International Journal of ChemTech Research
CODEN (USA): IJCRGG ISSN: 0974-4290
Vol.8, No.4, pp 2234-2240, 2015

The mass spectral fragmentation of substituted m-terphenyl and biarylderivatives

Periyasamy Murugan*

Department of Chemistry,Vel Tech University,Avadi , Chennai- 600 062, India.

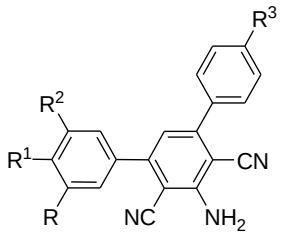
Abstract: A series of m-terphenyl and biaryl derivatives have been investigated by EI mass spectrometry because of due to their versatile wide applications such as laser dyes, OLED, liquid crystals, solar cells and NLO properties. Mass spectral fragmentation of m-terphenyl and biaryl derivatives were thoroughly analyzed in this article. In general, all the compounds except **3b**, showed the molecular ion peak. Loss of CH_3 group from the Ar-CH_2CH_3 or N-CH_2CH_3 has been observed from their parent skeleton compounds **2a-g**. The most common loss of CN,NH_2,HCN,C_2H_4 groups were observed from the compounds**1a-e, 2a-g, 3a-c**, which are depicted in the **scheme (I,II,III& IV)**. The loss of CHO group is the characteristic of furfuryl moiety has been observed in compound **3c**(m/z 194).As a representative fragmentation pattern of compound **1a** depicted in **Scheme-V**.
Key words: M-terphenyl, biaryl,OLED, NLO, furfuryl, HCN, CN,CHO.

Introduction

Mass spectrometry (MS) is unequivocally a powerful tool of characterization of organic compounds. In recent years, we have witnessed a significant development in the utilization of the terphenyls, particularly m-terphenyl[1] which are useful intermediate for building blocks for cyclophanes[2] to create a large molecular cavity[3]and host-guest complexes[4]. The biaryl unit is represented in several types of compounds of current interest including natural products, polymers, advanced materials, liquid crystals, ligands and molecules of medicinal interest[5]. In continuation of our work on the synthesis of m-terphenyl and biaryl compounds having laser dyes[6] and NLO properties[7]. In this paper, we would like to report the mass spectral fragmentation pattern of m-terphenyl and biaryl compounds **1 a-e , 2 a-g** and **3 a-c**. Similar loss of CH_3, HCHO and HCN groups were observed both methyl substituted compounds **1b** and **1d**.The characteristic loss of CHO group was observed in compound **3c**, it shows presence of furfuryl moiety.

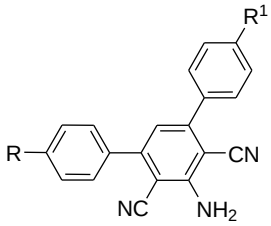
Experimental

The mass spectra were recorded with Jeol-JMS-DX 303 HF and GCMS QP 5000 Shimadzu instruments. Synthesis of m-terphenyl and biaryl compounds **1a-e, 2a-g, 3a-c** were previously reported[8] by our research group.



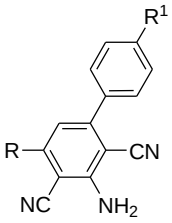
1a-e

Compounds	R	R^1	R^2	R^3
1a	H	H	H	H
1b	OCH_3	OCH_3	OCH_3	H
1c	H	Cl	H	H
1d	OCH_3	OCH_3	OCH_3	CH_3
1e	H	H	H	CH_3



2a-g

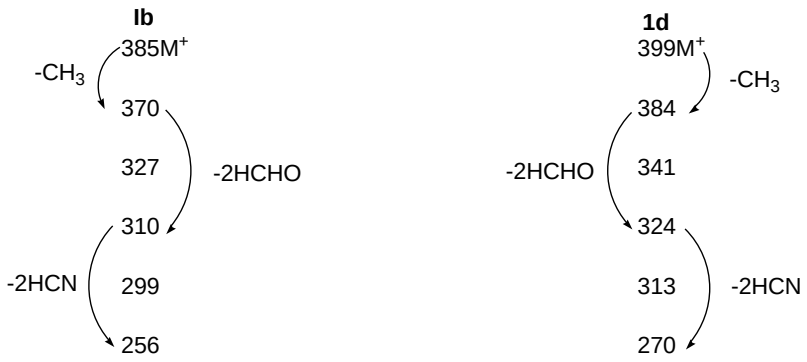
COMPOUND	R	R^1
2a	$N(CH_2CH_3)_2$	CH_3
2b	$N(CH_2CH_3)_2$	CH_2CH_3
2c	$N(CH_3)_3$	CH_2CH_3
2d	OCH_3	CH_3
2e	CH_3	CH_3
2f	CH_3	CH_2CH_3
2g	H	CH_2CH_3



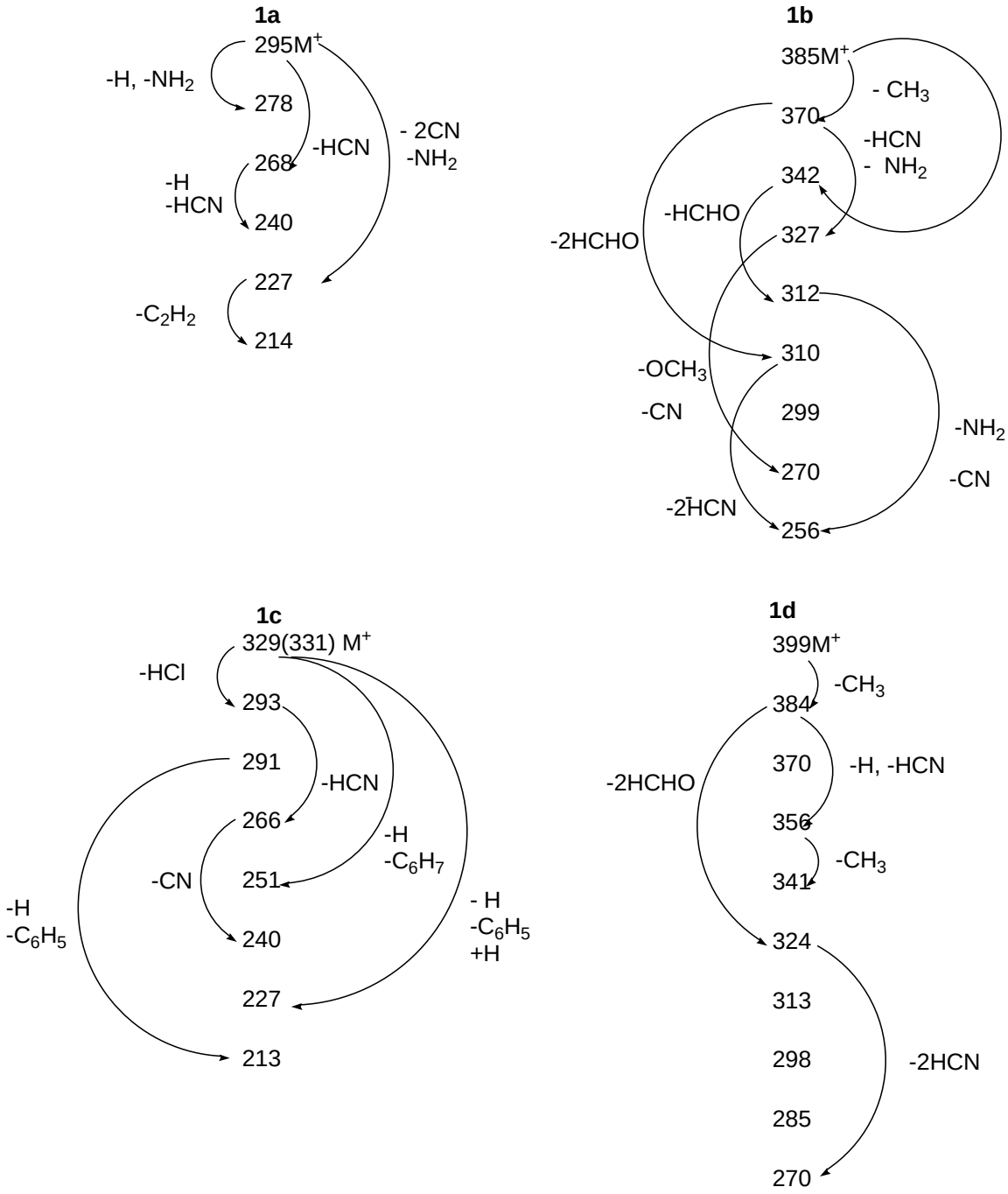
3a-c

COMPOUND	**R**	**R^1**
3a	C_6H_5	H
3b	C_6H_5	CH_3
3c	Furfuryl	CH_3

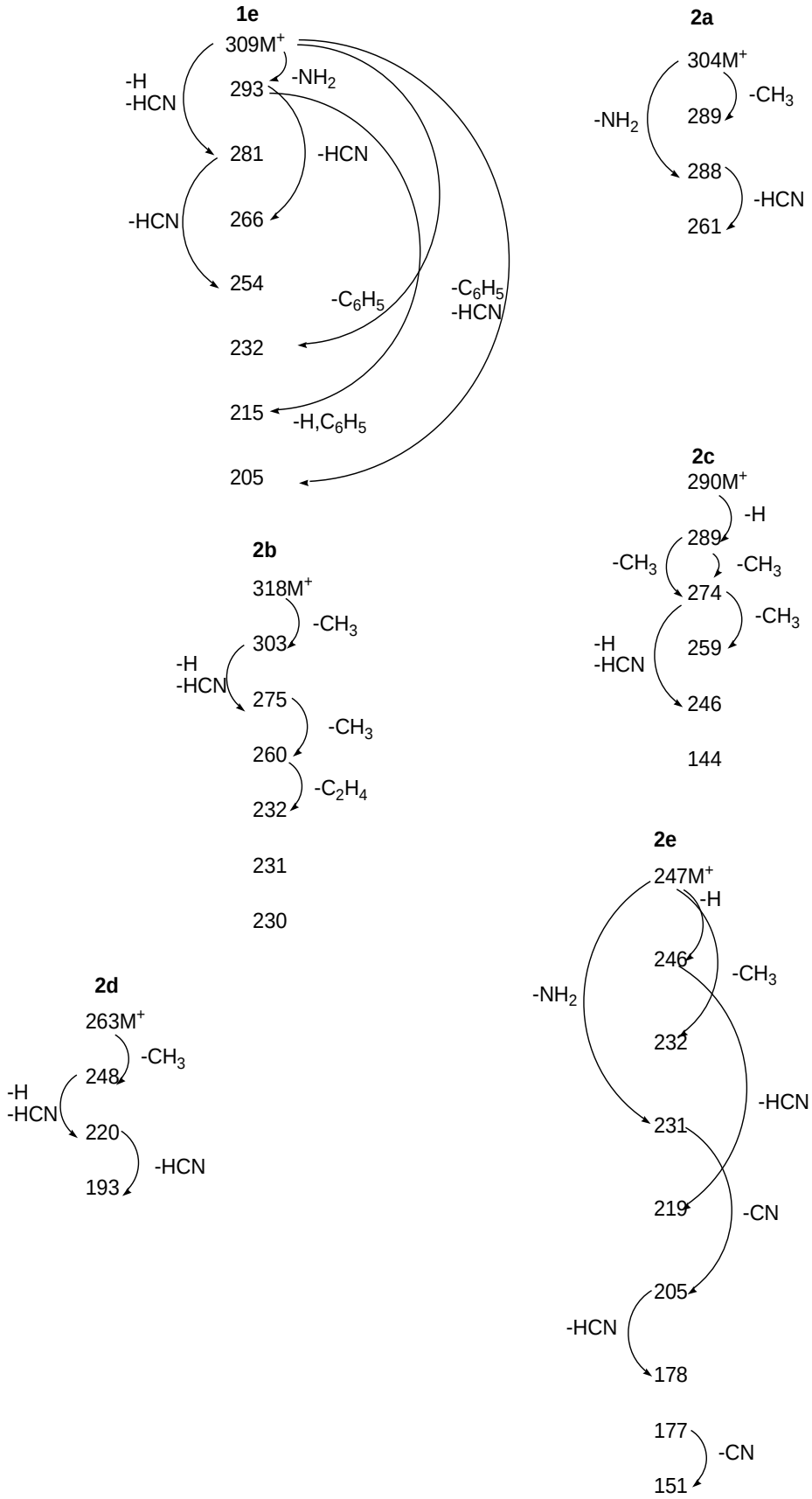
Similar loss of CH_3 , HCHO and HCN was observed both methyl substituted compounds **1b** and **1d** from the molecular ion shown in **scheme -I.** A successive loss of phenyl groups were observed compound **1c**and fragmentation pattern of m-terphenyl compounds**1b**and **1c**is depicted in **scheme** –II.



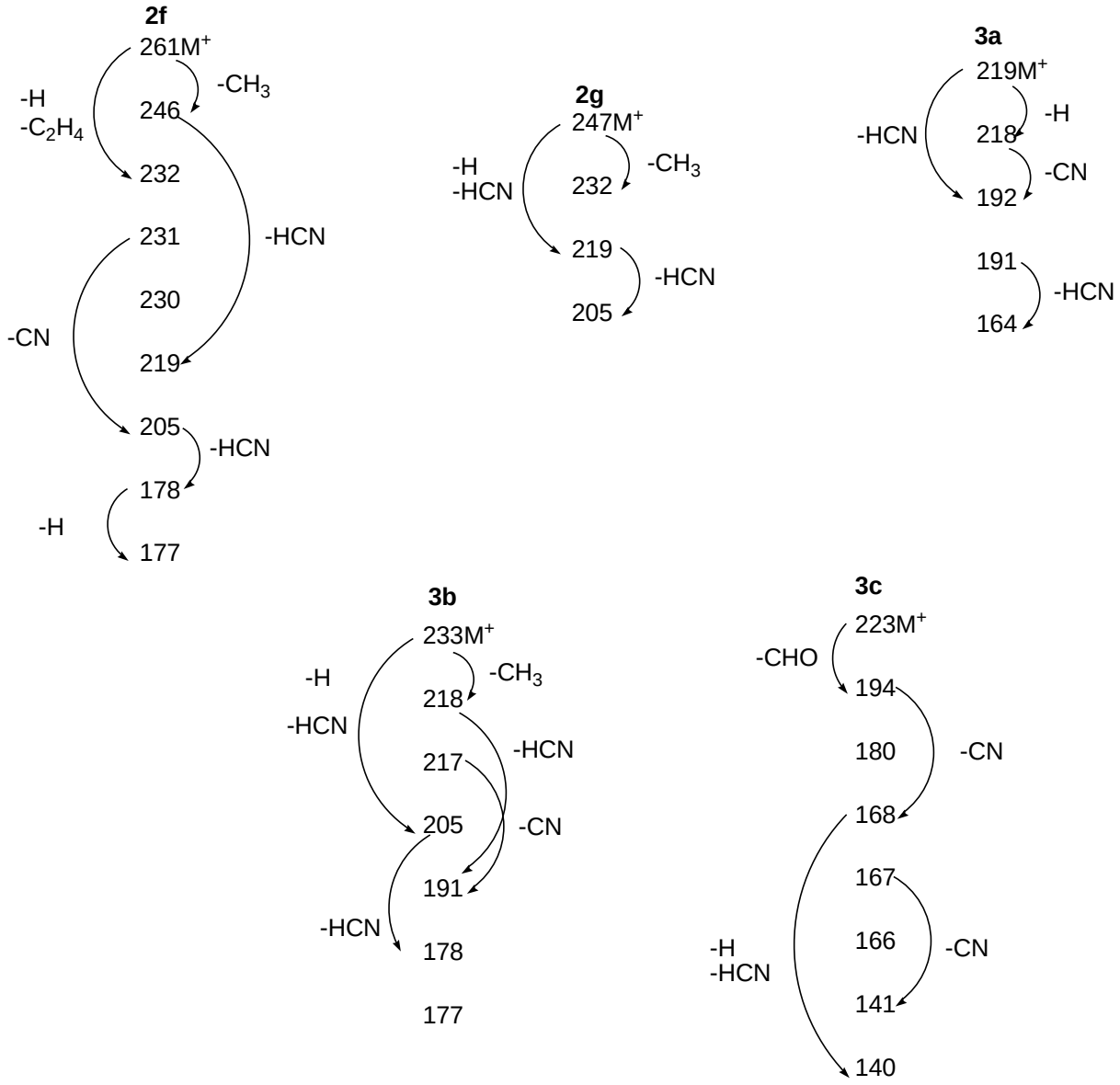
Scheme - I


1a
295M+
-H, -NH2
278
-HCN
- 2CN
-NH2
268
-H
-HCN
240
227
-C2H2
214
1b
385M+
- CH3
370
-H
-HCN
-NH2
-HCN
- NH2
342
-HCHO
-2HCHO
327
312
310
-OCH3
-CN
299
-NH2
270
-CN
-2HCN
256
1c
329(331) M+
-HCl
293
291
-HCN
266
-H
-C6H7
-CN
251
-H
-C6H5
- H
-C6H5
+H
240
227
213
1d
399M+
-CH3
384
370
-H, -HCN
-2HCHO
356
-CH3
341
324
313
298
-2HCN
285
270

Scheme- II

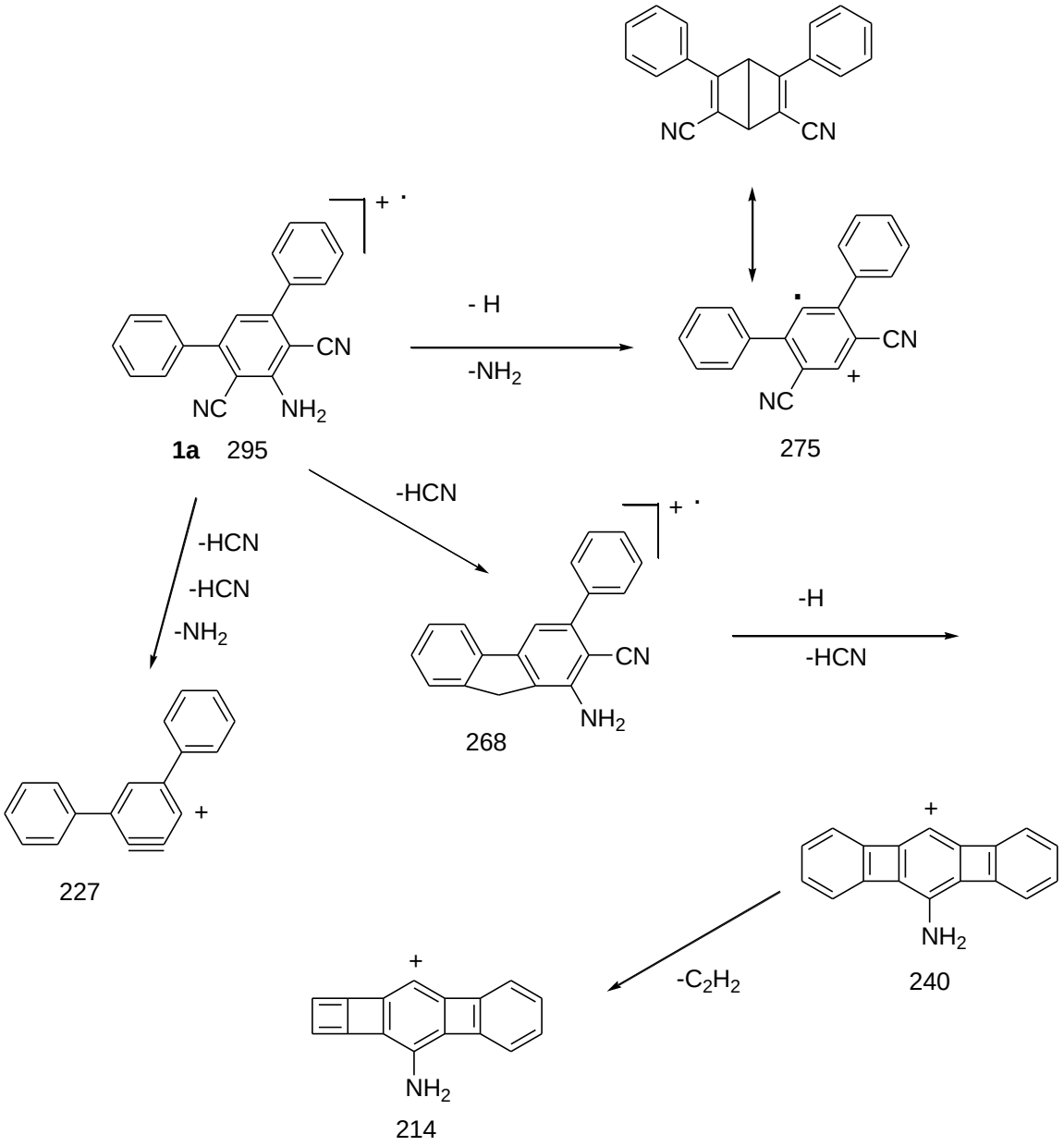

1e
309M+
-NH2
293
-H
-HCN
281
-HCN
-HCN
266
254
-C6H5
-C6H5
-HCN
232
215
-H,C6H5
205
2a
304M+
-CH3
289
-NH2
288
-HCN
261
2c
290M+
-H
289
-CH3
-CH3
274
-CH3
-H
-HCN
259
246
144
2b
318M+
-CH3
303
-H
-HCN
275
-CH3
260
-C2H4
232
231
230
2e
247M+
-H
246
-CH3
-NH2
232
-HCN
231
219
-CN
205
-HCN
178
177
-CN
151
2d
263M+
-CH3
248
-H
-HCN
220
-HCN
193

Scheme –III



Scheme –IV

The representative fragmentation pattern of m- terphenyl compound **1a** is furnished in **scheme-V**.



Scheme- V

Conclusion

Totally **15** m-terphenyl and biaryl derivatives were studied for their mass spectral fragmentation pattern. Molecular mass information and fragmentation pattern are easily obtained under the electron ionization (EI) condition. The most common loss of CN,NH_2,HCN,C_2H_4 groups were observed from all the compounds **1a-e, 2a-g, 3a-c**.Similar loss of CH_3 , HCHO and HCN groups were identified both methyl substituted compounds **1b** and **1d** from the molecular ions. Successive lossof phenyl groups were observed in compound **1c** and the loss of CHO group is the characteristic of furfurylmoiety has been observed in compound **3c** (m/z 194).

Acknowledgment

We thank the DST, India for the financial support of this work and Prof V.T. Ramakrishnan for generous support for all my work.

References

1. Saednya. A, Hart.H,Synthesis,1996,1455-1459.

2. (a) Hart. H,Rajakumar, P. Tetrahedron,34,1995,4407-4413 (b) Rajakumar. P,Srisailas.M, Tetra hedron Lett,34,1993,5323 – 5326.
3. Rajakumar. P, Kannan. A,Tetrahedron let,34,1993,4407-4409.
4. Bringmann.G, Walte,R, Weirich,R, Synthesis,1990,977-984.
5. Catellani. M, Motti. E,Minari.M,Chem.Comm,2000,157-160.
6. a)Murugan.P, Shanmugasundaram.P, Ramakrishnan.VT, Venkatachalapathy. B,Srividya,N, Ramamurthy.P, Gunasekaran.K, Velmurugan.D,J.Chem.Soc.Perkin Trans.2,1998,999-1007 ; b)Shanmugasundaram.P, Murugan.P, Ramakrishnan. VT, Heteroatom Chemistry,7,.1996,17-23.
7. Murugan,P, Ramakishnan,VT, Srividya,N, Ramamurthy.P, Indian J.Chem,37B,1998,737-742.
8. a)Murugan.P, Raghukumar. V,Ramakrishnan.VT,Synth.Commun,29,1999,3881-3886. b) Raghukumar. V, Murugan,P, Ramakrishnan.VT,Synth.Commun,31,2001,3497-3482.

*****