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Electronic Supporting Information (ESI)

Infrared Spectra and Structures of Protonated Amantadine Isomers: Detection of Ammonium and Open-Cage Iminium Ions

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Table S1. Computed vibrational frequencies (in cm^{-1}, B3LYP-D3/cc-pVTZ) of $AmaH^+$(**I-IV**) compared to experimental values of $AmaH^+Ar$ (Figure 1 and 2).[a] Maxima of convoluted bands are given in bold. The experimental values are given with peak width (fwhm in parenthesis) and are assigned to the most dominant vibrations.

Mode[b]	$AmaH^+$(**I**) C_{3v}	$AmaH^+$(**II**) C_s	$AmaH^+$(**III**) C_s	$AmaH^+$(**IV**) C_S	$AmaH^+Ar$ Exp.
τ_{CH2}, ρ_{CH2}	**1117** 1117 (6) 1117 (6) 1118 (0) 1127 (0)	**1113** 1112 (0.3) 1113 (15)	**1106** 1106 (8) 1116 (1) 1123 (2)	**1117** 1108 (0.7) 1117 (22) 1134 (2)	
τ_{CH2}		**1156** (2)	**1150** (4)	**1151** (0.8)	
τ_{CH2}	**1206** 1206 (4) 1206 (4)	**1203** 1199 (0.2) 1203 (15)	**1192** 1192 (29) 1203 (2) 1214 (0.1)	**1220** 1197 (0.9) 1220 (5)	**A** 1187 (12) **B** 1209 (2)
τ_{CH2}		**1251** 1248 (2) 1253 (2)	**1235** (15)		
τ_{CH2}, γ_{CH2}	**1294** 1278 (0.02) 1278 (0.02) 1285 (0) 1294 (27) 1297 (0.5) 1297 (0.5) 1321 (0.1) 1321 (0.1) 1325 (0)	**1297** 1283 (3) 1297 (14) 1302 (2) 1314 (1.4) 1324 (2) 1330 (1)	**1281** 1281 (10) 1285 (1) 1300 (0.8) **1308** 1307 (4) 1314 (1) 1327 (0.4)	**1279** 1261 (1) 1267 (0.2) 1279 (3) 1299 (3) **1324** 1315 (2) 1324 (10) 1334 (1) 1340 (8)	**C** 1322 (8)
γ_{CH2}, τ_{CH2}	**1359** 1355 (0.7) 1355 (0.7) 1359 (18) 1371 (0.7) 1371 (0.7)	**1346** 1346 (13) 1355 (1) 1356 (2) 1369 (1)	**1349** 1338 (0.5) 1349 (2) 1357 (0.5) 1369 (0.4)		**D** 1377 (11)
ρ_{NH2}, γ_{CH2}, β_{CH2}		**1415** 1390 (16) 1393 (2) 1409 (12) 1417 (23)	**1396** 1392 (4) 1397 (10)	**1384** 1356 (1) 1364 (3) 1365 0.1) 1368 (1) 1382 (33) 1395 (6) 1399 (19) 1401 (0.3)	
β_{CH2}			**1441** 1436 (17) 1443 (21)	**1455** 1452 (4) 1452 (13) 1459 (2) 1469 (12) 1476 (5)	**E** 1453 (13)

$\gamma_{NH3\ (umbrella)}$, β_{CH2}	**1441** 1441 (130) 1450 (0.07) 1450 (0.07)				**E** 1453 (13)
β_{CH2} β_{CH3}	**1469** 1463 (13) 1463 (13) 1472 (39) 1493 (7)	**1462** 1450 (4) 1453 (10) 1463 (8) 1465 (10) 1476 (9)	**1468** 1455 (0.2) 1462 (8) 1465 (6) 1469 (16) 1474 (7)		**F** 1474 (6) **G** 1483 (5)
ν_{CN} [c]		**1534** (7)	**1541** (3)	**1534** (5)	
β_{NH3}	**1611** 1611 (39) 1611 (39)				**H** 1611 (12)
β_{NH2} [c]		**1664** (219)	**1669** (206)	**1665** (203)	**I** 1714 (15)
ν_{CH}		**2848** (60)			**J** 2853 (10)
$\nu_{CH/CH2}$	**2899** 2892 (11) 2892 (12) 2899 (47) 2916 (25) 2916 (25) 2917 (0.3) 2930 (0)		**2882** 2883 (24) 2884 (9)	**2874** 2871 (8) 2876 (11)	**K** 2872 (7)
ν_{CH2}		**2913** 2885 (5) 2891 (10) 2908 (19) 2910 (4) 2915 (37) 2917 (9)	**2917** 2904 (6) 2913 (0.4) 2915 (33) 2919 (9) 2929 (17)	**2916** 2911 (3) 2913 (20) 2914 (22) 2924 (10) 2930 (17)	**L** 2921 (14)
ν_{CH2}	**2956** 2935 (34) 2935 (34) 2953 (38) 2953 (38) 2955 (0) 2958 (1) 2958 (1) 2964 (43)	**2952** 2942 (10) 2944 (19) 2952 (6) 2953 (14) 2954 (26) 2955 (7) 2966 (13)		**2948** 2944 (20) 2946 (2) 2948 (0.6) 2948 (14) 2949 (6) 2950 (31) 2966 (15)	**M** 2949 (17)
ν_{CH3}		**2977** 2977 (25) 2982 (18)	**2972** 2954 (0.3) 2955 (8) 2666 (17) 2969 (25) 2971 (9) 2972 (9) 2974 (9) 2977 (21) 2983 (16)	**2998** 2979 (16) 2998 (50)	**N** 2973 (5)
$2\beta_{NH3}$	3222				**O** 3164 (7) **P** 3185 (5)
ν_{NH3}^{s}	**3214** (26)				**Q** 3238 (13)
ν_{NH3}^{a}	**3301** 3301 (52) 3301 (52)				**R** 3317 (21)
ν_{NH2}^{s}		**3331** (136)	**3330** (129)	**3329** (129)	**S** 3344 (7)

$2\beta_{NH2}$ [c]		3328	3338	3330	**T** 3428 (11)
ν_{NH2} [a]		**3435** (77)	**3433** (76)	**3432** (78)	**U** 3451 (10)

[a] IR intensities in km mol^{-1} are given in parentheses. [b] Stretching (ν), bending (β), torsion (τ), wagging (γ), rocking (ρ). [c] Coupled β_{NH2}/ν_{CN} modes.

Table S2. Various energies of $AmaH^+$(**I-IV**) isomers (in kJ mol^{-1}) calculated at the B3LYP-D3/cc-pVTZ level.

	E_0	E_e
$AmaH^+$(**I**)	0	0
$AmaH^+$(**II**)	3.03	15.72
$AmaH^+$(**III**)	27.39	39.42
$AmaH^+$(**IV**)	29.50	42.50
TS I-IV	262.90	287.47
TS III-IV	43.48	56.33

Table S3. Computed vibrational frequencies (in cm^{-1}, B3LYP-D3/cc-pVTZ) of Ama compared to calculated vibrational frequencies of $AmaH^+$(**I-IV**) (Figure S4).[a] Maxima of convoluted bands are given in bold. Stretching (ν), bending (β), torsion (τ), wagging (γ), rocking (ρ).

Mode of Ama	Ama	Mode of Ama^+	$AmaH^+$(**I**)	$AmaH^+$(**II**)	$AmaH^+$(**III**)	$AmaH^+$(**IV**)
τ_{CH2}, γ_{CH2}	**1256** 1256 (4) 1274 (0.0) 1277 (0.2) 1279 (0.0)	τ_{CH2}, ρ_{CH2}	**1117** 1117 (6) 1117 (6) 1118 (0) 1127 (0)	**1113** 1112 (0.3) 1113 (15)	**1106** 1106 (8) 1116 (1) 1123 (2)	**1117** 1108 (0.7) 1117 (22) 1134 (2)
		τ_{CH2},		**1156** (2)	**1150** (4)	**1151** (0.8)
		τ_{CH2}	**1206** 1206 (4) 1206 (4)	**1203** 1199 (0.2) 1203 (15)	**1192** 1192 (29) 1203 (2) 1214 (0.1)	
γ_{CH2}	**1308** 1308 (5) 1311 (1) 1313 (1) 1319 (0.0) 1320 (0.0)	τ_{CH2}		**1251** 1248 (2) 1253 (2)	**1235** (15)	**1220** 1197 (0.9) 1220 (5)
		τ_{CH2}, γ_{CH2},	**1294** 1278 (0.02) 1278 (0.02) 1285 (0) 1294 (27) 1297 (0.5) 1297 (0.5) 1321 (0.1) 1321 (0.1) 1325 (0)	**1297** 1283 (3) 1297 (14) 1302 (2) 1314 (1.4) 1324 (2) 1330 (1)	**1281** 1281 (10) 1285 (1) 1300 (0.8) **1307** 1307 (4) 1314 (1) 1327 (0.4)	**1279** 1261 (1) 1267 (0.2) 1279 (3) 1299 (3) **1324** 1315 (2) 1324 (10) 1334 (1) 1340 (8)
τ_{CH2}, γ_{CH2}, τ_{NH2}	**1360** 1342 (0.2) 1351 (1) 1358 (3) 1364 (2) 1373 (0.1)	τ_{CH2}, γ_{CH2},	**1359** 1355 (0.7) 1355 (0.7) 1359 (18) 1371 (0.7) 1371 (0.7)	**1346** 1346 (13) 1355 (1) 1356 (2) 1369 (1)	**1349** 1338 (0.5) 1349 (2) 1357 (0.5) 1369 (0.4)	
β_{CH2}	**1461** 1446 (0.0) 1448 (0.0) 1461 (8) 1461 (10) 1463 (8) 1486 (0.1)	ρ_{NH2} γ_{CH3} (umbrella), γ_{CH2}, β_{CH2}		**1415** 1390 (16) 1393 (2) 1409 (12) 1417 (23)	**1396** 1392 (4) 1397 (10)	**1384** 1356 (1) 1364 (3) 1365 0.1) 1368 (1) 1382 (33) 1395 (6) 1399 (19) 1401 (0.3)
		$\gamma_{NH3\ (umbrella)}$, β_{CH2}	**1441** 1441 (130) 1450 (0.1) 1450 (0.1)		**1441** 1436 (17) 1443 (21)	**1455** 1452 (4) 1452 (13) 1459 (2) 1469 (12) 1476 (5)
		β_{CH3}, β_{CH2}	**1469** 1463 (13) 1463 (13)	**1462** 1450 (4) 1453 (10)	**1467** 1455 (0.2) 1462 (8)	

			1472 (39) 1493 (7)	1463 (8) 1465 (10) 1476 (9)	1465 (6) 1469 (16) 1474 (7)	
β_{NH2}	**1609** (34)	β_{NH3}	**1611** 1611 (39) 1611 (39)			
		ν_{CN} [b]		**1534** (7)	**1541** (3)	**1534** (5)
		β_{NH2} [b]		**1664** (219)	**1669** (206)	**1665** (203)
ν_{CH}, ν_{CH2}	**2890** 2880 (15) 2885 (28) 2890 (60) 2891 (4) 2892 (19) 2893 (28)	ν_{CH}		**2848** (60)		
		$\nu_{CH/CH2}$	**2899** 2892 (11) 2892 (12) 2899 (47) 2916 (25) 2916 (25) 2917 (0.3) 2930 (0)		**2882** 2883 (24) 2884 (9)	**2874** 2871 (8) 2876 (11)
	2917 2913 (113) 2914 (68) 2916 (92) 2922 (28) 2926 (12) 2926 (46) 2932 (100) 2936 (5) 2941 (81)	ν_{CH2}		**2913** 2885 (5) 2891 (10) 2908 (19) 2910 (4) 2915 (37) 2917 (9)	**2917** 2904 (6) 2913 (0.4) 2915 (33) 2919 (9) 2929 (17)	**2916** 2911 (3) 2913 (20) 2914 (22) 2924 (10) 2930 (17)
		ν_{CH2}	**2956** 2935 (34) 2935 (34) 2953 (38) 2953 (38) 2955 (0) 2958 (1) 2958 (1) 2964 (43)	**2952** 2942 (10) 2944 (19) 2952 (6) 2953 (14) 2954 (26) 2955 (7) 2966 (13)	**2972** 2954 (0.3) 2955 (8) 2666 (17) 2969 (25) 2971 (9) 2972 (9) 2974 (9) 2977 (21) 2983 (16)	**2948** 2944 (20) 2946 (2) 2948 (0.6) 2948 (14) 2949 (6) 2950 (31) 2966 (15)
		ν_{CH3}		**2977** 2977 (25) 2982 (18)		**2998** 2979 (16) 2998 (50)
ν_{NH2}^{s}	**3285** (3)	ν_{NH3}^{s}	**3214** (26)			
		ν_{NH2}^{s}		**3331** (136)	**3330** (129)	**3329** (129)
ν_{NH2}^{a}	**3359** (0.2)	ν_{NH3}^{a}	**3301** 3301 (52) 3301 (52)			
		ν_{NH2}^{a}		**3435** (77)	**3433** (76)	**3432** (78)

[a] IR intensities in km mol^{-1} are given in parentheses. [b] Coupled β_{NH2}/ν_{CN} modes.

Table S4. Computed vibrational frequencies (in cm^{-1}, B3LYP-D3/cc-pVTZ) of Ama^+(**I-III**) compared to experimental values of Ama^+Ar.[a] Maxima of convoluted bands are given in bold. The experimental values are given with peak width (fwhm in parenthesis) and are assigned to the most dominant vibrations.

Mode [d]	Ama^+(**I**)	Ama^+(**II**)	Ama^+(**III**)	Ama^+-Ar Exp.
ρ_{NH2}, τ_{CH2}, γ_{CH2},	**1226** 1226 (22) 1243 (0.001)		**1226** 1218 (2) 1227 (10)	**R** 1228 (15)
γ_{CH2}		**1247** (22)		
τ_{CH2}, γ_{CH2}	**1274** 1254 (1.3) 1271 (0.01) 1273 (0.1) 1274 (26) 1296 (5) 1307 (0.4)	**1285** 1283 (1) 1285 (4)	**1301** 1261 (1) 1280 (3) 1292 (1) 1301 (14) 1316 (5)	
γ_{CH2}	**1346** 1320 (0.1) 1325 (2) 1345 (2) 1345 (1) 1352 (2) 1362 (0.2)	**1310** 1306 (3) 1311 (2) 1323 (1) 1330 (0.1) 1333 (0.2) 1350 (1) 1360 (0.2)	**1336** 1332 (4) 1338 (7) 1348 (2)	
ρ_{NH2}, γ_{CH2}, γ_{CH3}		**1397** (10)	**1372** 1363 (15) 1378 (12) 1380 (4)	**S** 1368 (35)
β_{CH2}, β_{CH3}	**1458** 1435 (5) 1439 (1) 1450 (15) 1460 (12) 1463 (14) 1484 (1)	**1441** 1430 (1) 1438 (17) 1445 (20) **1469** 1464 (3) 1469 (17) 1473 (3)	**1440** 1421 (6) 1430 (0) 1431 (16) 1442 (11) 1442 (28) 1447 (5) 1467 (5)	**P** 1458 (25)
ν_{CN} [e]			**1500** (93)	**T** 1551 (7)
ν_{CN} [e]		**1542** (4)		
β_{NH2}	**1595** (70)			**Q_1** 1599 (6)
β_{NH2} [e]			**1641** (216)	**Q_2** 1664 (13)
β_{NH2} [e]		**1670** (208)		**Q_3** 1717 (7)
ν_{CH}		**2821** (8)		**A** 2842 (4)
ν_{CH}	**2840** (75)			**B** 2864 (11)
ν_{CH2}, ν_{CH3}			**2878** 2858 (0.3) 2873 (2) 2878 (16)	**B** 2864 (11)
ν_{CH2}, ν_{CH3}	**2920** 2908 (4) 2912 (16) 2921 (16) 2923 (20) 2925 (10)	**2901** 2898 (10) 2901 (40) **2926** 2916 (0.3) 2921 (8) 2929 (11)	**2905** 2898 (0) 2905 (9) **2926** 2925 (10) 2930 (6)	**C** 2920 (6)
ν_{CHn}	**2955** 2949 (5) 2950 (28) 2951 (1) 2952 (10)	**2972** 2955 (0) 2956 (13) 2970 (25) 2971 (5)	**2961** 2951 (5) 2953 (11) 2957 (11) 2959 (20)	**D** 2947 (25) **E** 2959 (6) **F** 2978 (4)

	2961 (6) 2962 (11) 2966 (4) 2971 (27)	2974 (8) 2974 (9) 2976 (8)	2963 (7) 2965 (28) 2966 (4) 2977 (17)	
ν_{CH2}	3024 (6)	3021 (6)		**G** 3008 (6)
ν_{CH2}		3121 (4)		
$2\beta_{NH2}$	3190[b] 3200 (12)[c]			**H** 3151 (9)
$2\beta_{NH2}$[e]			3282[b] 3262 (0.7)[c]	**I** 3267 (8)
$2\beta_{NH2}$[e]		3339[b] 3289 (0.3)[c]		
ν_{NH2}^{s}	**3322** (223)			$\mathbf{J_1}$ 3321 (16)
ν_{NH2}^{s}		**3329** (131)		$\mathbf{J_2}$ 3345 (8)
ν_{NH2}^{s}			**3358** (173)	$\mathbf{J_3}$ 3381 (17)
ν_{NH2}^{a}	**3438** (68)			$\mathbf{K_1}$ 3425 (9)
ν_{NH2}^{a}		**3433** (76)		$\mathbf{K_2}$ 3451 (7)
ν_{NH2}^{a}			**3467** (63)	$\mathbf{K_3}$ 3477 (11)

[a] IR intensities in km mol^{-1} are given in parentheses (M. A. R. George, O. Dopfer, *J. Phys. Chem. Lett.* **2022**, *13*, 449). [b] Harmonic value. [c] Result of anharmonic calculation.

[d] Stretching (ν), bending (β), torsion (τ), wagging (γ), rocking (ρ). [e] Coupled β_{NH2}/ν_{CN} modes.

Table S5. Computed vibrational frequencies (in cm^{-1}, B3LYP-D3/cc-pVTZ) of $AmaH^+$(**I-IV**)-Ar(**I**) compared to experimental values of $AmaH^+Ar$ (Figure S7-S10).[a] Maxima of convoluted bands are given in bold. The experimental values are given with peak width (fwhm in parenthesis) and are assigned to the most dominant vibrations.

Mode[b]	$AmaH^+$(**I**)-Ar(**I**)	$AmaH^+$(**II**)-Ar(**I**)	$AmaH^+$(**III**)-Ar(**I**)	$AmaH^+$(**IV**)-Ar(**I**)	$AmaH^+$-Ar Exp.
τ_{CH2}, ρ_{CH2}	**1117** 1116 (4) 1117 (5) 1118 (2) 1126 (0.1)	**1113** 1111 (0.3) 1113 (16)	**1106** 1106 (7) 1116 (1) 1124 (2)	**1118** 1109 (0.9) 1118 (21) 1134 (1)	
τ_{CH2},		**1155** (2)	**1150** (5)	**1152** (0.7)	
τ_{CH2}	**1206** 1205 (3) 1206 (3)	**1203** 1199 (0.5) 1203 (14)	**1191** 1191 (29) 1203 (2) 1214 (0.1)	**1221** 1197 (1) 1221 (4)	**A** 1187 (12) **B** 1209 (2)
τ_{CH2}		**1251** 1250 (2) 1253 (1)	**1234** (13)		
τ_{CH2}, γ_{CH2}	**1296** 1278 (0.05) 1279 (0.03) 1285 (0) 1296 (26) 1297 (1) 1300 (2) 1320 (0.2) 1322 (0.2) 1324 (0.01)	**1297** 1282 (3) 1297 (13) 1301 (2) 1316 (2) 1324 (1) 1331 (0.5)	**1282** 1281 (11) 1285 (2) 1297 (0.6) **1308** 1307 (3) 1314 (2) 1325 (0.4)	**1280** 1261 (1) 1267 (0.3) 1280 (3) 1300 (3) **1329** 1316 (2) 1325 (9) 1334 (1) 1341 (8)	**C** 1322 (8)
γ_{CH2}, τ_{CH2}	**1360** 1354 (1) 1355 (0.4) 1360 (19) 1372 (0.6) 1373 (1)	**1349** 1349 (10) 1352 (2) 1356 (2) 1369 (1)	**1348** 1337 (0.6) 1348 (2) 1357 (0.5) 1368 (0.4)		**D** 1377 (11)
ρ_{NH2} γ_{CH3} (umbrella), γ_{CH2}, β_{CH2}		**1416** 1392 (16) 1394 (2) 1411 (11) 1419 (23)	**1396** 1391 (4) 1398 (11)	**1384** 1357 (0.8) 1365 (3) 1365 (0.3) 1368 (2) 1384 (31) 1391 (3) 1401 (18) 1403 (1)	
β_{CH2}			**1441** 1438 (15) 1446 (19)	**1461** 1452 (2) 1453 (11) 1459 (5) 1469 (13) 1480 (7)	**E** 1453 (13)

$\gamma_{NH3\ (umbrella)}$, β_{CH2}	**1442** 1442 (110) 1448 (0.7) 1453 (0.7)				**E** 1453 (13)
β_{CH2} β_{CH3}	**1470** 1460 (17) 1465 (13) 1474 (31) 1493 (5)	**1463** 1451 (4) 1453 (10) 1464 (7) 1465 (10) 1475 (11)	**1470** 1457 (0.8) 1463 (9) 1468 (6) 1471 (18) 1474 (4)		**F** 1474 (6) **G** 1483 (5)
ν_{CN} [c]		**1537** (8)	**1544** (6)	**1534** (8)	
β_{NH3}	**1612** 1611 (32) 1613 (30)				**H** 1611 (12)
β_{NH2} [c]		**1667** (206)	**1671** (185)	**1668** (187)	**I** 1714 (15)
ν_{CH}		**2860** (53)			**J** 2853 (10)
$\nu_{CH/CH2}$	**2905** 2893 (10) 2896 (10) 2901 (43) 2915 (26) 2915 (26) 2917 (0.6) 2933 (8)		**2886** 2883 (17) 2891 (11)	**2874** 2871 (8) 2876 (11)	**K** 2872 (7)
ν_{CH2}		**2913** 2887 (5) 2893 (9) 2908 (15) 2910 (4) 2915 (40) 2917 (9)	**2917** 2904 (5) 2915 (33) 2916 (3) 2922 (9) 2927 (14)	**2916** 2910 (3) 2914 (23) 2914 (20) 2924 (11) 2931 (19)	**L** 2921 (14)
ν_{CH2}	**2952** 2938 (24) 2941 (32) 2953 (38) 2953 (41) 2955 (0.2) 2958 (2) 2958 (2) 2964 (46)	**2953** 2943 (13) 2947 (19) 2952 (13) 2953 (13) 2954 (26) 2955 (15) 2962 (11) 2966 (12)		**2948** 2944 (22) 2945 (2) 2948 (3) 2948 (9) 2949 (31) 2958 (5) 2966 (15)	**M** 2949 (17)
ν_{CH3}		**2977** 2976 (27) 2980 (18)	**2973** 2953 (0.7) 2954 (8) 2666 (15) 2969 (23) 2971 (15) 2974 (11) 2977 (19) 2983 (3) 2983 (21)	**3009** 2980 (17) 3009 (47)	**N** 2973 (5)
$2\beta_{NH3}$	3222				**O** 3164 (7)
$2\beta_{NH3}$	3226				**P** 3185 (5)
ν_{NH3} [s]	**3210** (53)				**Q** 3238 (13)
ν_{NH3} [a]	**3301** 3289 (123)				**R** 3317 (21)

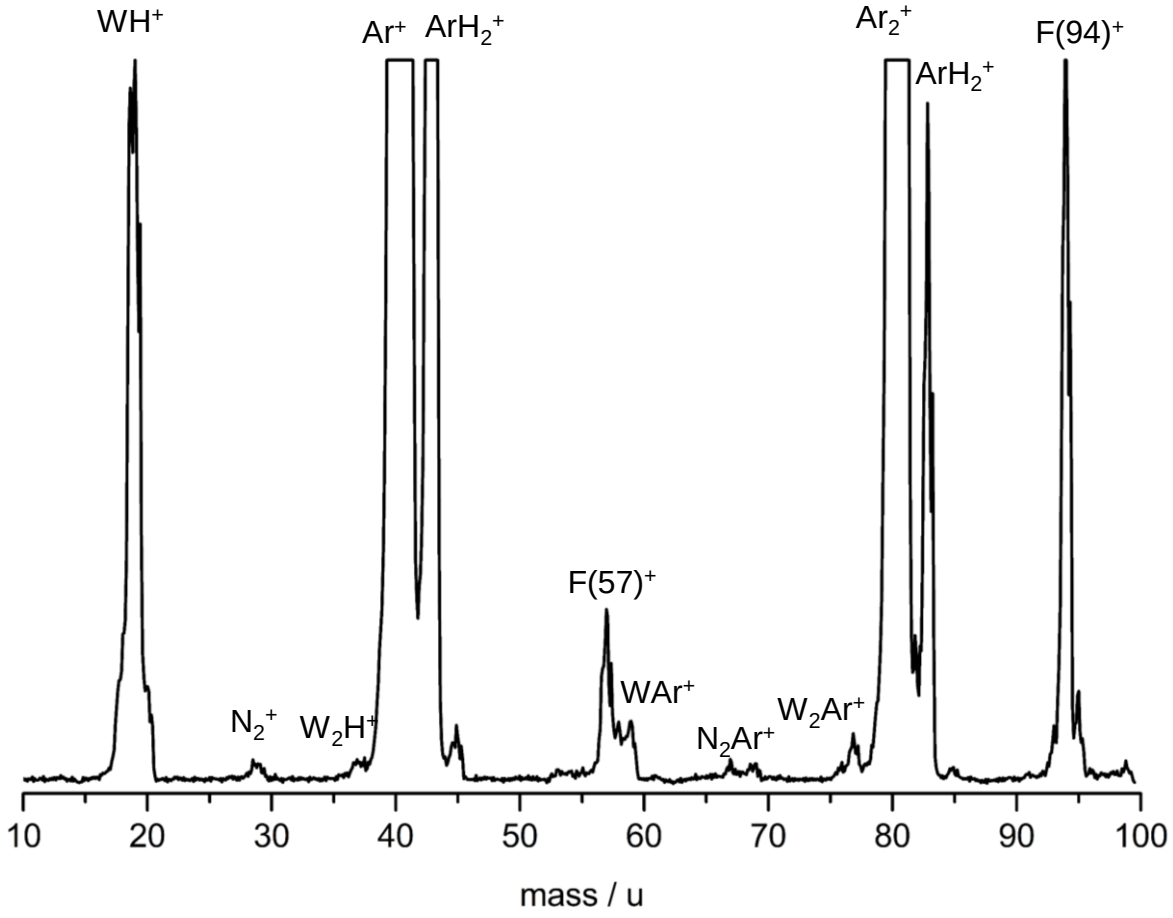
	3302 (50)				
$\nu_{NH2}{}^{s}$		**3333** (130)	**3324** (159)	**3328** (139)	**S** 3344 (7)
$2\beta_{NH2}{}^{c}$		3334	3342	3336	**T** 3428 (11)
$\nu_{NH2}{}^{a}$		**3437** (82)	**3428** (116)	**3432** (99)	**U** 3451 (10)

[a] IR intensities in km mol^{-1} are given in parentheses. [b] Stretching (ν), bending (β), torsion (τ), wagging (γ), rocking (ρ). [c] Coupled β_{NH2}/ν_{CN} modes.

Table S6. Various energies of the AmaH$^+$(**I-IV**)-Ar(**I-VI**) isomers (in kJ mol^{-1}) calculated at the B3LYP-D3/cc-pVTZ level.

	E_0	E_e	D_0	E_0^{total}
AmaH$^+$(**I**)-Ar(**I**)	0.00	0.00	10.15	0.00
AmaH$^+$(**I**)-Ar(**II**)	4.10	5.04	6.05	4.10
AmaH$^+$(**I**)-Ar(**III**)	4.17	4.86	5.98	4.17
AmaH$^+$(**I**)-Ar(**IV**)	4.94	5.30	5.21	4.94
AmaH$^+$(**I**)-Ar(**V**)	5.04	5.10	5.11	5.04
AmaH$^+$(**II**)-Ar(**I**)	0.00	0.00	9.76	3.42
AmaH$^+$(**II**)-Ar(**II**)	2.34	2.63	7.42	5.77
AmaH$^+$(**II**)-Ar(**III**)	2.99	3.48	6.77	6.41
AmaH$^+$(**II**)-Ar(**IV**)	3.38	4.06	6.38	6.81
AmaH$^+$(**II**)-Ar(**V**)	3.40	3.91	6.36	6.82
AmaH$^+$(**II**)-Ar(**VI**)	3.56	3.91	6.20	6.98
AmaH$^+$(**III**)-Ar(**I**)	0.00	0.00	8.98	28.57
AmaH$^+$(**III**)-Ar(**II**)	0.34	-0.06	8.65	28.90
AmaH$^+$(**III**)-Ar(**III**)	2.07	2.57	6.92	30.63
AmaH$^+$(**III**)-Ar(**IV**)	2.75	2.79	6.24	31.31
AmaH$^+$(**III**)-Ar(**V**)	4.39	4.28	4.58	32.96
AmaH$^+$(**III**)-Ar(**VI**)	6.86	7.06	2.13	35.42
AmaH$^+$(**IV**)-Ar(**I**)	0.00	0.00	8.94	30.72
AmaH$^+$(**IV**)-Ar(**II**)	0.24	0.51	8.70	30.96
AmaH$^+$(**IV**)-Ar(**III**)	0.98	1.59	7.96	31.70
AmaH$^+$(**IV**)-Ar(**IV**)	2.48	2.99	6.45	33.20
AmaH$^+$(**IV**)-Ar(**V**)	2.53	3.27	6.41	33.24
AmaH$^+$(**IV**)-Ar(**VI**)	2.96	3.14	5.98	33.68

Figure S1


WH+
Ar+
ArH2+
Ar2+
ArH2+
F(94)+
F(57)+
WAr+
N2+
W2H+
N2Ar+
W2Ar+
10
20
30
40
50
60
70
80
90
100
mass / u

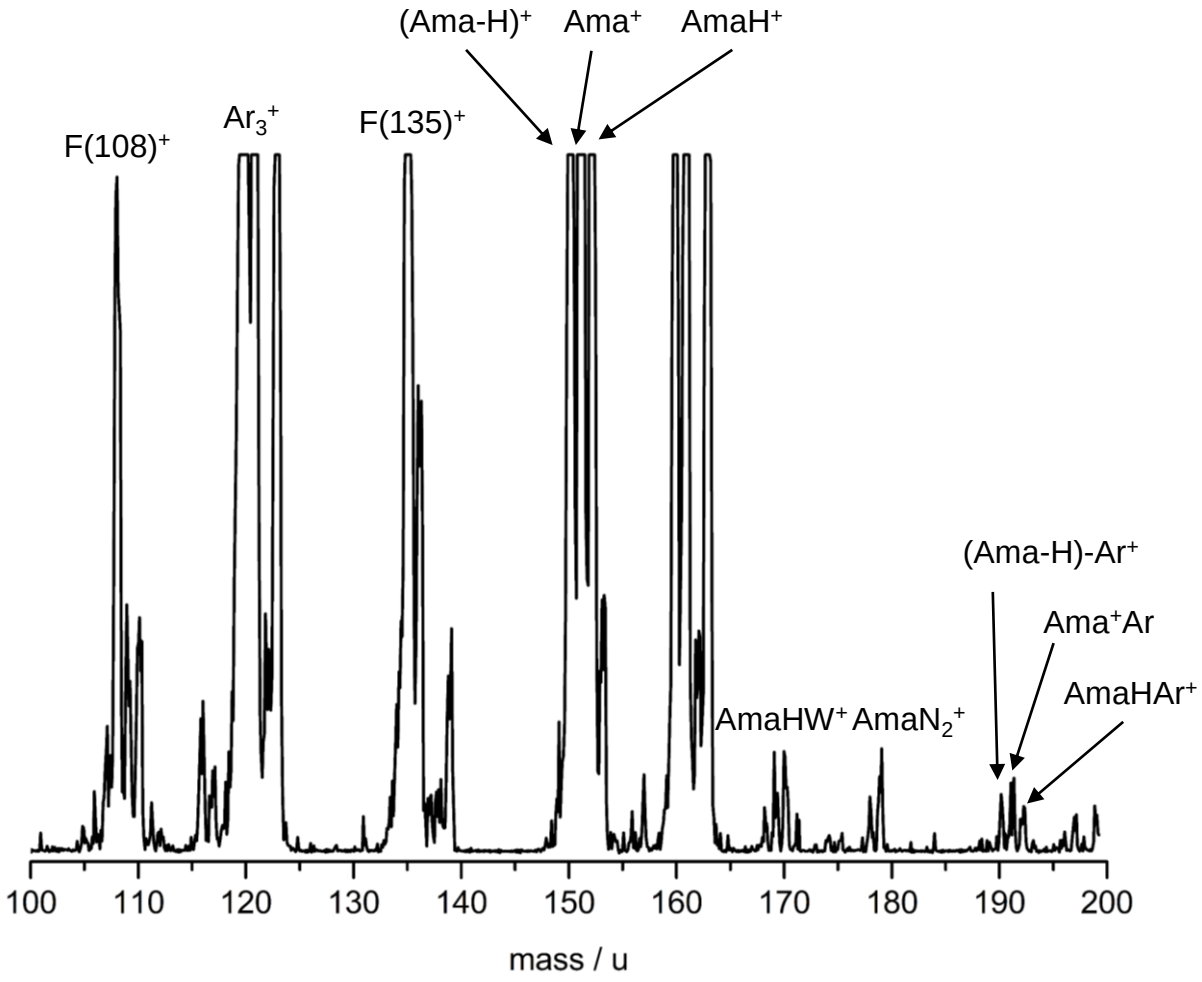

(Ama-H)+
Ama+
AmaH+
F(108)+
Ar3+
F(135)+
(Ama-H)-Ar+
Ama+Ar
AmaHAr+
AmaHW+
AmaN2+
100
110
120
130
140
150
160
170
180
190
200
mass / u

Figure S2

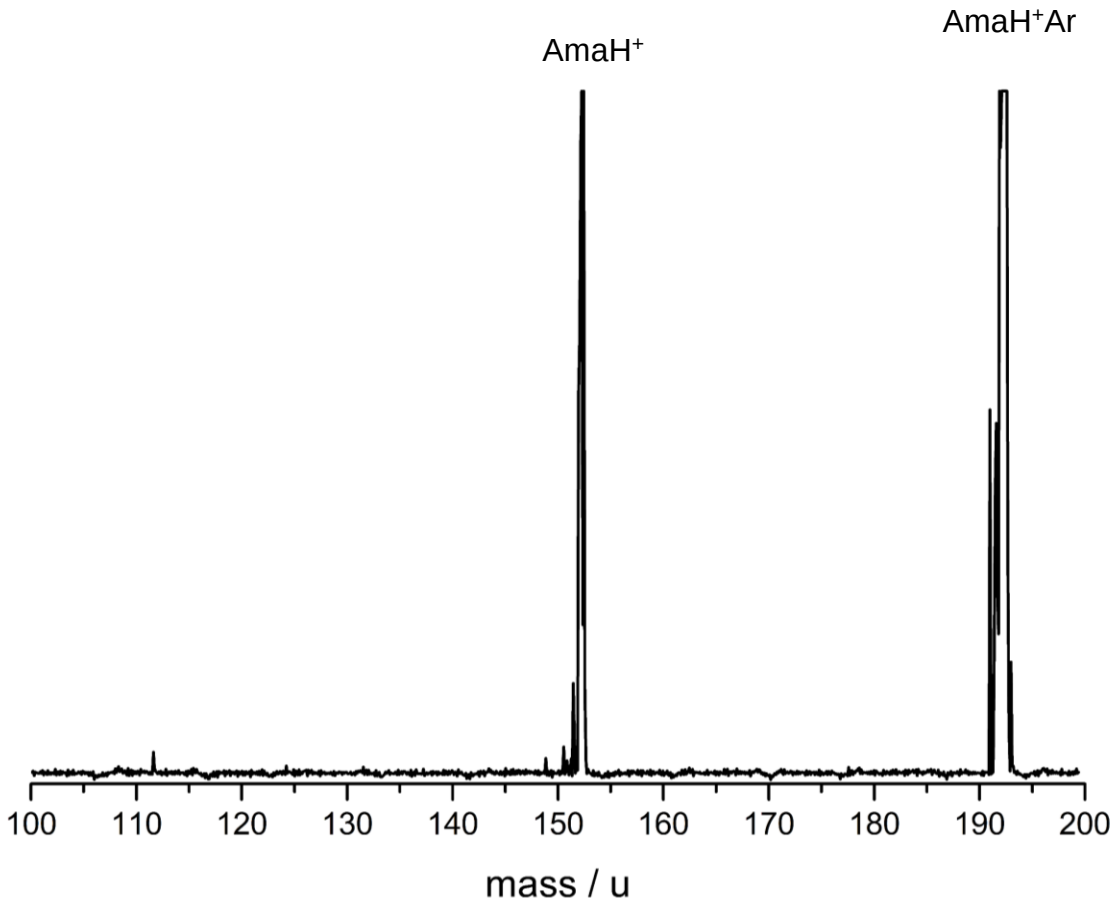
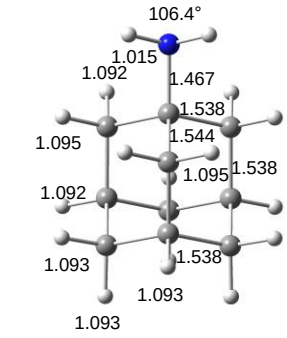
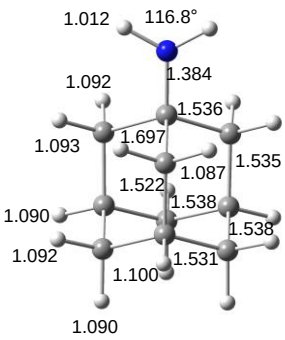


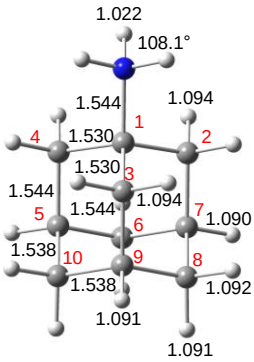
Figure S3



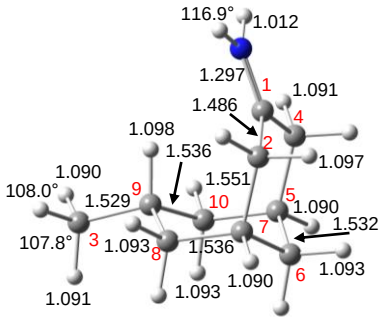
Ama (C_s)



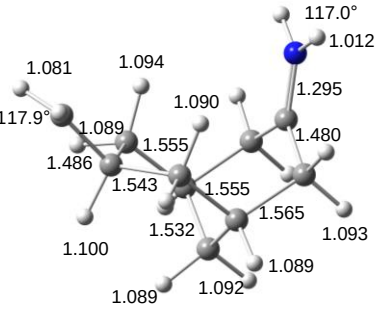
Ama$^+$(**I**) (C_s)



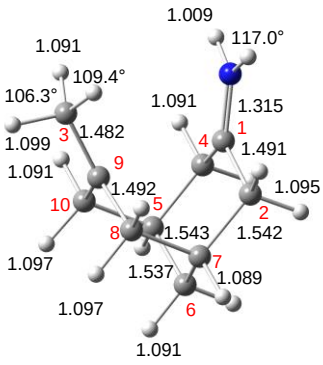
AmaH$^+$(**I**) (C_{3v})



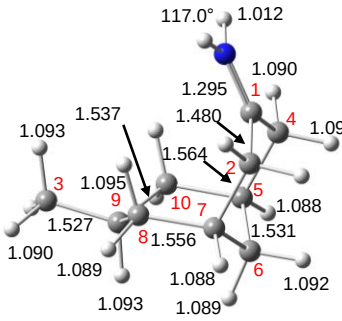
AmaH$^+$(**II**) (C_s)



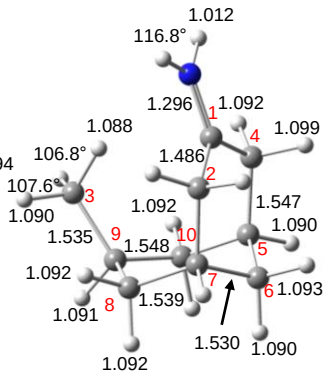
Ama$^+$(**II**) (C_s)



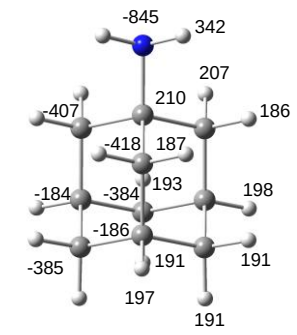
Ama$^+$(**III**) (C_s)



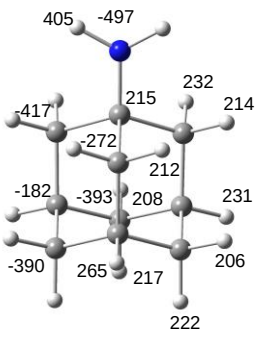
AmaH$^+$(**III**) (C_s)



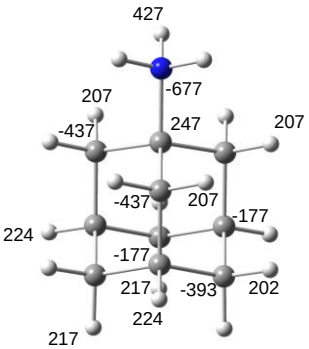
AmaH$^+$(**IV**) (C_s)



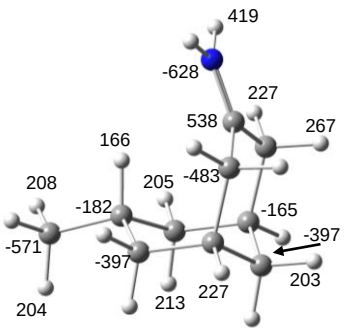
Ama (C_s)



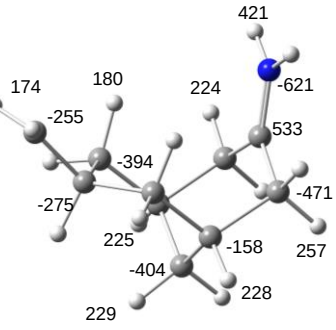
Ama$^+$(**I**) (C_s)



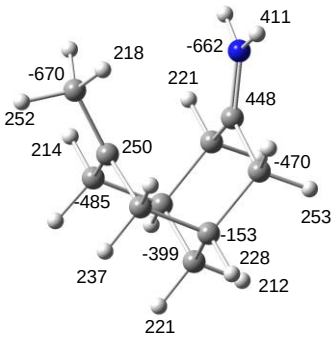
AmaH$^+$(**I**) (C_{3v})



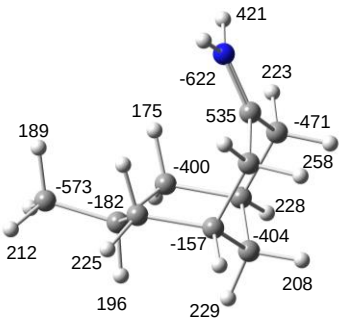
AmaH$^+$(**II**) (C_s)



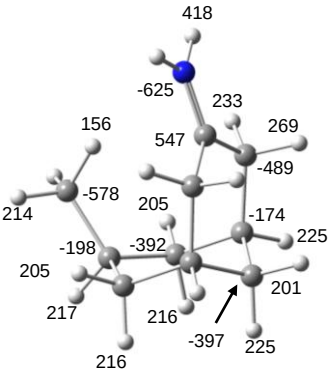
Ama$^+$(**II**) (C_s)



Ama$^+$(**III**) (C_s)



AmaH$^+$(**III**) (C_s)



AmaH$^+$(**IV**) (C_s)

Figure S4

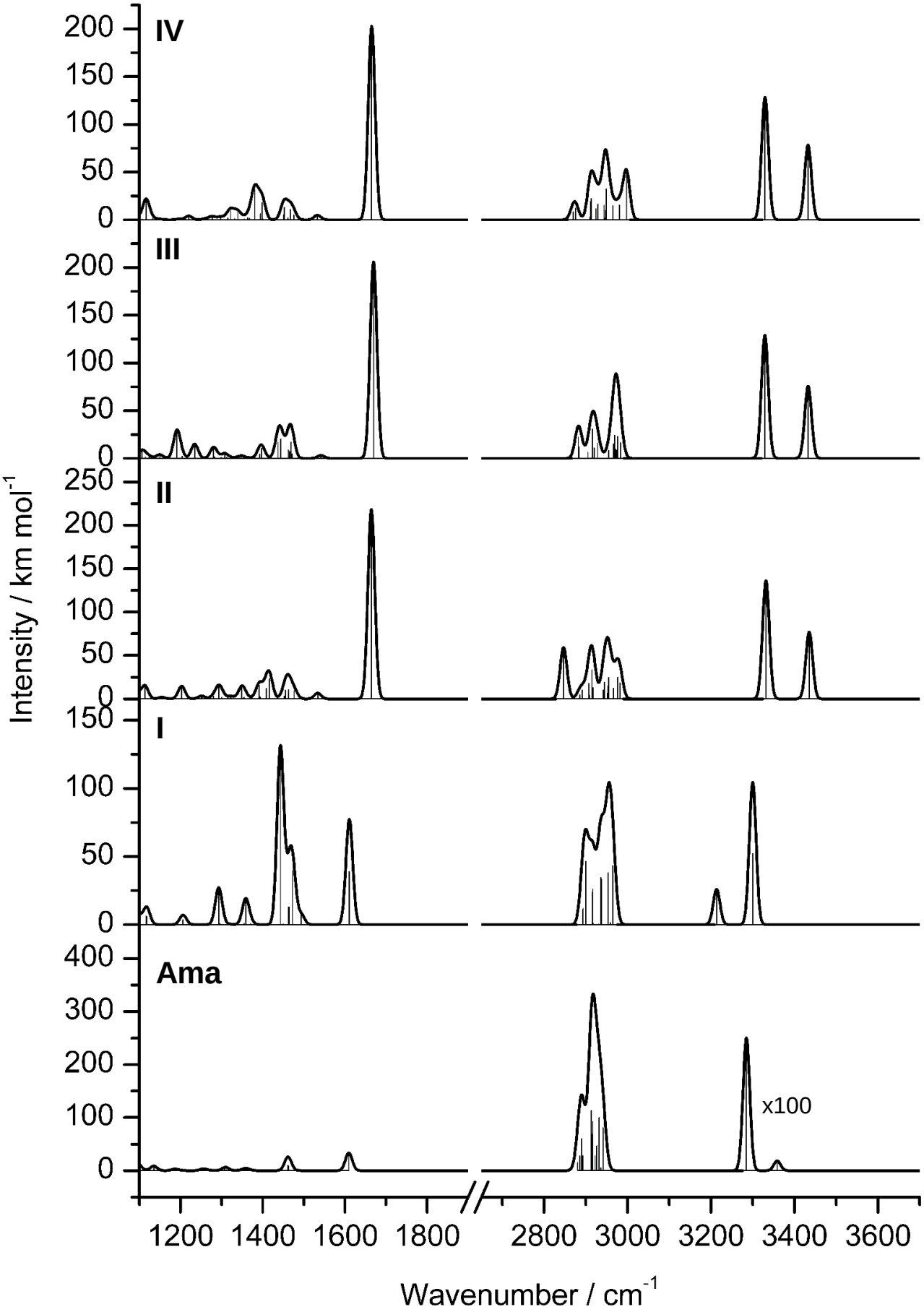
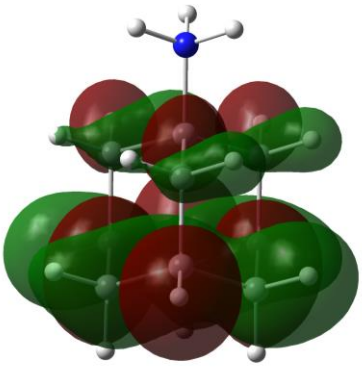
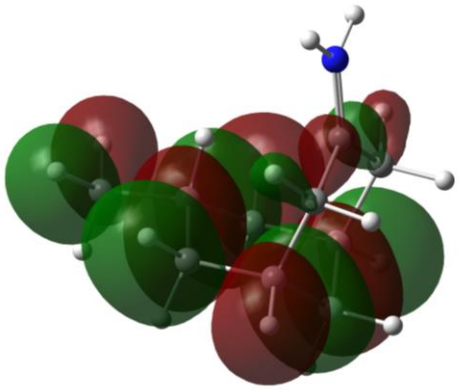

IV
III
II
I
Ama
x100
Intensity / km mol-1
Wavenumber / cm-1
1200 1400 1600 1800
2800 3000 3200 3400 3600

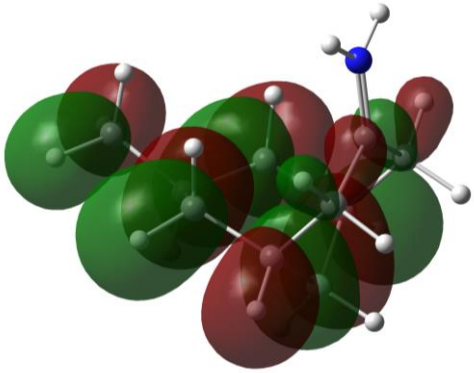
Figure S5



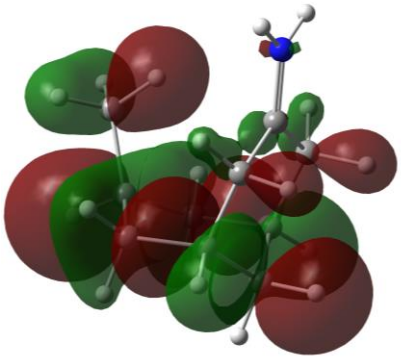
$AmaH^+$(**I**) (C_{3v})



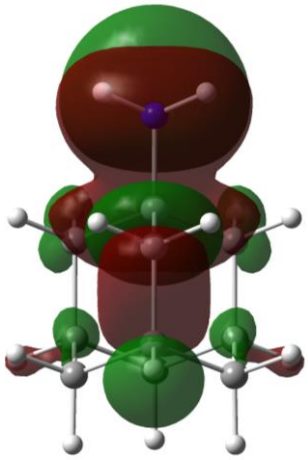
$AmaH^+$(**II**) (C_s)



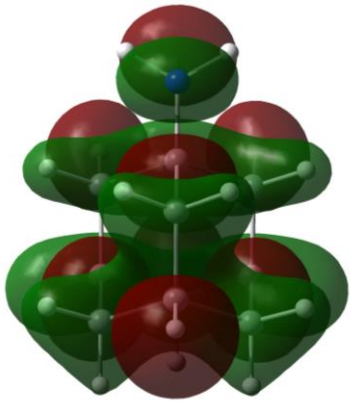
$AmaH^+$(**III**) (C_s)



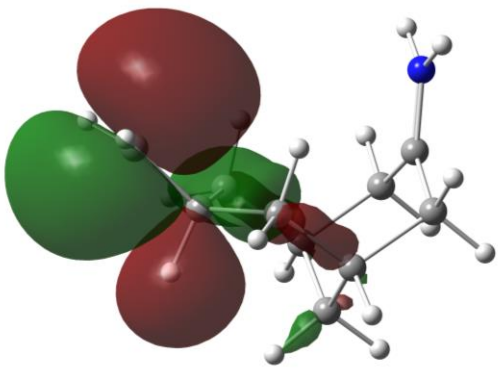
$AmaH^+$(**IV**) (C_s)



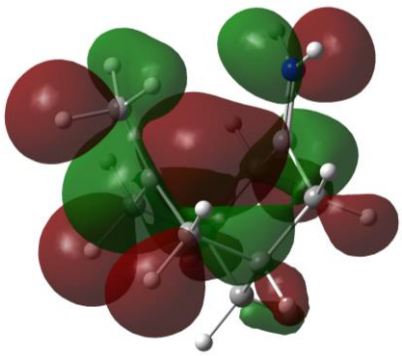
Ama (C_s)



Ama^+(**I**) (C_s)

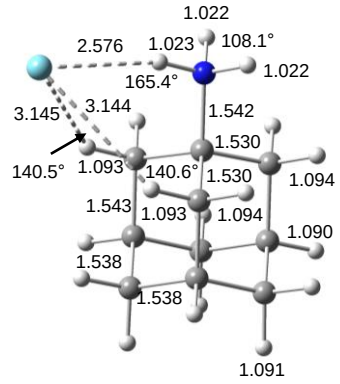


Ama^+(**II**) (C_s)

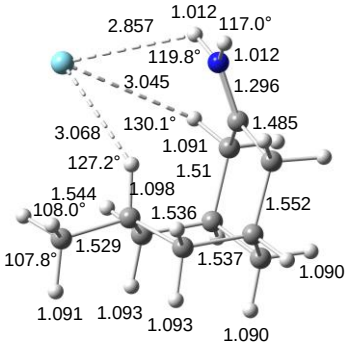


Ama^+(**III**) (C_s)

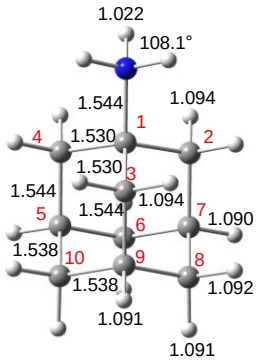
Figure S6



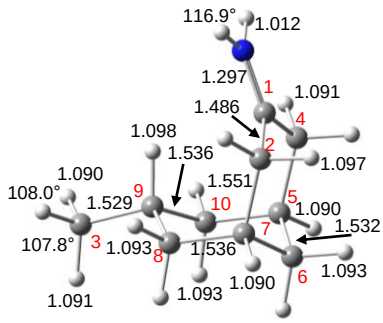
AmaH$^+$(**I**)-Ar(**I**)



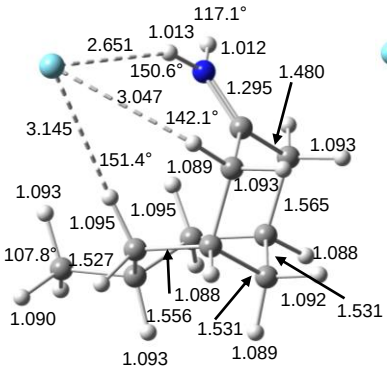
AmaH$^+$(**II**)-Ar(**I**)



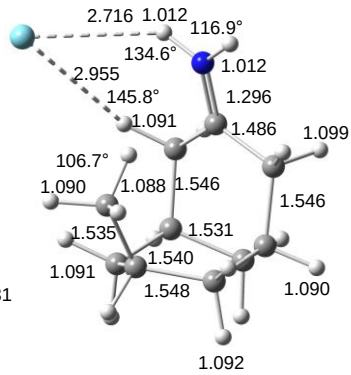
AmaH$^+$(**I**) (C_{3v})



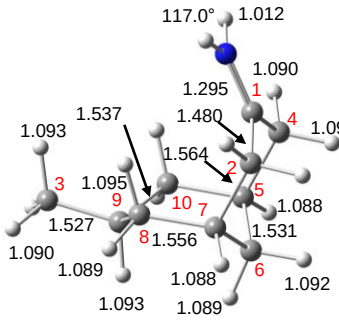
AmaH$^+$(**II**) (C_s)



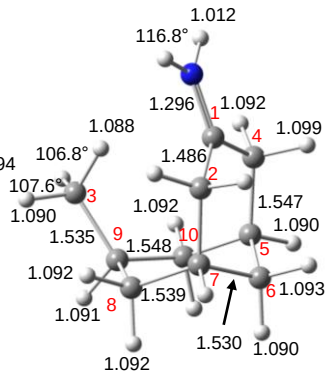
AmaH$^+$(**III**)-Ar(**I**)



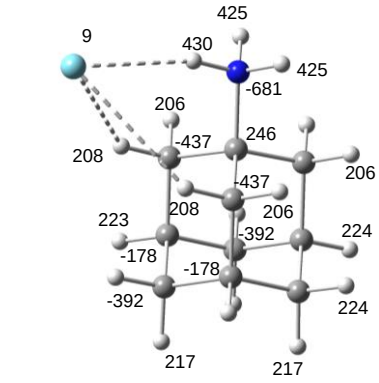
AmaH$^+$(**IV**)-Ar(**I**)



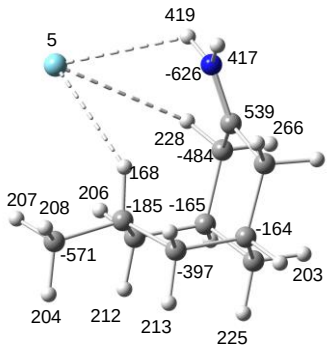
AmaH$^+$(**III**) (C_s)



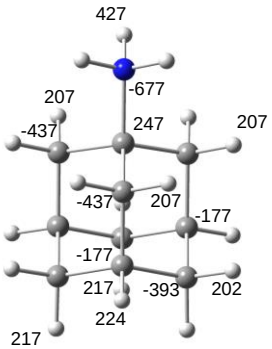
AmaH$^+$(**IV**) (C_s)



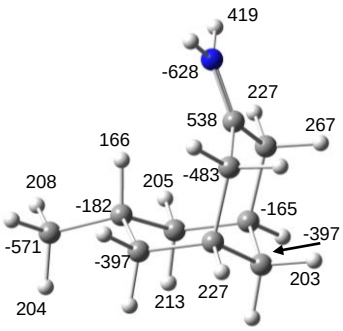
AmaH$^+$(**I**)-Ar(**I**)



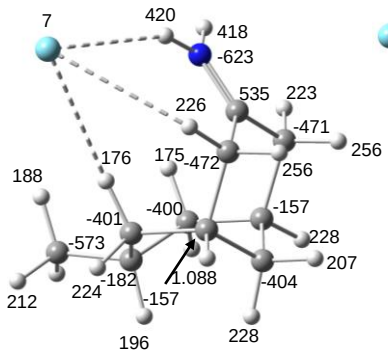
AmaH$^+$(**II**)-Ar(**I**)



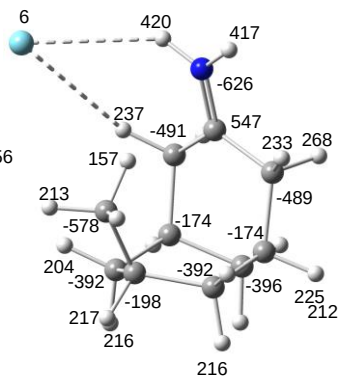
AmaH$^+$(**I**) (C_{3v})



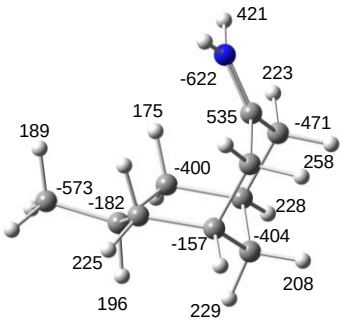
AmaH$^+$(**II**) (C_s)



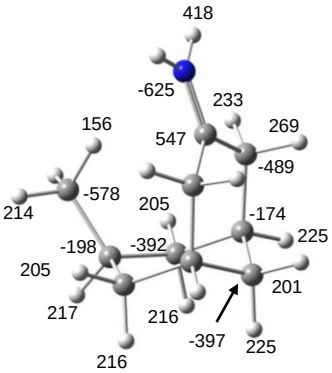
AmaH$^+$(**III**)-Ar(**I**)



AmaH$^+$(**IV**)-Ar(**I**)



AmaH$^+$(**III**) (C_s)



AmaH$^+$(**IV**) (C_s)

Figure S7

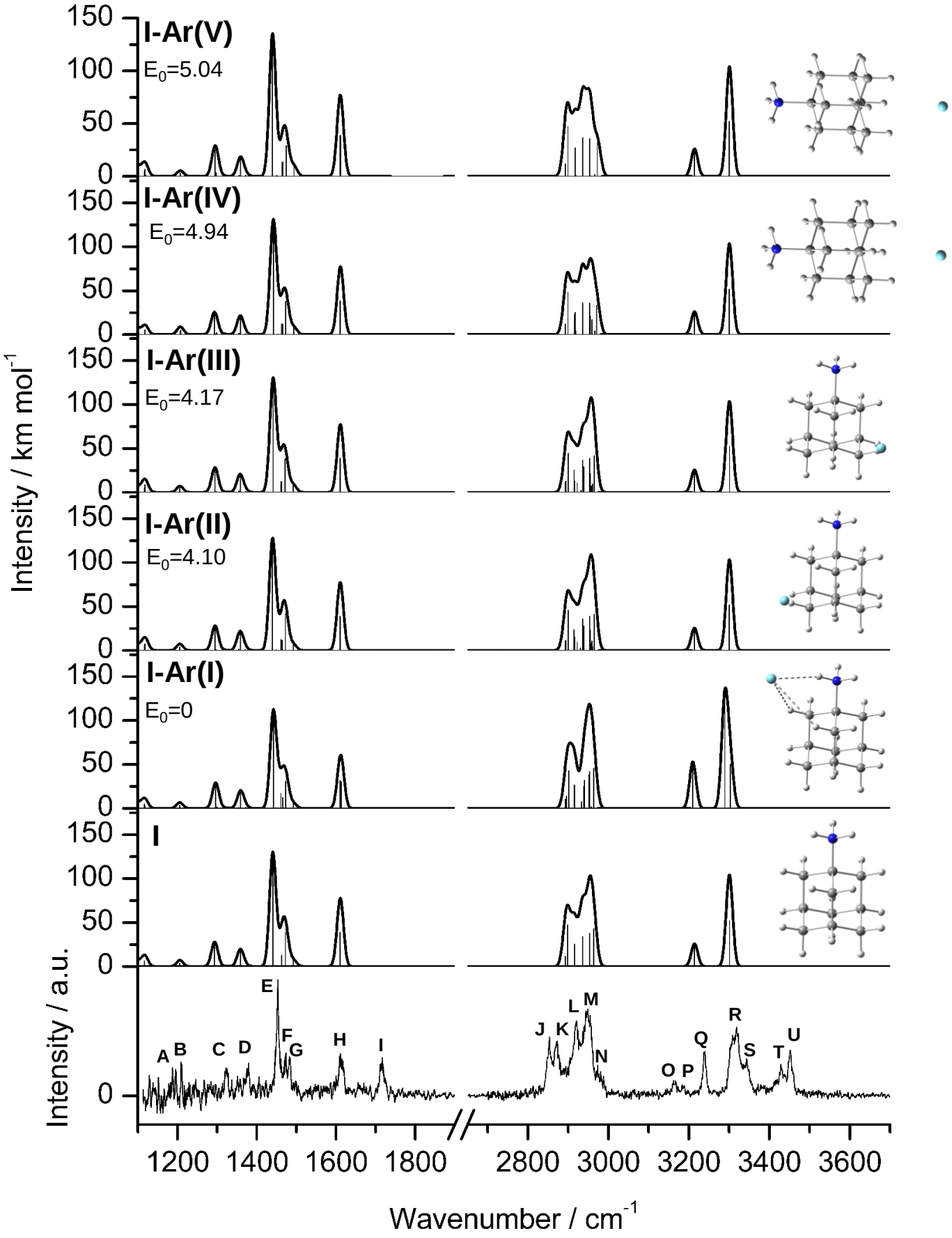

I-Ar(V)
E0=5.04
I-Ar(IV)
E0=4.94
I-Ar(III)
E0=4.17
I-Ar(II)
E0=4.10
I-Ar(I)
E0=0
I
Intensity / km mol-1
Intensity / a.u.
A B C D E F G H I
J K L M N O P Q R S T U
1200 1400 1600 1800 2800 3000 3200 3400 3600
Wavenumber / cm-1

Figure S8

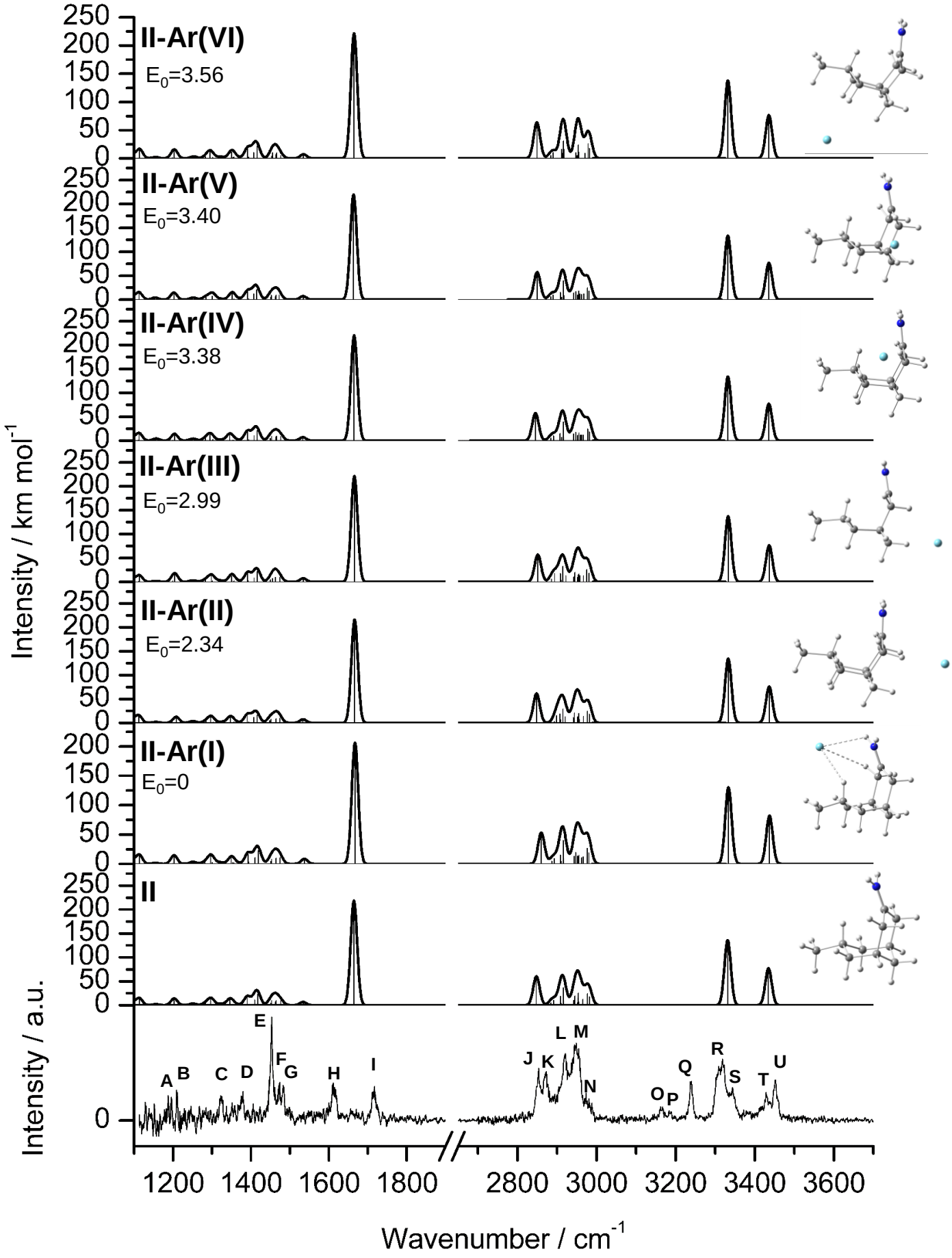

II-Ar(VI)
E0=3.56
II-Ar(V)
E0=3.40
II-Ar(IV)
E0=3.38
II-Ar(III)
E0=2.99
II-Ar(II)
E0=2.34
II-Ar(I)
E0=0
II
Intensity / km mol-1
Intensity / a.u.
A B C D E F G H I
J K L M N O P Q R S T U
1200 1400 1600 1800 2800 3000 3200 3400 3600
Wavenumber / cm-1

Figure S9

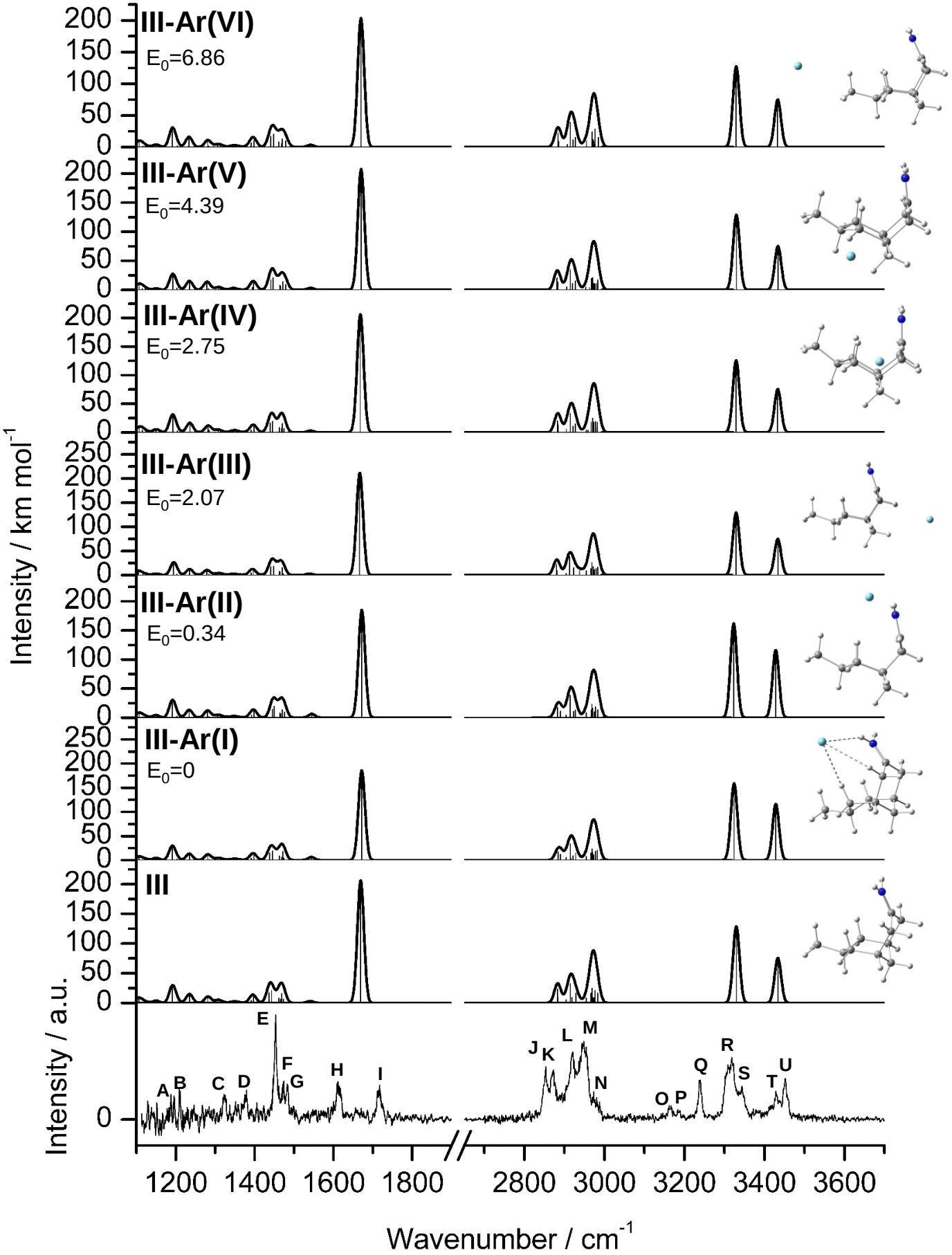
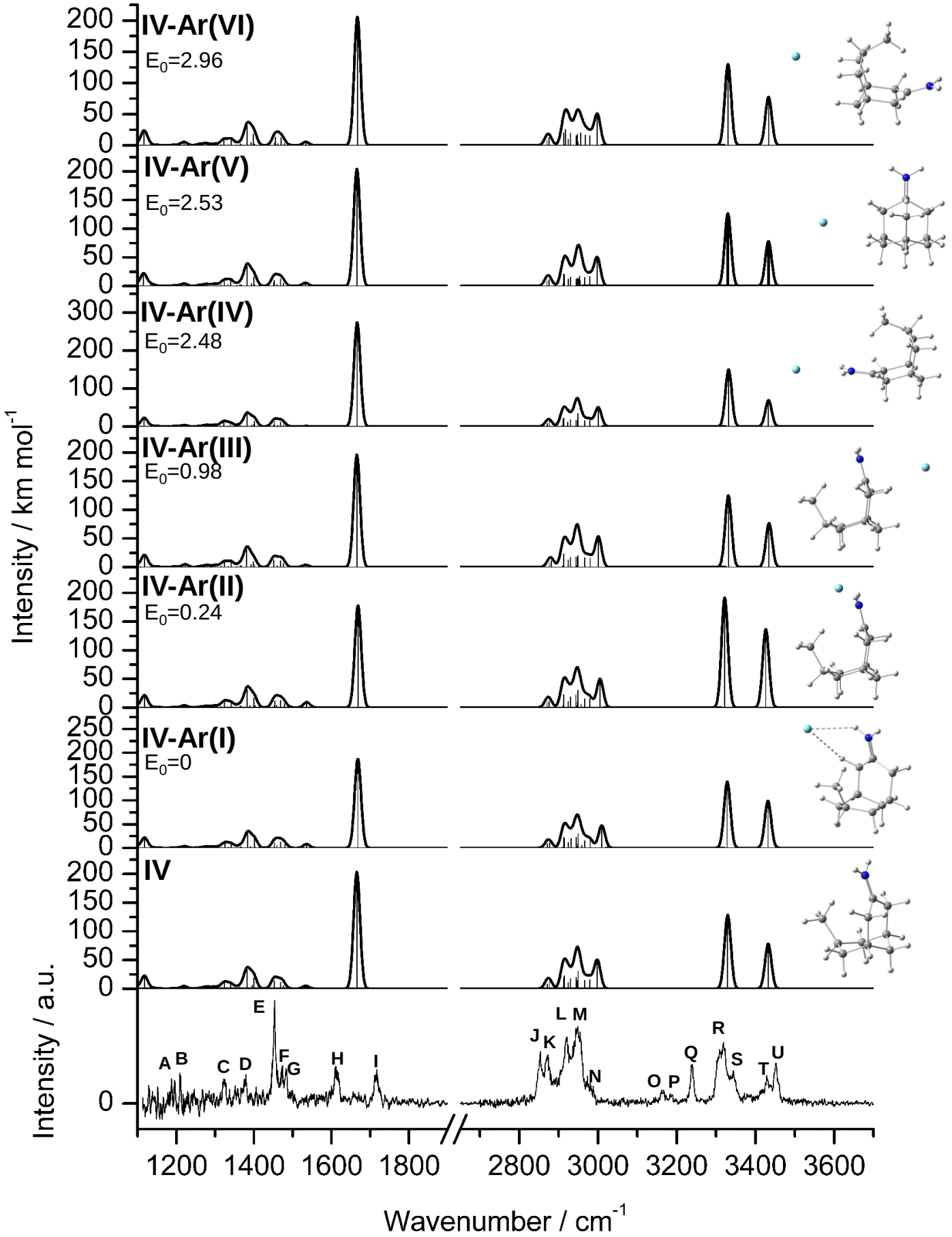

III-Ar(VI)
E0=6.86
III-Ar(V)
E0=4.39
III-Ar(IV)
E0=2.75
III-Ar(III)
E0=2.07
III-Ar(II)
E0=0.34
III-Ar(I)
E0=0
III
Intensity / km mol-1
Intensity / a.u.
A
B
C
D
E
F
G
H
I
J
K
L
M
N
O
P
Q
R
S
T
U
1200
1400
1600
1800
2800
3000
3200
3400
3600
Wavenumber / cm-1

Figure S10


IV-Ar(VI)
E0=2.96
IV-Ar(V)
E0=2.53
IV-Ar(IV)
E0=2.48
IV-Ar(III)
E0=0.98
IV-Ar(II)
E0=0.24
IV-Ar(I)
E0=0
IV
Intensity / km mol-1
Intensity / a.u.
A B C D E F G H I
J K L M N O P Q R S T U
1200 1400 1600 1800 2800 3000 3200 3400 3600
Wavenumber / cm-1

Cartesian coordiantes (Å) and energies (hartree) of relevant structures (B3LYP-D3/cc-pVTZ)

Ar

Sum of electronic and zero-point Energies= -527.559372
Sum of electronic and thermal Energies= -527.557955
Sum of electronic and thermal Enthalpies= -527.557011
Sum of electronic and thermal Free Energies= -527.574583

Ama

1	6	0	-1.011128	1.127081	1.255703
2	1	0	-0.514261	1.502017	2.154656
3	1	0	-2.038105	1.501352	1.276200
4	6	0	-1.011128	-0.410783	1.256075
5	1	0	-1.521728	-0.777686	2.149414
6	6	0	-0.287239	1.641427	0.000000
7	1	0	-0.281288	2.733996	0.000000
8	6	0	1.158945	1.116612	0.000000
9	1	0	1.696050	1.483603	0.880296
10	1	0	1.696050	1.483603	-0.880296
11	6	0	0.437377	-0.927013	1.249983
12	1	0	0.460778	-2.018647	1.262920
13	1	0	0.962767	-0.582715	2.146909
14	6	0	1.182128	-0.427579	0.000000
15	6	0	0.437377	-0.927013	-1.249983
16	1	0	0.962767	-0.582715	-2.146909
17	1	0	0.460778	-2.018647	-1.262920
18	6	0	-1.736812	-0.921403	0.000000
19	1	0	-2.774040	-0.575535	0.000000
20	1	0	-1.762177	-2.014271	0.000000
21	6	0	-1.011128	1.127081	-1.255703
22	1	0	-2.038105	1.501352	-1.276200
23	1	0	-0.514261	1.502017	-2.154656
24	6	0	-1.011128	-0.410783	-1.256075
25	1	0	-1.521728	-0.777686	-2.149414
26	7	0	2.535235	-0.993222	0.000000
27	1	0	3.048130	-0.666622	-0.812633
28	1	0	3.048130	-0.666622	0.812633

Sum of electronic and zero-point Energies= -445.999992
Sum of electronic and thermal Energies= -445.991746
Sum of electronic and thermal Enthalpies= -445.990802
Sum of electronic and thermal Free Energies= -446.032017

AmaH$^+$(I)

1	7	0	0.000000	0.000000	2.705063
2	1	0	0.000000	-0.955384	3.067886
3	1	0	-0.827387	0.477692	3.067886
4	1	0	0.827387	0.477692	3.067886
5	6	0	0.000000	0.000000	1.161528
6	6	0	0.000000	1.454567	0.688278
7	1	0	-0.884328	1.977269	1.063861
8	1	0	0.884328	1.977269	1.063861
9	6	0	-1.259692	-0.727284	0.688278
10	1	0	-1.270201	-1.754485	1.063861
11	1	0	-2.154529	-0.222784	1.063861
12	6	0	1.259692	-0.727284	0.688278
13	1	0	2.154529	-0.222784	1.063861
14	1	0	1.270201	-1.754485	1.063861
15	6	0	0.000000	1.452026	-0.855237
16	1	0	0.000000	2.485024	-1.201872
17	6	0	-1.257491	-0.726013	-0.855237
18	1	0	-2.152094	-1.242512	-1.201872
19	6	0	1.257491	-0.726013	-0.855237
20	1	0	2.152094	-1.242512	-1.201872
21	6	0	-1.258890	0.726821	-1.359309
22	6	0	1.258890	0.726821	-1.359309
23	6	0	-0.000000	-1.453641	-1.359309
24	1	0	-2.158547	1.246238	-1.021366
25	1	0	-1.278091	0.737906	-2.449633
26	1	0	2.158547	1.246238	-1.021366
27	1	0	1.278091	0.737906	-2.449633
28	1	0	-0.000000	-2.492475	-1.021366
29	1	0	-0.000000	-1.475813	-2.449633

Sum of electronic and zero-point Energies= -446.364241
Sum of electronic and thermal Energies= -446.355795

Sum of electronic and thermal Enthalpies= -446.354850
Sum of electronic and thermal Free Energies= -446.395459

AmaH$^+$(II)

1	6	0	-1.032218	-0.080276	1.248536
2	6	0	-1.920024	-0.103457	0.000000
3	6	0	-1.032218	-0.080276	-1.248536
4	6	0	-0.174398	1.193527	-1.268059
5	6	0	0.671935	1.384485	0.000000
6	6	0	-0.174398	1.193527	1.268059
7	6	0	-0.174398	-1.372459	1.283463
8	6	0	1.378998	2.740017	0.000000
9	6	0	0.523455	-1.643946	0.000000
10	6	0	-0.174398	-1.372459	-1.283463
11	7	0	1.710185	-2.166783	0.000000
12	1	0	-1.651876	-0.102280	2.144793
13	1	0	-2.569775	-0.981990	0.000000
14	1	0	-2.571968	0.770259	0.000000
15	1	0	-1.651876	-0.102280	-2.144793
16	1	0	0.471257	1.202982	-2.149429
17	1	0	-0.848000	2.047625	-1.374939
18	1	0	0.648746	3.551113	0.000000
19	1	0	0.471257	1.202982	2.149429
20	1	0	-0.848000	2.047625	1.374939
21	1	0	0.529042	-1.376449	2.117771
22	1	0	-0.851518	-2.223682	1.429220
23	1	0	2.008692	2.857719	-0.882285
24	1	0	2.008692	2.857719	0.882285
25	1	0	0.529042	-1.376449	-2.117771
26	1	0	-0.851518	-2.223682	-1.429220
27	1	0	2.195815	-2.378022	0.862392
28	1	0	2.195815	-2.378022	-0.862392
29	1	0	1.460851	0.620205	0.000000

Sum of electronic and zero-point Energies= -446.363086
Sum of electronic and thermal Energies= -446.353254
Sum of electronic and thermal Enthalpies= -446.352309
Sum of electronic and thermal Free Energies= -446.397259

AmaH$^+$(III)

1	6	0	0.906969	-0.296697	1.246490
2	6	0	1.667525	-0.757854	0.000000
3	6	0	0.906969	-0.296697	-1.246490
4	6	0	-0.539532	-0.868885	-1.270651
5	6	0	-0.913395	-1.649556	0.000000
6	6	0	-0.539532	-0.868885	1.270651
7	6	0	0.906969	1.267387	1.271436
8	6	0	-2.392481	-2.030142	0.000000
9	6	0	0.344785	1.775760	0.000000
10	6	0	0.906969	1.267387	-1.271436
11	7	0	-0.681722	2.565511	0.000000
12	1	0	1.442834	-0.603444	2.142869
13	1	0	2.684396	-0.359833	0.000000
14	1	0	1.764590	-1.842406	0.000000
15	1	0	1.442834	-0.603444	-2.142869
16	1	0	-1.265617	-0.060210	-1.407496
17	1	0	-0.662583	-1.517986	-2.136895
18	1	0	-0.335073	-2.576938	0.000000
19	1	0	-1.265617	-0.060210	1.407496
20	1	0	-0.662583	-1.517986	2.136895
21	1	0	0.363962	1.650985	2.135132
22	1	0	1.942799	1.612172	1.337199
23	1	0	-2.647755	-2.619608	-0.880911
24	1	0	-2.647755	-2.619608	0.880911
25	1	0	0.363962	1.650985	-2.135132
26	1	0	1.942799	1.612172	-1.337199
27	1	0	-1.097319	2.892752	0.863023
28	1	0	-1.097319	2.892752	-0.863023
29	1	0	-3.025964	-1.139628	0.000000

Sum of electronic and zero-point Energies= -446.353807
Sum of electronic and thermal Energies= -446.343818
Sum of electronic and thermal Enthalpies= -446.342874
Sum of electronic and thermal Free Energies= -446.388567

AmaH$^+$(IV)

1	6	0	-0.573444	-1.316962	1.284082
2	1	0	-1.137686	-0.941170	2.140379
3	1	0	-0.401991	-2.376871	1.482034
4	6	0	0.821153	-0.667853	1.243741
5	1	0	1.355380	-0.986435	2.139060
6	6	0	-1.428799	-1.193903	0.000000
7	1	0	-2.092472	-2.060100	0.000000
8	6	0	-2.371882	0.017165	0.000000
9	1	0	-3.015790	-0.001197	0.879919
10	1	0	-1.865043	0.980393	0.000000
11	6	0	0.821153	0.878044	1.290438
12	1	0	1.846003	1.204899	1.515446
13	1	0	0.189284	1.270896	2.089518
14	6	0	0.497875	1.540261	0.000000
15	6	0	0.821153	0.878044	-1.290438
16	1	0	0.189284	1.270896	-2.089518
17	1	0	1.846003	1.204899	-1.515446
18	6	0	1.584049	-1.129779	0.000000
19	1	0	1.662105	-2.216994	0.000000
20	1	0	2.605267	-0.739745	0.000000
21	6	0	-0.573444	-1.316962	-1.284082
22	1	0	-0.401991	-2.376871	-1.482034
23	1	0	-1.137686	-0.941170	-2.140379
24	6	0	0.821153	-0.667853	-1.243741
25	1	0	1.355380	-0.986435	-2.139060
26	7	0	-0.007701	2.733743	0.000000
27	1	0	-0.220072	3.219394	-0.862291
28	1	0	-0.220072	3.219394	0.862291
29	1	0	-3.015790	-0.001197	-0.879919

Sum of electronic and zero-point Energies= -446.353004
Sum of electronic and thermal Energies= -446.342963
Sum of electronic and thermal Enthalpies= -446.342018
Sum of electronic and thermal Free Energies= -446.387553

Ama$^+$(I)

1	6	0	-1.009933	1.119927	1.260815
2	1	0	-0.519111	1.502470	2.157785
3	1	0	-2.034331	1.491912	1.270028
4	6	0	-1.009933	-0.418569	1.258258
5	1	0	-1.512657	-0.782974	2.154281
6	6	0	-0.292961	1.610622	0.000000
7	1	0	-0.245778	2.709641	0.000000
8	6	0	1.169160	1.189049	0.000000
9	1	0	1.708022	1.497285	0.892533
10	1	0	1.708022	1.497285	-0.892533
11	6	0	0.436294	-0.931980	1.280099
12	1	0	0.450942	-2.023690	1.314481
13	1	0	0.966411	-0.567549	2.163360
14	6	0	1.172297	-0.507942	0.000000
15	6	0	0.436294	-0.931980	-1.280099
16	1	0	0.966411	-0.567549	-2.163360
17	1	0	0.450942	-2.023690	-1.314481
18	6	0	-1.725250	-0.938846	0.000000
19	1	0	-2.762343	-0.601654	0.000000
20	1	0	-1.747492	-2.030538	0.000000
21	6	0	-1.009933	1.119927	-1.260815
22	1	0	-2.034331	1.491912	-1.270028
23	1	0	-0.519111	1.502470	-2.157785
24	6	0	-1.009933	-0.418569	-1.258258
25	1	0	-1.512657	-0.782974	-2.154281
26	7	0	2.515855	-0.841720	0.000000
27	1	0	3.044730	-0.885075	-0.862169
28	1	0	3.044730	-0.885075	0.862169

Sum of electronic and zero-point Energies= -445.710234
Sum of electronic and thermal Energies= -445.701526
Sum of electronic and thermal Enthalpies= -445.700582
Sum of electronic and thermal Free Energies= -445.743151

Ama^{+}(II)

1	6	0	0.878102	-0.318597	1.247668
2	6	0	1.635327	-0.783226	0.000000
3	6	0	0.878102	-0.318597	-1.247668
4	6	0	-0.568901	-0.886083	-1.279077
5	6	0	-0.955442	-1.657448	0.000000
6	6	0	-0.568901	-0.886083	1.279077
7	6	0	0.878102	1.245884	1.270499
8	6	0	-2.392771	-2.036083	0.000000
9	6	0	0.309242	1.748203	0.000000
10	6	0	0.878102	1.245884	-1.270499
11	7	0	-0.730363	2.520450	0.000000
12	1	0	1.416275	-0.624513	2.143007
13	1	0	2.653570	-0.389067	0.000000
14	1	0	1.727499	-1.868303	0.000000
15	1	0	1.416275	-0.624513	-2.143007
16	1	0	-1.294078	-0.080902	-1.429269
17	1	0	-0.686147	-1.547069	-2.136958
18	1	0	-0.364623	-2.585563	0.000000
19	1	0	-1.294078	-0.080902	1.429269
20	1	0	-0.686147	-1.547069	2.136958
21	1	0	0.337490	1.629612	2.135471
22	1	0	1.913834	1.590934	1.332043
23	1	0	-2.899004	-2.268577	-0.926112
24	1	0	-2.899004	-2.268577	0.926112
25	1	0	0.337490	1.629612	-2.135471
26	1	0	1.913834	1.590934	-1.332043
27	1	0	-1.153201	2.838847	0.862911
28	1	0	-1.153201	2.838847	-0.862911

Sum of electronic and zero-point Energies= -445.694426
Sum of electronic and thermal Energies= -445.684131
Sum of electronic and thermal Enthalpies= -445.683187
Sum of electronic and thermal Free Energies= -445.730175

Ama^{+}(III)

1	6	0	0.923219	-0.687401	1.262057
2	6	0	1.637589	-1.195743	0.000000
3	6	0	0.923219	-0.687401	-1.262057
4	6	0	-0.547317	-1.154933	-1.263904
5	6	0	-1.207910	-0.715660	0.000000
6	6	0	-0.547317	-1.154933	1.263904
7	6	0	0.923219	0.854630	1.276496
8	6	0	-2.594709	-0.193357	0.000000
9	6	0	0.358830	1.379799	0.000000
10	6	0	0.923219	0.854630	-1.276496
11	7	0	-0.415579	2.442147	0.000000
12	1	0	1.432506	-1.047956	2.154616
13	1	0	2.679262	-0.869158	0.000000
14	1	0	1.650442	-2.286200	0.000000
15	1	0	1.432506	-1.047956	-2.154616
16	1	0	-1.072493	-0.775868	-2.141394
17	1	0	-0.569959	-2.249855	-1.329234
18	1	0	-1.072493	-0.775868	2.141394
19	1	0	-0.569959	-2.249855	1.329234
20	1	0	0.380399	1.243863	2.139094
21	1	0	1.953469	1.219584	1.347374
22	1	0	0.380399	1.243863	-2.139094
23	1	0	1.953469	1.219584	-1.347374
24	1	0	-0.742050	2.856458	0.860499
25	1	0	-0.742050	2.856458	-0.860499
26	1	0	-2.812381	0.398211	-0.890584
27	1	0	-2.812381	0.398211	0.890584
28	1	0	-3.311898	-1.026340	0.000000

Sum of electronic and zero-point Energies= -445.727708
Sum of electronic and thermal Energies= -445.717586
Sum of electronic and thermal Enthalpies= -445.716642
Sum of electronic and thermal Free Energies= -445.762902

AmaH$^+$(I)-Ar(I)

1	6	0	-2.647295	0.362184	-1.289414
2	1	0	-2.655463	1.109472	-2.086291
3	1	0	-3.541061	-0.249047	-1.420106
4	6	0	-2.682966	1.046241	0.087306
5	1	0	-3.564609	1.681739	0.165642
6	6	0	-1.393736	-0.521170	-1.398032
7	1	0	-1.358289	-1.000844	-2.375801
8	6	0	-0.136391	0.358792	-1.239284
9	1	0	-0.105183	1.116008	-2.028138
10	1	0	0.765582	-0.252515	-1.325510
11	6	0	-1.427348	1.929262	0.247616
12	1	0	-1.442794	2.433084	1.218222
13	1	0	-1.406576	2.697574	-0.530493
14	6	0	-0.197537	1.026817	0.135660
15	6	0	-0.188604	-0.021373	1.250780
16	1	0	0.712961	-0.636004	1.187981
17	1	0	-0.195542	0.466316	2.229923
18	6	0	-2.698548	-0.017690	1.197951
19	1	0	-3.593361	-0.634104	1.104535
20	1	0	-2.742766	0.458463	2.180203
21	6	0	-1.407079	-1.586956	-0.288876
22	1	0	-2.281389	-2.228363	-0.404698
23	1	0	-0.527957	-2.230534	-0.368335
24	6	0	-1.445274	-0.900886	1.086850
25	1	0	-1.446645	-1.650337	1.877873
26	7	0	1.059263	1.905471	0.295294
27	1	0	1.907579	1.337440	0.232027
28	1	0	1.097636	2.618351	-0.435570
29	1	0	1.058797	2.378268	1.200955
30	18	0	3.611771	-0.576660	-0.030223

Sum of electronic and zero-point Energies= -973.927480
Sum of electronic and thermal Energies= -973.916548
Sum of electronic and thermal Enthalpies= -973.915604
Sum of electronic and thermal Free Energies= -973.965796

AmaH$^+$(II)-Ar(I)

1	6	0	-2.255515	0.101817	-0.504154
2	6	0	-2.311848	0.163062	1.026147
3	6	0	-0.885086	0.122000	1.583156
4	6	0	-0.188743	-1.181086	1.163576
5	6	0	-0.178381	-1.407516	-0.355328
6	6	0	-1.575128	-1.198566	-0.959448
7	6	0	-1.530646	1.368436	-1.032993
8	6	0	0.382927	-2.784868	-0.709920
9	6	0	-0.231057	1.613824	-0.356963
10	6	0	-0.115481	1.381753	1.105893
11	7	0	0.777935	2.074866	-1.027428
12	1	0	-3.264496	0.135243	-0.914637
13	1	0	-2.835056	1.061976	1.360861
14	1	0	-2.875519	-0.689653	1.404915
15	1	0	-0.909739	0.174553	2.671431
16	1	0	0.832743	-1.206941	1.548745
17	1	0	-0.716593	-2.010573	1.640960
18	1	0	-0.244278	-3.573448	-0.290693
19	1	0	-1.516590	-1.234567	-2.049886
20	1	0	-2.217090	-2.031494	-0.661305
21	1	0	-1.409329	1.349059	-2.117288
22	1	0	-2.153892	2.238873	-0.793081
23	1	0	1.390769	-2.914332	-0.314160
24	1	0	0.423867	-2.929399	-1.789920
25	1	0	0.930048	1.366105	1.415830
26	1	0	-0.578104	2.259538	1.574322
27	1	0	0.714959	2.254748	-2.021144
28	1	0	1.673310	2.241545	-0.586418
29	1	0	0.502004	-0.671995	-0.803623
30	18	0	3.341178	0.032420	0.119849

Sum of electronic and zero-point Energies= -973.926176
Sum of electronic and thermal Energies= -973.913831
Sum of electronic and thermal Enthalpies= -973.912887
Sum of electronic and thermal Free Energies= -973.966243

AmaH$^+$(III)-Ar(I)

1	6	0	-0.590637	-0.252460	1.537625
2	6	0	-2.038611	-0.636345	1.219681
3	6	0	-2.217208	-0.689673	-0.300410
4	6	0	-1.880903	0.679274	-0.957491
5	6	0	-1.329093	1.719770	0.031317
6	6	0	-0.222223	1.126796	0.919154
7	6	0	0.348115	-1.387374	1.009212
8	6	0	-0.841869	2.970132	-0.697682
9	6	0	0.084942	-1.600045	-0.431649
10	6	0	-1.311258	-1.835479	-0.862394
11	7	0	1.033762	-1.470188	-1.302886
12	1	0	-0.441347	-0.227724	2.615531
13	1	0	-2.289364	-1.598496	1.670836
14	1	0	-2.722842	0.092241	1.651768
15	1	0	-3.238038	-0.978039	-0.544446
16	1	0	-1.152110	0.545476	-1.764225
17	1	0	-2.771388	1.083672	-1.437492
18	1	0	-2.151201	2.019564	0.685979
19	1	0	0.694682	1.043835	0.326806
20	1	0	0.011583	1.833914	1.714357
21	1	0	1.395671	-1.156845	1.198085
22	1	0	0.099613	-2.314391	1.533059
23	1	0	-1.639410	3.415432	-1.292928
24	1	0	-0.490345	3.725022	0.006025
25	1	0	-1.392960	-1.909362	-1.946725
26	1	0	-1.641214	-2.782800	-0.427529
27	1	0	1.983282	-1.255904	-1.022529
28	1	0	0.858199	-1.574881	-2.294186
29	1	0	-0.015700	2.732351	-1.372364
30	18	0	3.758835	0.390592	0.056444

Sum of electronic and zero-point Energies= -973.916600
Sum of electronic and thermal Energies= -973.904127
Sum of electronic and thermal Enthalpies= -973.903182
Sum of electronic and thermal Free Energies= -973.957628

AmaH$^+$(IV)-Ar(I)

1	6	0	2.454299	-0.247942	1.398047
2	1	0	2.326827	0.068957	2.435535
3	1	0	3.439684	-0.715334	1.348217
4	6	0	2.526525	0.981163	0.474523
5	1	0	3.420379	1.542302	0.747822
6	6	0	1.392016	-1.316016	1.043313
7	1	0	1.778236	-2.259544	1.432696
8	6	0	0.050141	-1.121521	1.763054
9	1	0	0.198790	-1.077265	2.842384
10	1	0	-0.485398	-0.217915	1.479550
11	6	0	1.351743	1.974770	0.621639
12	1	0	1.639640	2.909818	0.121372
13	1	0	1.151336	2.231398	1.663759
14	6	0	0.097573	1.560466	-0.059436
15	6	0	0.142546	0.701425	-1.271130
16	1	0	-0.804374	0.174470	-1.398407
17	1	0	0.216195	1.412864	-2.105568
18	6	0	2.626476	0.537942	-0.987431
19	1	0	3.502537	-0.097148	-1.119248
20	1	0	2.756824	1.398341	-1.648871
21	6	0	1.255294	-1.513595	-0.484985
22	1	0	2.060252	-2.170910	-0.819664
23	1	0	0.326102	-2.042969	-0.707272
24	6	0	1.362319	-0.244762	-1.351164
25	1	0	1.417163	-0.564416	-2.391979
26	7	0	-1.041600	2.006554	0.367132
27	1	0	-1.912575	1.742326	-0.076282
28	1	0	-1.104049	2.609259	1.177713
29	1	0	-0.616584	-1.959000	1.555711
30	18	0	-3.394136	-0.532126	-0.164087

Sum of electronic and zero-point Energies= -973.915781
Sum of electronic and thermal Energies= -973.903230
Sum of electronic and thermal Enthalpies= -973.902285
Sum of electronic and thermal Free Energies= -973.956552