Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
This journal is © The Owner Societies 2013

Supplementary Information

Formation and Infrared Absorption of Protonated Naphthalene (1-$C_{10}H_9^+$ and 2-$C_{10}H_9^+$) and Their Neutral Counterparts in Solid *Para*-Hydrogen

Mohammed Bahou,[a] Yu-Jong Wu,[b,*] and Yuan-Pern Lee[a,c,*]

[a]Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, 1001, Ta-Hsueh Road, Hsinchu 30010, Taiwan.

[b]National Synchrotron Radiation Research Center, 101, Hsin-Ann Road, Hsinchu 30076, Taiwan.

[c] Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan.

Author E-mail address:
yjwu@nsrrc.org.tw;yplee@mail.nctu.edu.tw

Received xx xxxx. 2012

This journal is © The Owner Societies 2013

Table S1 Comparison of geometric parameters of isomers of $C_{10}H_9^+$ predicted with B3PW91/6-311++G(2d,2p). The atomic numbering is according to Fig. S1. The unit of Bond lengths is Å and the unit of angles is degree.

$C_{10}H_9^+$ geometry	1-$C_{10}H_9^+$	2-$C_{10}H_9^+$	4a-$C_{10}H_9^+$
r(C_1C_2)	1.471	1.465	1.353
r(C_2C_3)	1.362	1.478	1.426
r(C_3C_4)	1.409	1.348	1.374
r(C_4C_5)	1.402	1.435	1.407
r(C_5C_6)	1.428	1.451	1.487
r(C_1C_6)	1.492	1.372	1.483
r(C_7C_8)	1.373	1.384	1.374
r(C_8C_9)	1.404	1.415	1.426
r(C_6C_{10})	1.387	1.433	1.483
r(C_1H_{11})	1.101	1.084	1.082
r(C_3H_{13})	1.080	1.081	1.082
r(C_8H_{16})	1.080	1.082	1.082
r($C_{10}H_{18}$)	1.082	1.081	1.082
r(C_xH_{19})[a]	1.101	1.103	1.131
∠$H_{11}C_1H_{19}$	102.15		
∠$H_{12}C_2H_{19}$		101.04	
∠$C_5C_6H_{19}$			99.33
∠$C_1C_2C_3$	122.18	116.34	120.39
∠$C_2C_3C_4$	119.32	121.21	122.17
∠$C_4C_5C_6$	119.07	119.98	118.50
∠$C_7C_8C_9$	119.59	122.04	121.17
∠$C_{10}C_6C_5$	118.86	119.83	116.69

[a] The x mark denotes the carbon that attached with proton.

Table S2 Comparison of geometric parameters of isomers of $C_{10}H_9$ predicted with B3PW91/6-311++G(2d,2p). The atomic numbering is according to Fig. S1. The unit of Bond lengths is Å and the unit of angles is degree.

$C_{10}H_9$ geometry	1-$C_{10}H_9$	2-$C_{10}H_9$	4a-$C_{10}H_9$
r(C_1C_2)	1.496	1.493	1.348
r(C_2C_3)	1.366	1.499	1.432
r(C_3C_4)	1.403	1.340	1.376
r(C_4C_5)	1.432	1.451	1.403
r(C_5C_6)	1.417	1.438	1.511
r(C_1C_6)	1.454	1.395	1.499
r(C_7C_8)	1.382	1.391	1.376
r(C_8C_9)	1.396	1.404	1.432

$r(C_6C_{10})$	1.391	1.424	1.499
$r(C_1H_{11})$	1.100	1.083	1.084
$r(C_3H_{13})$	1.083	1.083	1.082
$r(C_8H_{16})$	1.082	1.081	1.082
$r(C_{10}H_{18})$	1.084	1.082	1.084
$r(C_xH_{19})$[a]	1.100	1.101	1.120
$\angle H_{11}C_1H_{19}$	103.95		
$\angle H_{12}C_2H_{19}$		103.27	
$\angle C_5C_6H_{19}$			104.48
$\angle C_1C_2C_3$	122.07	113.55	121.08
$\angle C_2C_3C_4$	121.82	122.53	120.33
$\angle C_4C_5C_6$	119.95	118.45	118.51
$\angle C_7C_8C_9$	119.84	119.70	120.33
$\angle C_{10}C_6C_5$	119.21	117.88	113.27

[a] The x mark denotes the carbon that attached with proton.

Table S3 Comparison of geometric parameters of transition states predicted with B3PW91/6-311++G(2d,2p). The atomic numbering is according to Fig. S2 and the corresponding potential energy surfaces are shown in Fig. S3. The unit of Bond lengths is Å and the unit of angles is degree.

TS geometry	TSA	TSB	TSC	TSD
$r(C_1C_2)$	1.429	1.381	1.491	1.382
$r(C_2C_3)$	1.423	1.398	1.422	1.461
$r(C_3C_4)$	1.364	1.382	1.361	1.363
$r(C_4C_5)$	1.423	1.401	1.453	1.438
$r(C_5C_6)$	1.428	1.454	1.426	1.453
$r(C_1C_6)$	1.422	1.472	1.438	1.460
$r(C_7C_8)$	1.375	1.367	1.396	1.394
$r(C_8C_9)$	1.406	1.421	1.386	1.400
$r(C_6C_{10})$	1.405	1.440	1.399	1.436
$r(C_1H_{11})$	1.084	1.083	1.080	1.083
$r(C_3H_{13})$	1.081	1.082	1.083	1.083
$r(C_8H_{16})$	1.082	1.082	1.082	1.081
$r(C_{10}H_{18})$	1.083	1.083	1.084	1.083
$r(C_1H_{19})$	1.338	1.430	1.331	1.483
$\angle H_{11}C_1H_{19}$	103.87	105.29	107.24	102.76
$\angle C_1C_2C_3$	119.90	120.41	118.09	118.59
$\angle C_2C_3C_4$	119.32	121.18	121.40	121.92
$\angle C_4C_5C_6$	119.63	118.78	119.27	117.32
$\angle C_7C_8C_9$	120.91	121.35	119.59	119.31
$\angle C_{10}C_6C_5$	120.18	119.46	118.87	117.67

This journal is © The Owner Societies 2013

Table S4 Vibrational wavenumbers (cm^{-1}) and intensities (km mol^{-1}) of 1-$C_{10}H_9^+$ and 2-$C_{10}H_9^+$ predicted with B3PW91/6-311++G(2d,2p).

mode	sym	1-$C_{10}H_9^+$		2-$C_{10}H_9^+$	
		Harmonic	Anharmonic	Harmonic	Anharmonic
ν_1	A'	3221 (1)	3102	3221 (1)	3097
ν_2	A'	3220 (2)	3087	3213 (1)	3086
ν_3	A'	3206 (0)	3090	3210 (1)	3095
ν_4	A'	3200 (0)	3079	3201 (0)	3084
ν_5	A'	3194 (2)	3076	3197 (1)	3076
ν_6	A'	3192 (0)	3049	3195 (0)	3065
ν_7	A'	3182 (0)	3032	3185 (1)	3072
ν_8	A'	2992 (31)	2850	2978 (62)	2841
ν_9	A'	1663 (86)	1625	1669 (236)	1627
ν_{10}	A'	1617 (67)	1571	1646 (25)	1610
ν_{11}	A'	1594 (12)	1558	1584 (5)	1563
ν_{12}	A'	1550 (231)	1515	1541 (31)	1507
ν_{13}	A'	1495 (127)	1458	1511 (116)	1471
ν_{14}	A'	1475 (1)	1449	1470 (2)	1440
ν_{15}	A'	1451 (30)	1420	1435 (12)	1405
ν_{16}	A'	1405 (81)	1365	1432 (98)	1402
ν_{17}	A'	1382 (17)	1346	1383 (32)	1335
ν_{18}	A'	1333 (105)	1286	1319 (50)	1289
ν_{19}	A'	1300 (22)	1278	1302 (131)	1268
ν_{20}	A'	1269 (24)	1252	1271 (5)	1249
ν_{21}	A'	1219 (8)	1201	1240 (5)	1218
ν_{22}	A'	1197 (10)	1182	1200 (17)	1185
ν_{23}	A'	1188 (30)	1170	1182 (20)	1167
ν_{24}	A'	1157 (7)	1141	1163 (5)	1148
ν_{25}	A'	1115 (8)	1099	1051 (15)	1025
ν_{26}	A'	1053 (2)	1037	1043 (3)	1025
ν_{27}	A'	978 (14)	963	941 (7)	930
ν_{28}	A'	929 (1)	920	937 (21)	926
ν_{29}	A'	800 (0)	791	785 (5)	778
ν_{30}	A'	755 (4)	745	753 (4)	745

ν_{31}	A'	608 (2)	603	615 (2)	609
ν_{32}	A'	503 (8)	496	509 (1)	502
ν_{33}	A'	502 (8)	497	501 (4)	496
ν_{34}	A'	355 (1)	352	360 (2)	358
ν_{35}	A"	3002 (11)	2844	2980 (14)	2824
ν_{36}	A"	1175 (1)	1138	1159 (0)	1120
ν_{37}	A"	1044 (0)	1018	1041 (1)	1019
ν_{38}	A"	1036 (0)	1016	1025 (1)	1001
ν_{39}	A"	1022 (5)	1000	1012 (3)	992
ν_{40}	A"	997 (0)	977	958 (17)	937
ν_{41}	A"	928 (1)	904	914 (10)	891
ν_{42}	A"	860 (7)	840	817 (17)	796
ν_{43}	A"	788 (54)	773	801 (1)	778
ν_{44}	A"	745 (28)	726	784 (44)	768
ν_{45}	A"	673 (0)	653	672 (2)	653
ν_{46}	A"	488 (0)	472	485 (22)	471
ν_{47}	A"	432 (13)	423	447 (3)	434
ν_{48}	A"	402 (0)	393	375 (1)	365
ν_{49}	A"	246 (13)	245	265 (2)	264
ν_{50}	A"	171 (1)	169	167 (1)	163
ν_{51}	A"	117 (0)	119	134 (6)	135

This journal is © The Owner Societies 2013

Table S5 Vibrational wavenumbers (cm^{-1}) and intensities (km mol^{-1}) of 1-$C_{10}H_9$ and 2-$C_{10}H_9$ predicted with B3PW91/6-311++G(2d,2p).

mode	sym	1-$C_{10}H_9$		2-$C_{10}H_9$	
		Harmonic	Anharmonic	Harmonic	Anharmonic
ν_1	A'	3201 (14)	3054	3202 (16)	3069
ν_2	A'	3197 (23)	3074	3187 (23)	3062
ν_3	A'	3187 (28)	3061	3182 (23)	3048
ν_4	A'	3186 (6)	3067	3174 (8)	3050
ν_5	A'	3172 (1)	3048	3171 (10)	3047
ν_6	A'	3168 (4)	3023	3168 (5)	3043
ν_7	A'	3163 (9)	3048	3160 (3)	2988
ν_8	A'	2974 (26)	2865	2947 (50)	2844
ν_9	A'	1638 (0)	1597	1682 (0)	1639
ν_{10}	A'	1609 (0)	1555	1611 (0)	1564
ν_{11}	A'	1565 (2)	1523	1571 (2)	1533
ν_{12}	A'	1522 (8)	1488	1509 (5)	1475
ν_{13}	A'	1477 (7)	1448	1463 (4)	1434
ν_{14}	A'	1444 (0)	1410	1449 (3)	1420
ν_{15}	A'	1438 (11)	1409	1436 (6)	1407
ν_{16}	A'	1396 (1)	1363	1415 (3)	1386
ν_{17}	A'	1366 (0)	1337	1365 (5)	1327
ν_{18}	A'	1324 (5)	1294	1355 (0)	1326
ν_{19}	A'	1279 (3)	1255	1295 (5)	1274
ν_{20}	A'	1235 (1)	1213	1250 (1)	1225
ν_{21}	A'	1206 (2)	1182	1205 (0)	1184
ν_{22}	A'	1176 (0)	1163	1176 (0)	1161
ν_{23}	A'	1173 (0)	1157	1162 (1)	1147
ν_{24}	A'	1140 (2)	1127	1140 (2)	1121
ν_{25}	A'	1094 (2)	1079	1056 (3)	1040
ν_{26}	A'	1060 (3)	1042	1041 (4)	1024
ν_{27}	A'	960 (11)	945	929 (1)	910
ν_{28}	A'	924 (0)	913	908 (17)	894
ν_{29}	A'	795 (1)	784	785 (1)	771
ν_{30}	A'	752 (0)	743	755 (0)	744

ν_{31}	A'	609 (1)	603	611 (2)	604
ν_{32}	A'	505 (1)	497	504 (0)	498
ν_{33}	A'	486 (0)	480	497 (1)	483
ν_{34}	A'	356 (1)	354	355 (1)	353
ν_{35}	A"	2979 (10)	2817	2939 (13)	2773
ν_{36}	A"	1199 (1)	1173	1183 (1)	1154
ν_{37}	A"	990 (0)	982	996 (1)	974
ν_{38}	A"	966 (0)	951	978 (0)	970
ν_{39}	A"	964 (2)	946	948 (7)	937
ν_{40}	A"	929 (2)	915	923 (9)	904
ν_{41}	A"	871 (1)	857	864 (0)	854
ν_{42}	A"	793 (19)	781	790 (17)	773
ν_{43}	A"	750 (56)	742	759 (75)	749
ν_{44}	A"	714 (10)	700	700 (0)	686
ν_{45}	A"	658 (28)	649	685 (1)	673
ν_{46}	A"	540 (1)	533	543 (6)	530
ν_{47}	A"	469 (2)	464	456 (18)	448
ν_{48}	A"	427 (8)	420	392 (0)	385
ν_{49}	A"	249 (6)	249	255 (0)	247
ν_{50}	A"	170 (1)	167	171 (2)	166
ν_{51}	A"	83 (0)	92	122 (1)	121

This journal is © The Owner Societies 2013

Table S6 Vibrational wavenumbers (cm^{-1}) and intensities (km mol^{-1}) of 4a-$C_{10}H_9^+$ and 4a-$C_{10}H_9$ predicted with B3PW91/6-311++G(2d,2p).

mode	sym	4a-$C_{10}H_9^+$		4a-$C_{10}H_9$	
		Harmonic	Anharmonic	Harmonic	Anharmonic
ν_1	A'	3219 (0)	3072	3202 (2)	3063
ν_2	A'	3210 (2)	3070	3188 (37)	3034
ν_3	A'	3200 (0)	3054	3171 (3)	3043
ν_4	A'	3196 (1)	3017	3167 (10)	3006
ν_5	A'	2747 (51)	2548	2718 (20)	2526
ν_6	A'	1652 (35)	1621	1636 (1)	1592
ν_7	A'	1593 (14)	1564	1521 (1)	1481
ν_8	A'	1488 (0)	1467	1473 (0)	1441
ν_9	A'	1428 (18)	1433	1404 (1)	1371
ν_{10}	A'	1389 (0)	1365	1351 (0)	1317
ν_{11}	A'	1266 (11)	1240	1263 (10)	1230
ν_{12}	A'	1194 (2)	1185	1170 (0)	1146
ν_{13}	A'	1148 (0)	1140	1157 (1)	1143
ν_{14}	A'	1043 (2)	1107	1076 (10)	1052
ν_{15}	A'	1029 (1)	1018	1004 (0)	990
ν_{16}	A'	1020 (2)	917	974 (2)	954
ν_{17}	A'	921 (13)	853	955 (5)	935
ν_{18}	A'	902 (25)	584	871 (3)	853
ν_{19}	A'	807 (73)	993	794 (30)	778
ν_{20}	A'	783 (4)	786	772 (22)	760
ν_{21}	A'	717 (2)	710	708 (65)	699
ν_{22}	A'	705 (34)	515	670 (1)	664
ν_{23}	A'	508 (1)	506	513 (3)	507
ν_{24}	A'	463 (15)	367	466 (14)	456
ν_{25}	A'	424 (2)	556	438 (5)	433
ν_{26}	A'	342 (0)	358	323 (0)	322
ν_{27}	A'	155 (2)	190	151 (1)	150
ν_{28}	A"	3219 (5)	3073	3201 (25)	3063
ν_{29}	A"	3209 (0)	3068	3187 (4)	3035

ν_{30}	A"	3199 (0)	3052	3169 (5)	3044
ν_{31}	A"	3195 (0)	3005	3164 (1)	3027
ν_{32}	A"	1667 (54)	1611	1636 (0)	1589
ν_{33}	A"	1537 (14)	1494	1512 (3)	1478
ν_{34}	A"	1476 (190)	1427	1421 (3)	1391
ν_{35}	A"	1433 (178)	1399	1340 (2)	1312
ν_{36}	A"	1275 (16)	1264	1258 (0)	1235
ν_{37}	A"	1204 (27)	1187	1202 (7)	1173
ν_{38}	A"	1198 (0)	1148	1180 (0)	1161
ν_{39}	A"	1175 (9)	1125	1111 (11)	1093
ν_{40}	A"	1040 (0)	1051	1074 (1)	1051
ν_{41}	A"	1024 (0)	1059	1003 (11)	995
ν_{42}	A"	1016 (2)	986	971 (1)	950
ν_{43}	A"	930 (7)	907	929 (0)	911
ν_{44}	A"	908 (25)	796	920 (3)	905
ν_{45}	A"	828 (31)	823	781 (0)	767
ν_{46}	A"	706 (28)	659	677 (14)	664
ν_{47}	A"	609 (2)	613	605 (1)	600
ν_{48}	A"	546 (0)	682	564 (0)	554
ν_{49}	A"	490 (9)	469	469 (3)	464
ν_{50}	A"	335 (0)	540	350 (1)	338
ν_{51}	A"	152 (0)	137	115 (0)	109

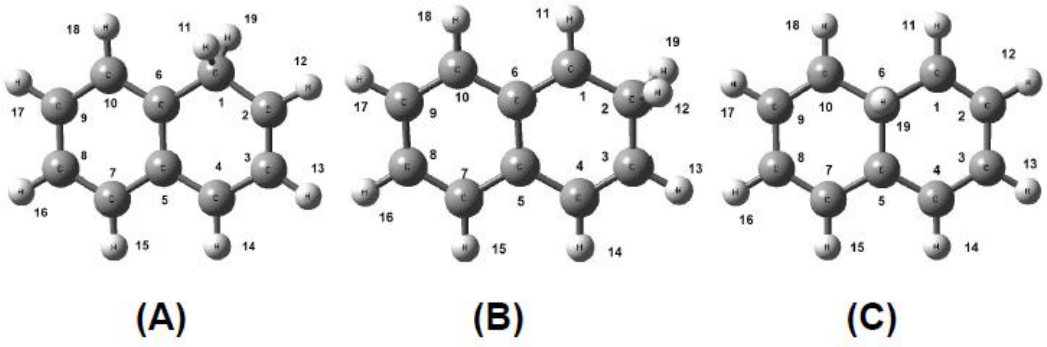

Fig. S1 Atomic numbering of (A)1-$C_{10}H_9^+$ and 1-$C_{10}H_9$, (B) 2-$C_{10}H_9^+$ and 2-$C_{10}H_9$, (C) 4a-$C_{10}H_9^+$ and 4a-$C_{10}H_9$.

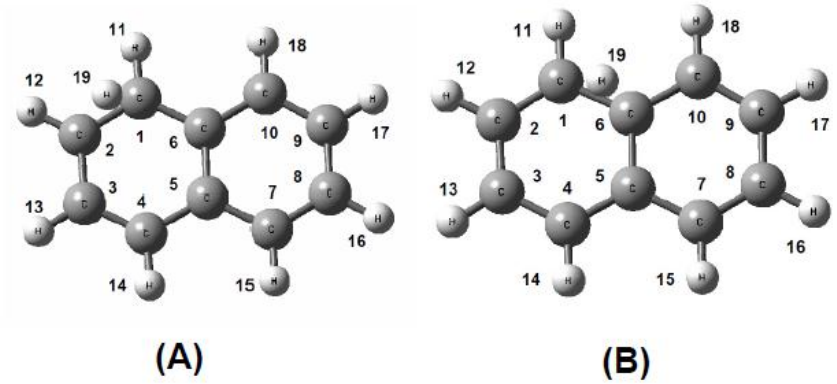

Fig. S2 Atomic numbering for (A) TSA and TSC, (B) TSB and TSD.

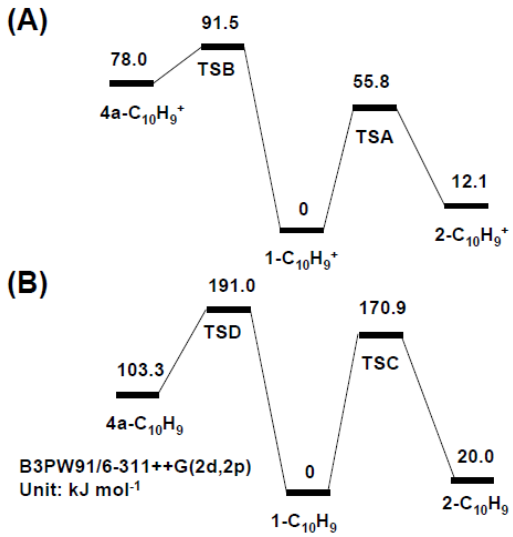

Fig. S3 Potential energy surfaces of isomerization of (A) $C_{10}H_9^+$ and (B) $C_{10}H_9$.