548	-2.9410757109	0.4027599630
9	N	0.8872523720	3.8922057615	-0.2287737547
10	H	1.6268775063	0.4732754893	0.0481038720
11	H	-1.2743822237	1.5204772032	-0.1498264428
12	H	-3.0334126616	-1.6586059206	-0.8605073775

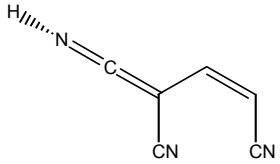
INFRARED SPECTRUM

mode no.	unscaled frequency	absolute intensity	relative intensity[#]	scaled frequency[*#]
1	76.8541	1.6974	0	73
2	90.6411	6.5505	1	87
3	110.1403	5.8029	0	105
4	125.0945	2.849	0	120
5	210.72	2.2229	0	202
6	260.1435	4.1032	0	250
7	364.6609	0.7909	0	350
8	433.2893	19.9524	3	416
9	483.0529	2.4559	0	464
10	487.8568	5.7822	0	468
11	548.1444	3.7216	0	526
12	600.4468	5.9387	0	577
13	631.9834	6.9537	1	607
14	728.4593	85.2299	13	700
15	825.389	22.3223	3	793
16	846.5084	14.8442	2	813
17	864.9672	522.486	79	831
18	985.8321	39.9931	6	947
19	1031.165	0.445	0	991
20	1200.463	5.9429	0	1154
21	1316.323	6.4731	0	1265
22	1338.409	1.2204	0	1286
23	1386.744	18.2756	2	1333

24	1667.866	81.1127	12	1603
25	2131.348	654.8864	100	2048
26	2324.904	63.413	9	2234
27	2333.929	30.3808	4	2243
28	3183.085	3.523	0	3059
29	3209.908	1.7886	0	3085
30	3483.373	69.6608	10	3348

* scaled by 0.9613. - # normalized to most prominent peak (=100)

s-Z-cis-2,4-dicyanovinylketeniminediene s-Z-cis-11



GAUSSIAN 98; B3LYP/6-31+G*; POINT GROUP C_1

ZERO POINT VIBRATIONAL ENERGY = 47.76994 kcal/mol

ELECTRONIC ENERGY = -394.6060764 H

ZERO POINT CORRECTION = 0.076126 H

SUM OF ELECTRONIC AND ZERO POINT ENERGIES = -394.52995 H

STANDARD ORIENTATION

centre no.	**atom type**			**coordinates [Å]**
		x	**y**	**z**
1	C	-1.8155604095	0.7512005518	-0.8529275881
2	N	-2.8993949070	1.1595959293	-1.2083999670
3	C	-0.6863248880	0.2780060820	-0.2965336232
4	C	0.2394962913	1.2632872477	0.1762991911
5	N	0.9532698658	2.1061391264	0.5429171335
6	C	-0.4814422925	-1.1665102872	-0.2305551538
7	C	0.5794262465	-1.8649787578	0.2329411705
8	C	1.7939542490	-1.3442231864	0.7663967860
9	N	2.8179913913	-1.0100707095	1.2098047477
10	H	-1.3175312657	-1.7504453693	-0.6067453891
11	H	0.5253059213	-2.9502237534	0.2038555318
12	H	-3.0881342872	1.4103287989	-2.1810882381

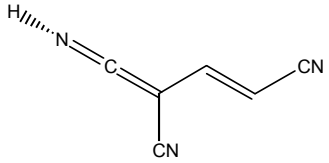
INFRARED SPECTRUM

mode no.	**unscaled frequency**	**absolute intensity**	**relative intensity#**	**scaled frequency*#**
1	36.2695	1.6547	0	34

2	107.8058	1.3505	0	103
3	135.486	3.9682	0	130
4	174.8591	4.8067	0	168
5	180.9993	3.0083	0	173
6	325.7814	3.0348	0	313
7	363.8064	0.9543	0	349
8	429.4725	17.9695	2	412
9	487.5256	0.3813	0	468
10	507.6215	11.4222	1	487
11	634.073	9.0531	1	609
12	636.3419	4.5905	0	611
13	667.3479	3.9358	0	641
14	726.4715	81.4392	9	698
15	765.9266	13.5386	1	736
16	773.0146	43.7857	5	743
17	879.153	615.557	72	845
18	964.9118	5.4092	0	927
19	979.3325	0.2554	0	941
20	1220.252	2.678	0	1173
21	1287.405	1.6996	0	1237
22	1343.774	25.2607	2	1291
23	1451.922	2.4341	0	1395
24	1669.22	75.9596	8	1604
25	2130.039	852.3666	100	2047
26	2326.01	13.6129	1	2235
27	2337.386	14.0749	1	2246
28	3187.178	2.7951	0	3063
29	3202.986	2.3298	0	3079
30	3483.183	66.8972	7	3348

* scaled by 0.9613. - # normalized to most prominent peak (=100)

s-Z-trans-2,4-dicyanovinylketenimine s-Z-trans-11



GAUSSIAN 98; B3LYP/6-31+G*; POINT GROUP C_1

ZERO POINT VIBRATIONAL ENERGY = 47.72167 kcal/mol

ELECTRONIC ENERGY = -394.6123775 H

ZERO POINT CORRECTION = 0.076049 H

SUM OF ELECTRONIC AND ZERO POINT ENERGIES = -394.536328 H

STANDARD ORIENTATION

centre no.	**atom type**			**coordinates [Å]**
		x	**y**	**z**
1	C	-0.9204200343	-0.1788157815	0.0131984199
2	C	-0.9279396447	-1.6084533881	-0.0370799923
3	C	1.5586853334	0.0106436710	-0.0315132953
4	C	0.3318495824	0.5743958353	0.0121773040
5	C	2.7453371395	0.7988046631	-0.0377911776
6	C	-2.1042204143	0.4513503650	0.0889836145
7	N	-3.1621526687	1.0340772800	-0.0043278830
8	N	-0.8957338949	-2.7715893887	-0.0743252364
9	N	3.7268779349	1.4267483215	-0.0421652017
10	H	1.6871074095	-1.0688972886	-0.0648351859
11	H	0.2362348854	1.6564880442	0.0435073852
12	H	-3.7060336655	1.3002035660	0.8192068093

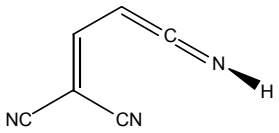
INFRARED SPECTRUM

mode no.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	89.6985	4.781	0	86
2	105.6151	5.8929	0	101
3	125.277	1.85	0	120
4	137.9294	3.898	0	132
5	212.7483	4.0769	0	204
6	268.5653	3.7809	0	258
7	360.0216	2.4585	0	346
8	429.9595	19.1472	2	413
9	487.8433	7.5112	0	468
10	501.9872	1.5263	0	482
11	545.9379	0.3454	0	524
12	600.4253	3.2634	0	577
13	628.5688	5.1402	0	604
14	735.1319	89.5497	10	706
15	804.0945	17.0361	1	772
16	853.9029	15.0107	1	820
17	877.5037	616.0248	71	843
18	979.7152	42.7083	4	941
19	1031.869	2.3227	0	991

20	1263.477	0.4558	0	1214
21	1269.387	15.559	1	1220
22	1339.836	2.7561	0	1287
23	1386.291	5.1877	0	1332
24	1669.916	89.9147	10	1605
25	2134.477	859.0689	100	2051
26	2325.607	49.4941	5	2235
27	2334.215	20.3576	2	2243
28	3194.506	2.4342	0	3070
29	3204.717	2.1971	0	3080
30	3482.57	70.5782	8	3347

* scaled by 0.9613. - # normalized to most prominent peak (=100)

s-Z-4,4-dicyanovinylketenimine s-Z-18



GAUSSIAN 98; B3LYP/6-31+G*; POINT GROUP C_1

ZERO POINT VIBRATIONAL ENERGY = 47.60677 kcal/mol

ELECTRONIC ENERGY = -394.6110774 H

ZERO POINT CORRECTION = 0.075866 H

SUM OF ELECTRONIC AND ZERO POINT ENERGIES = -394.535211 H

STANDARD ORIENTATION

centre no.	**atom type**			**coordinates [Å]**
		x	**y**	**z**
1	C	0.9417560618	-1.6327951696	0.0451836925
2	C	2.0057489135	-0.8881789446	-0.2898791831
3	N	2.9581078912	-0.3094977816	-0.7585973929
4	C	-0.4152774931	-1.1816108136	0.1417284483
5	C	-0.9095373215	0.0998417662	0.1428291995
6	C	-2.3203574207	0.3256926196	0.2220274259
7	C	-0.0621276558	1.2508807171	0.1109396993
8	N	-3.4697469168	0.5012053329	0.2871133935
9	N	0.6514403286	2.1715274711	0.1112511537
10	H	1.1437233451	-2.6819990721	0.2457076705
11	H	3.5889329131	0.2701584923	-0.2043102393

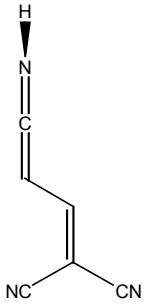
12	H	-1.1524958842	-1.9737856274	0.2432567951

INFRARED SPECTRUM

mode no.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	46.3875	1.4304	0	44
2	109.6101	2.1189	0	105
3	139.6943	8.8207	1	134
4	174.2774	1.9046	0	167
5	182.0059	8.1009	1	174
6	332.8008	5.799	0	319
7	376.8695	0.7985	0	362
8	448.1916	89.7314	11	430
9	465.9032	3.1407	0	447
10	489.846	0.3428	0	470
11	600.8608	26.0869	3	577
12	605.6872	1.5154	0	582
13	646.46	12.9637	1	621
14	691.8076	9.055	1	665
15	789.3607	10.5082	1	758
16	822.7464	174.429	21	790
17	859.4872	459.4353	56	826
18	954.4374	7.9915	0	917
19	1016.978	23.8988	2	977
20	1198.402	2.9254	0	1152
21	1205.566	2.8837	0	1158
22	1383.062	25.811	3	1329
23	1462.994	60.2808	7	1406
24	1607.468	219.084	27	1545
25	2127.613	808.8117	100	2045
26	2318.118	28.3668	3	2228
27	2333.947	38.5125	4	2243
28	3191.994	4.6243	0	3068
29	3205.612	1.219	0	3081
30	3513.226	93.0472	11	3377

[*] scaled by 0.9613. - [#] normalized to most prominent peak (=100)

s-E-4,4-dicyanovinylketenimine s-E-18



GAUSSIAN 98; B3LYP/6-31+G*; POINT GROUP C_1

ZERO POINT VIBRATIONAL ENERGY = 47.68737 kcal/mol

ELECTRONIC ENERGY = -394.6147178 H

ZERO POINT CORRECTION = 0.075995 H

SUM OF ELECTRONIC AND ZERO POINT ENERGIES = -394.538723 H

STANDARD ORIENTATION

centre no.	**atom type**			**coordinates [Å]**
		x	**y**	**z**
1	C	-0.3759092737	-0.1238717659	0.4067906243
2	C	-0.4059610635	0.2713273691	-0.9066370536
3	C	0.7977410302	0.4972065477	-1.6467533048
4	C	0.8154112064	-0.3584244669	1.1642565185
5	C	0.7729289911	-0.7186653859	2.4508073365
6	N	0.7427967322	-1.1866153053	3.5702475543
7	C	-1.6520630611	0.4727148116	-1.5794575006
8	N	1.7984579952	0.6728964647	-2.2157193241
9	N	-2.6716959758	0.6355047288	-2.1177920787
10	H	-1.3322695640	-0.2724554916	0.9013916457
11	H	1.7945816606	-0.2308893148	0.7074387319
12	H	0.7378896665	-0.5908790691	4.3999768409

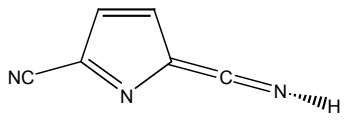
INFRARED SPECTRUM

mode no.	**unscaled frequency**	**absolute intensity**	**relative intensity#**	**scaled frequency*#**
1	89.9442	1.4556	0	86
2	90.168	4.0357	0	86
3	129.5476	7.2648	0	124
4	176.7822	8.562	0	169
5	211.1505	0.597	0	202
6	282.8905	11.6799	0	271
7	364.1082	0.7666	0	350
8	457.7442	19.9821	1	440

9	467.0608	20.6369	1	448
10	499.8829	0.7313	0	480
11	580.7363	6.22	0	558
12	602.8129	0.6532	0	579
13	624.5287	18.5614	1	600
14	674.7066	54.3818	4	648
15	816.6353	0.4733	0	785
16	857.7668	49.5094	4	824
17	884.471	759.8765	63	850
18	957.7315	22.7065	1	920
19	1097.51	25.4699	2	1055
20	1184.608	0.6531	0	1138
21	1234.855	41.2039	3	1187
22	1350.276	17.2977	1	1298
23	1427.842	5.1112	0	1372
24	1620.885	301.3617	25	1558
25	2129.013	1201.952	100	2046
26	2322.13	24.6885	2	2232
27	2335.746	39.3036	3	2245
28	3190.002	6.427	0	3066
29	3205.928	3.1271	0	3081
30	3490.331	73.2671	6	3355

* scaled by 0.9613. - # normalized to most prominent peak (=100)

5-Cyano-2*H*-pyrrol-2-ylidenemethanimine 22



GAUSSIAN 98; B3LYP/6-31+G*; POINT GROUP C_1

ZERO POINT VIBRATIONAL ENERGY = 48.9091 kcal/mol

ELECTRONIC ENERGY = -394.6232051 H

ZERO POINT CORRECTION = 0.077942 H

SUM OF ELECTRONIC AND ZERO POINT ENERGIES = -394.545264 H

STANDARD ORIENTATION

centre no.	**atom type**			**coordinates [Å]**
		x	**y**	**z**
1	C	-1.1176582061	-0.6255510758	1.0070178261
2	C	-1.0756312774	0.2381898238	-0.1577524243
3	N	0.1475219442	0.4469611606	-0.6188424240

4	C	0.9579643124	-0.2854186909	0.2488571540
5	C	0.1808228899	-0.9652570009	1.2667128195
6	C	2.2935458821	-0.3344491602	0.0719550878
7	N	3.4954094570	-0.2689870548	0.0167794464
8	C	-2.2208325704	0.8299194198	-0.7815981970
9	N	-3.1793424544	1.2886045369	-1.2555475848
10	H	-2.0071078816	-0.9236635661	1.5469609359
11	H	0.5680270155	-1.5932923694	2.0584654039
12	H	4.0846920550	-0.8936944580	-0.5333059999

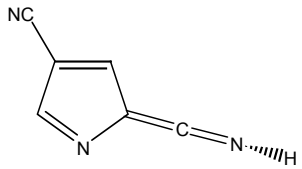
INFRARED SPECTRUM

mode no.	**unscaled frequency**	**absolute intensity**	**relative intensity**[#]	**scaled frequency**[*#]
1	104.9151	3.5799	0	100
2	114.6654	0.6555	0	110
3	200.1356	6.5144	0	192
4	204.8221	3.9796	0	196
5	461.9301	30.2552	2	444
6	475.7824	9.2521	0	457
7	502.7828	5.3162	0	483
8	547.6811	3.2666	0	526
9	602.6744	2.3643	0	579
10	639.6358	17.7406	1	614
11	656.7764	8.406	0	631
12	667.256	41.306	3	641
13	728.3713	46.93	3	700
14	776.0073	75.0694	6	745
15	798.483	838.1171	70	767
16	908.075	0.5534	0	872
17	949.7378	15.014	1	912
18	979.5688	8.6129	0	941
19	1084.77	12.8002	1	1042
20	1198.155	1.0617	0	1151
21	1263.346	17.4363	1	1214
22	1375.012	87.1319	7	1321
23	1438.964	38.2189	3	1383
24	1440.941	6.5829	0	1385
25	1559.728	19.1379	1	1499
26	2146.906	1181.764	100	2063
27	2341.014	12.2683	1	2250
28	3253.653	0.067	0	3127

29	3271.803	1.1521	0	3145
30	3518.815	117.8936	9	3382

[*] scaled by 0.9613. - [#] normalized to most prominent peak (=100)

4-Cyano-2*H*-pyrrol-2-ylidenemethanimine



GAUSSIAN 98; B3LYP/6-31+G*; POINT GROUP C_1

ZERO POINT VIBRATIONAL ENERGY = 49.04061 kcal/mol

ELECTRONIC ENERGY = -394.6262238 H

ZERO POINT CORRECTION = 0.078151 H

SUM OF ELECTRONIC AND ZERO POINT ENERGIES = -394.548073 H

STANDARD ORIENTATION

centre no.	**atom type**			**coordinates [Å]**
		x	**y**	**z**
1	C	-1.1064318919	-0.3924169562	0.0502138765
2	C	-1.0750391802	1.0552711749	-0.1124850560
3	N	0.1422967804	1.5343494023	-0.1735735955
4	C	0.9733358120	0.4074288045	-0.0479532309
5	C	0.2077076539	-0.8057474103	0.0878832309
6	C	2.3156820247	0.5116331492	-0.0922131044
7	N	3.5121083824	0.6090731936	0.0169664576
8	C	-2.2708106953	-1.2010517938	0.1512010711
9	N	-3.2369613497	-1.8471433406	0.2311261552
10	H	-1.9433331728	1.7024413021	-0.1787255029
11	H	0.5883124046	-1.8118912918	0.2024277029
12	H	4.1662517373	0.5847933928	-0.7652160440

INFRARED SPECTRUM

mode no.	**unscaled frequency**	**absolute intensity**	**relative intensity[#]**	**scaled frequency[*#]**
1	97.0372	2.1223	0	93
2	113.8776	1.4427	0	109
3	201.7324	4.9485	0	193
4	203.892	13.1405	1	196
5	455.3231	25.1069	2	437
6	482.0713	2.1941	0	463
7	495.6693	12.5137	1	476

8	537.4227	0.2225	0	516
9	613.7264	1.8914	0	589
10	622.4539	14.995	1	598
11	646.1952	36.2817	3	621
12	658.2673	14.8583	1	632
13	718.8431	71.2866	5	691
14	803.4269	842.5355	70	772
15	837.9354	19.5692	1	805
16	907.1674	15.6323	1	872
17	939.2768	24.088	2	902
18	986.1099	24.2385	2	947
19	1163.238	0.948	0	1118
20	1199.237	16.5967	1	1152
21	1274.764	8.9453	0	1225
22	1346.46	22.8667	1	1294
23	1442.135	9.5397	0	1386
24	1469.395	48.518	4	1412
25	1587.895	30.6638	2	1526
26	2147.035	1197.877	100	2063
27	2331.039	49.5371	4	2240
28	3234.431	2.599	0	3109
29	3270.498	0.3828	0	3143
30	3517.847	118.2806	9	3381

* scaled by 0.9613. - # normalized to most prominent peak (=100)