Supporting Information

DFT b3lyp D95V+(d,p)

Reactions:

A $RCOOH \rightarrow RCOO^- + H^+$

B $[RCOOHCs]^+ \rightarrow RCOOH + Cs+$

C $[RCOO^-Cs^+] \rightarrow RCOO^- + Cs^+$

D $[(RCOO^-Cs^+)Cs^+]^+ \rightarrow [RCOO^-Cs^+] + Cs^+$

1 au = 627.5095 kCal/mol = 2625.4997 kJ/mol
1 kCal/ol = 4.184 kJ/mol

	H (au)	G (au)		PA (kJ/mol) CsCA (kJ/mol)	GB (kJ/mol) CsCB (kJ/mol)	Structures
H^+	0.002360	-0.010650				
Cs^+	-19.999390	-20.018674				
Benzoic	-420.780895	-420.820977				
Benzoate	-420.242564	-420.282523	**A**	**1419.6**	**1385.7**	
Benzoic + Cs^+	-440.808640	-440.858181	**B**	**74.4**	**48.7**	On COO^-
Benzoate + Cs^+	-440.418087	-440.465992	**C**	**462.4**	**432.7**	
Benzoate + $2Cs^+$	-460.465140	-460.521848	**D**	**125.1**	**97.6**	In-out
	-460.464375	-460.519361	**D**	**123.1**	**91.1**	Propeller
	-460.461969	-460.519144	**D**	**116.8**	**90.5**	
3OH-benzoic	-496.019136	-496.062001				
3OH-benzoate	-495.484542	-495.527070	**A**	**1409.8**	**1376.5**	
3OH-benzoic + Cs^+	-516.048799	-516.101241	**B**	**79.5**	**54.0**	On COO^-
3OH-benzoate + Cs^+	-515.657803	-515.708324	**C**	**456.5**	**426.9**	
3OH-benzoate + $2Cs^+$	-535.705918	-535.765080	**D**	**127.9**	**100.0**	In-out
	-535.703688	-535.766091	**D**	**122.1**	**102.6**	Propeller
4OH-benzoic	-496.021836	-496.064498				
4OH-benzoate	-495.481822	-495.524582	**A**	**1424.0**	**1389.6**	
4OH-benzoic + Cs^+	-516.051827	-516.103961	**B**	**80.3**	**54.6**	On COO^-
			B			On
	-516.035160	-516.087781		**36.6**	**12.1**	Substituent
4OH-benzoate + Cs^+	-515.657851	-515.708472	**C**	**463.8**	**433.8**	
4OH-benzoate + $2Cs^+$	-535.705708	-535.764763		**127.3**	**98.8**	In-out
	-535.703347	-535.765045		**121.1**	**99.5**	Propeller
3COOH-benzoic	-609.386918	-609.434107				
3COOH-benzoate	-608.857808	-608.904917	**A**	**1395.4**	**1361.4**	
3COOH-benzoic + Cs^+	-629.417062	-629.473396	**B**	**80.7**	**54.1**	On COO^-
3COOH-benzoate + Cs^+	-629.027271	-629.082291	**C**	**446.5**	**416.7**	
3COOH-benzoate + $2Cs^+$	-649.077481	-649.140595	**D**	**133.4**	**104.0**	In-out
	-649.074486	-649.140075	**D**	**125.6**	**102.7**	Propeller
			D			On
	-649.067821	-649.132519		**108.1**	**82.8**	Substituent
4COOH-benzoic	-609.386319	-609.433621				
4COOH-benzoate	-608.858989	-608.906307	**A**	**1390.7**	**1356.5**	
4COOH-benzoic + Cs^+	-629.410787	-629.467596	**B**	**65.8**	**40.2**	On COO^-
4COOH-benzoate + Cs^+	-629.027097	-629.082398	**C**	**443.0**	**413.3**	
4COOH-benzoate + $2Cs^+$	-649.069685	-649.133805	**D**	**113.4**	**85.9**	In-out
	-649.068884	-649.134361	**D**	**111.3**	**87.4**	Propeller

			D			On
	-649.066482	-649.131193		**105.0**	**79.1**	Substituent
3CH3-benzoic	-460.076782	-460.121515				
3CH3-benzoate	-459.537081	-459.582256	**A**	**1423.2**	**1387.9**	
3CH3-benzoic + Cs^+	-480.105801	-480.160202	**B**	**77.8**	**52.5**	On COO^-
3CH3-benzoate + Cs^+	-479.713151	-479.766785	**C**	**463.9**	**435.5**	
3CH3-benzoate + $2Cs^+$	-499.761748	-499.822864	**D**	**129.2**	**98.2**	In-out
	-499.761278	-499.822661	**D**	**128.0**	**97.7**	In-out
	-499.759015	-499.823299	**D**	**122.0**	**99.3**	Propeller
4CH3-benzoic	-460.077351	-460.122302				
4CH3-benzoate	-459.536887	-459.582722	**A**	**1425.2**	**1388.7**	
4CH3-benzoic + Cs^+	-480.107084	-480.162028	**B**	**79.7**	**55.3**	On COO^-
4CH3-benzoate + Cs^+	-479.713360	-479.766513	**C**	**464.9**	**433.5**	
4CH3-benzoate + $2Cs^+$	-499.761971	-499.823793	**D**	**129.2**	**101.4**	In-out
	-499.761769	-499.819116	**D**	**128.7**	**89.1**	Propeller
3F-benzoic	-520.054248	-520.096438				
3F-benzoate	-519.522702	-519.564722	**A**	**1401.8**	**1368.1**	
3F-benzoic + Cs^+	-540.079725	-540.131539	**B**	**68.5**	**43.1**	On COO^-
			B			On
	-540.068702	-540.122227		**39.6**	**18.7**	Substituent
3F-benzoate + Cs^+	-539.694140	-539.744105	**C**	**451.7**	**421.9**	A
3F-benzoate + $2Cs^+$	-559.738001	-559.796810	**D**	**116.8**	**89.3**	In-out
	-559.737087	-559.798261	**D**	**114.4**	**93.2**	Propeller
			D			On
	-559.723316	-559.783719		**78.2**	**55.0**	Substituent
4F-benzoic	-520.055501	-520.097683				
4F-benzoate	-519.522162	-519.564242	**A**	**1406.5**	**1372.6**	
4F-benzoic + Cs^+	-540.080737	-540.132551	**B**	**67.9**	**42.5**	On COO^-
			B			On
	-540.067971	-540.117771		**34.3**	**3.7**	Substituent
4F-benzoate + Cs^+	-539.694336	-539.744429	**C**	**453.6**	**424.1**	
4F-benzoate + $2Cs^+$	-559.737273	-559.796136	**D**	**114.3**	**86.7**	In-out
	-559.736664	-559.797505	**D**	**112.7**	**90.3**	Propeller
3CF3-benzoic	-757.912370	-757.962948				
3CF3-benzoate	-757.386167	-757.436451	**A**	**1387.7**	**1354.4**	
3CF3-benzoic + Cs^+	-777.936569	-777.996019	**B**	**65.1**	**37.8**	On COO^-
			B			On
	-777.928187	-777.988309		**43.1**	**17.6**	Substituent
3CF3-benzoate + Cs^+	-777.554041	-777.612422	**C**	**442.4**	**413.0**	
3CF3-benzoate + $2Cs^+$	-797.597158	-797.663919	**D**	**114.8**	**86.2**	In-out
	-797.595623	-797.664348	**D**	**110.8**	**87.3**	Propeller
			D			On
	-797.582023	-797.649687		**75.1**	**48.8**	Substituent
4CF3-benzoic	-757.911914	-757.962454				
4CF3-benzoate	-757.386866	-757.437770	**A**	**1384.7**	**1349.6**	
4CF3-benzoic + Cs^+	-777.933799	-777.993734	**B**	**59.1**	**33.1**	On COO^-
			B			On
	-777.925282	-777.986979		**36.7**	**15.4**	Substituent
4CF3-benzoate + Cs^+	-777.553733	-777.612847	**C**	**439.7**	**410.6**	
			C			On
	-777.469697	-777.530866		**219.1**	**195.4**	Substituent
4CF3-benzoate + $2Cs^+$	-797.593461	-797.660915	**D**	**105.9**	**77.2**	In-out
	-797.593408	-797.662013	**D**	**105.8**	**80.1**	Propeller
			D			On
	-797.580864	-797.651394		**72.8**	**52.2**	Substituent
			D	**293.5**	**267.4**	

3NH2-benzoic	-476.135274	-476.178401				
3NH2-benzoate	-475.594230	-475.637320	**A**	**1426.7**	**1392.6**	
3NH2-benzoic + Cs^+	-496.164157	-496.216907	**B**	**77.4**	**52.1**	On COO^-
			B			On
	-496.153657	-496.206246		**49.9**	**24.1**	Substituent
3NH2-benzoate + Cs^+	-495.770970	-495.822060	**C**	**465.6**	**436.0**	
3NH2-benzoate + $2Cs^+$	-515.822896	-515.882652	**D**	**137.9**	**110.1**	In-out
4NH2-benzoic	-476.138415	-476.181537				
4NH2-benzoate	-475.593109	-475.636340	**A**	**1437.9**	**1403.5**	
4NH2-benzoic + Cs^+	-496.172692	-496.225719	**B**	**91.6**	**67.0**	On COO^-
4NH2-benzoate + Cs^+	-495.772051	-495.823095	**C**	**471.4**	**441.3**	
4NH2-benzoate + $2Cs^+$	-515.823848	-515.883232	**D**	**137.6**	**108.9**	In-out
	-515.821550	-515.879566	**D**	**131.6**	**99.2**	Propeller
3CN-benzoic	-513.031460	-513.076010				
3CN-benzoate	-512.509495	-512.553889	**A**	**1376.6**	**1342.9**	
3CN-benzoic + Cs^+	-533.053694	-533.107959	**B**	**60.0**	**34.9**	On COO^-
						On
	-533.061888	-533.116657		**81.5**	**57.7**	Substituent
3CN-benzoate + Cs^+	-532.674759	-532.727106	**C**	**435.5**	**405.8**	
3CN-benzoate + $2Cs^+$	-552.713832	-552.775401	**D**	**104.2**	**77.8**	In-out
	-552.714068	-552.777098	**D**	**104.8**	**82.2**	Propeller
			D			On
	-552.718003	-552.779829		**115.1**	**89.4**	Substituent
4CN-benzoic	-513.031314	-513.075928				
4CN-benzoate	-512.510605	-512.555153	**A**	**1373.3**	**1339.3**	
4CN-benzoic + Cs^+	-533.051315	-533.105514	**B**	**54.1**	**28.6**	On COO^-
			B			On
	-533.060247	-533.114832		**77.6**	**53.1**	Substituent
4CN-benzoate + Cs^+	-532.674498	-532.727096	**C**	**431.9**	**402.4**	
4CN-benzoate + $2Cs^+$	-552.711067	-552.772991	**D**	**97.6**	**71.5**	In-out
	-552.711795	-552.775644	**D**	**99.5**	**78.4**	Propeller
			D			On
	-552.717067	-552.782217		**113.4**	**95.7**	Substituent
3NO2-benzoic	-625.325375	-625.372244				
3NO2-benzoate	-624.805132	-624.851851	**A**	**1372.1**	**1338.3**	
3NO2-benzoic + Cs^+	-645.348791	-645.405208	**B**	**63.1**	**37.5**	On COO^-
			B			On
	-645.355417	-645.411299		**80.5**	**53.5**	Substituent
3NO2-benzoate + Cs^+	-644.969352	-645.023955	**C**	**432.8**	**402.8**	
3NO2-benzoate + $2Cs^+$	-665.011514	-665.074550	**D**	**112.3**	**83.8**	In-out
	-665.010311	-665.075375	**D**	**109.1**	**86.0**	Propeller
			D			On
	-665.014643	-665.078002		**120.5**	**92.9**	Substituent
4NO2-benzoic	-625.324686	-625.371670				
4NO2-benzoate	-624.807241	-624.854240	**A**	**1364.7**	**1330.6**	
4NO2-benzoic + Cs^+	-645.343397	-645.399933	**B**	**50.7**	**25.2**	On COO^-
			B			On
	-645.353456	-645.409800		**77.1**	**51.1**	Substituent
4NO2-benzoate + Cs^+	-644.969083	-645.024029	**C**	**426.5**	**396.8**	
			D			On
4NO2-benzoate + $2Cs^+$	-665.013991	-665.078721		**119.5**	**94.6**	Substituent
	-665.004443	-665.068559	**D**	**94.4**	**67.9**	In-out
	-665.005618	-665.070704	**D**	**97.5**	**73.5**	Propeller