Table 1 The calculated frequencies (in cm^{-1}) of HCOOArH and the transition states (TS1, TS2, TS3, TS4 and TS5) for HCOOArH dissociation reactions at the MP2(full)/AVTZ level.

Compound	υ^a(C-H1)	υ(C-O1)	υ(C-O2)	υ(Ar-O2)	υ(Ar-H2)	β^b	γ^c
trans-HCOOArH	2987.21	1615.53	1306.97	333.88	2307.96	172.71	174.64
						607.47	669.77
						781.69	1060.92
						1376.27	
cis-HCOOArH	2828.20	1711.20	1226.46	346.09	2062.90	137.66	100.82
						733.08	707.93
						766.87	1035.38
						1419.89	
TS1	2952.80			251.44	2771.82	-529.36	130.90
						300.78	357.90
						760.79	1065.53
						1347.32	
						1386.96	
						1584.42	
TS2	2961.59	1783.75	996.60	468.05	-903.93	158.64	248.84
						368.42	406.12
						729.64	983.17
						1297.30	
TS3	2150.64			254.77	2698.04	-244.90	115.18
						150.86	398.41
						746.47	991.01
						1237.94	
						1449.72	
						1771.80	
TS4	3077.25	1750.81	1117.64	724.51	-924.60	185.05	146.00
						407.34	452.62
						468.41	1008.61
						1377.82	
TS5	2636.81	1798.67	975.74	52.59		-1035.52	21.24
						67.04	218.77
						174.27	903.91
						516.94	
						-1232.50	

υ^a is stretching vibration

β^b is in-plane bending vibration

γ^c is out-of-plane bending vibration

Table 2 The calculated frequencies (in cm^{-1}) of HCOOKrH, HCOOKrD and the transition states (TS1, TS2, TS3, TS4 and TS5) for HCOOKrH dissociation reactions at the MP2(full)/AVTZ level.

Compound	υ^a(C-H1)	υ(C-O1)	υ(C-O2)	υ(Kr-O2)	υ(Kr-H2)	β^b	γ^c
trans-HCOOKrH	3000.46	1635.13	1290.09	334.09	2158.30	155.22	184.96
						614.56	667.68
						783.86	1061.07
						1377.05	
cis-HCOOKrH	2853.10	1722.71	1224.63	327.20	2055.89	138.16	105.72
						704.96	681.34
						762.09	1036.79
						1422.69	
trans-HCOOKrD	3000.14	1676.19	1288.59	332.79	1500.69	154.28	182.42
						451.50	491.30
						772.89	1061.00
						1373.17	
TS1	2946.32			219.32	2626.10	-517.10	91.47
						256.34	291.17
						752.77	1068.77
						1349.96	
						1391.22	
						1587.16	
TS2	2904.94	1806.20	957.69	376.83	-862.57	128.84	203.50
						228.31	317.88
						656.93	926.33
						1259.08	
TS3	2157.96			309.44	2531.89	-315.42	132.52
						204.25	364.76
						748.64	1000.52
						1251.80	
						1451.64	
						1766.25	
TS4	3128.10	1746.93	1082.74	612.07	-884.42	156.43	152.13
						282.51	287.81
						355.19	1000.56
						1343.56	
TS5	2652.95	1804.07	976.25	53.26		-1035.86	23.93
						69.31	220.58
						197.33	906.24
						511.37	
						1237.89	

υ^a is stretching vibration
β^b is in-plane bending vibration
γ^c is out-of-plane bending vibration

Table 3 The calculated frequencies (in cm^{-1}) of HCOOXeH, HCOOXD and the transition states (TS1, TS2, TS3, TS4 and TS5) for HCOOXeH dissociation reactions at the MP2(full)/AVTZ level.

Compound	υ^a(C-H1)	υ(C-O1)	υ(C-O2)	υ(Xe-O2)	υ(Xe-H2)	β^b	γ^c
trans-HCOOXeH	3016.43	1648.79	1282.82	327.35	2049.48	146.81	196.86
						571.85	622.19
						777.09	1064.20
						1378.13	
cis-HCOOXeH	2872.89	1732.10	1219.84	312.38	2015.53	135.80	103.30
						637.31	622.92
						759.01	1039.26
						1424.44	
trans-HCOOXeD	3016.20	1666.48	1281.19	324.62	1445.01	145.76	191.47
						413.81	452.33
						770.54	1062.65
						1372.91	
TS1	2942.51			207.38	2429.12	-387.18	22.29
						209.41	214.14
						747.16	1073.06
						1392.96	
						1353.37	
						1592.52	
TS2	2831.78	1797.51	937.21	301.73	-808.93	107.08	118.15
						127.63	277.08
						587.76	917.45
						1209.03	
TS3	2189.31			308.46	2354.37	-343.57	136.21
						192.37	320.26
						751.15	1006.03
						1256.58	
						1451.07	
						1758.31	
TS4	3159.26	1729.87	1080.24	492.75	-875.08	132.93	126.88
						174.23	199.55
						275.89	997.21
						1322.32	
TS5	2686.37	1812.45	973.11	57.48		-1043.31	28.56
						74.08	220.50
						218.31	911.34
						496.06	
						1253.35	

υ^a is stretching vibration
β^b is in-plane bending vibratio
γ^c is out-of-plane bending vibration

Cartesian coordinates for all optimized equilibrium and transition state structures

HCOOArH

trans-HCOOArH

C	1.22672100	0.81666400	0.00000000
O	1.61242100	-0.36064100	0.00000000
H	1.96813500	1.63305800	0.00000000
H	-1.84626800	-1.75228300	0.00000000
Ar	-1.13230900	-0.64772900	0.00000000
O	0.00000000	1.22043700	0.00000000

cis-HCOOArH

C	1.23866700	0.38076000	0.00000000
O	2.24261800	1.07293400	0.00000000
H	1.34666500	-0.72992800	0.00000000
O	0.00000000	0.79594100	0.00000000
Ar	-1.35889600	-0.81647100	0.00000000
H	-2.25948600	-1.80914800	0.00000000

TS1

C	-1.46434500	-0.00987600	-0.00005700
O	-0.86881400	-1.13051400	0.00005200
H	-2.56899300	-0.05030200	-0.00004700
H	1.75459200	1.13972100	0.00023800
O	-0.94013300	1.14110900	0.00001800
Ar	1.33733600	-0.06194000	-0.00002300

TS2

C	1.28142100	0.79543400	0.00000000
O	1.74503600	-0.30798500	0.00000000
H	1.85362200	1.74402100	0.00000000
H	-2.33921400	-2.23429200	0.00000000
Ar	-1.17573500	-0.63570300	0.00000000
O	0.00000000	1.20302600	0.00000000

TS3

C	-1.05547100	0.55336400	0.00000000
O	-1.97734200	1.36296900	0.00000000
H	0.00000000	1.08590400	0.00000000
O	-0.98397100	-0.70186100	0.00000000
Ar	1.54170000	-0.45505600	0.00000000
H	2.27273200	-1.50395600	0.00000000

TS4

C	1.25538400	0.35295300	0.00000000
O	2.19580600	1.10407900	0.00000000
H	1.30687500	-0.74127200	0.00000000
O	0.00000000	0.86422900	0.00000000
Ar	-1.32754400	-0.82728300	0.00000000
H	-2.50983000	-2.23181700	0.00000000

TS5

C	-1.09145200	1.17019900	0.00000000
O	-1.57949900	2.27470400	0.00000000
H	0.00000000	0.95719200	0.00000000
O	-1.48333300	-0.06368000	0.00000000
Ar	1.60284100	-1.52469200	0.00000000
H	2.20023500	1.77788200	0.00000000

HCOOKrH

trans-HCOOKrH

C	-0.10838200	-1.91865100	0.00000000
O	1.10792300	-1.71208500	0.00000000
H	-0.49855700	-2.94913500	0.00000000
H	0.60482200	2.27809200	0.00000000
Kr	0.00000000	0.94433400	0.00000000
O	-1.03991900	-1.01455000	0.00000000

cis-HCOOKrH

C	0.31700800	-1.78406100	0.00000000
O	0.21507900	-2.99714900	0.00000000
H	1.32873600	-1.31839300	0.00000000
O	-0.66989200	-0.92052000	0.00000000
Kr	0.00000000	1.13357200	0.00000000
H	0.40772300	2.55551200	0.00000000

TS1

C	1.94299000	0.00002100	0.00006700
O	1.37289900	-1.13070800	-0.00004800
H	3.04878500	-0.01124400	0.00042000
H	-1.22751000	1.34339500	0.00035100
O	1.39161000	1.14102700	-0.00009900
Kr	-0.98875800	-0.03930100	0.00000000

TS2

C	-0.07717500	-2.02511100	0.00000000
O	1.10890900	-1.90132900	0.00000000
H	-0.64633200	-2.98246400	0.00000000
H	0.90868000	3.23456700	0.00000000
O	-1.08382200	-1.13593300	0.00000000
Kr	0.00000000	1.00546300	0.00000000

TS3

C	-0.25840300	-1.70990900	0.00000000
O	-0.74663900	-2.83589300	0.00000000
H	-1.07824600	-0.86224800	0.00000000
O	0.91902700	-1.26208000	0.00000000
Kr	0.00000000	1.16877700	0.00000000
H	1.24955800	1.82951900	0.00000000

TS4

C	-0.37823500	-1.84233600	0.00000000
O	-0.22992500	-3.03514900	0.00000000
H	-1.31399800	-1.27995600	0.00000000
O	0.75930000	-1.09280500	0.00000000
H	-0.65159000	3.31521600	0.00000000
Kr	0.00000000	1.16784400	0.00000000

TS5

C	0.95552200	2.08312400	0.00000000
O	1.05209200	3.28610700	0.00000000
H	0.00000000	1.51490700	0.00000000
O	1.73612500	1.04841300	0.00000000
H	-2.33957400	1.60907400	0.00000000
Kr	-0.71386900	-1.39719100	0.00000000

HCOOXeH

trans-HCOOXeH

C	-0.10974700	-2.22100600	0.00000000
O	1.10540300	-2.02047600	0.00000000
H	-0.51189400	-3.24550100	0.00000000
H	0.60138900	2.29439700	0.00000000
Xe	0.00000000	0.75701400	0.00000000
O	-1.03428000	-1.30472700	0.00000000

cis-HCOOXeH

C	0.32302000	-2.13985200	0.00000000
O	0.18346400	-3.34712000	0.00000000
H	1.34409900	-1.69947600	0.00000000
O	-0.64520500	-1.24884400	0.00000000
Xe	0.00000000	0.90363300	0.00000000
H	0.41170800	2.51013900	0.00000000

TS1

C	2.28268400	0.02418800	0.02025800
O	1.76681900	-1.12687100	-0.02028500
H	3.38487900	0.07148100	0.10026700
H	-0.87489900	1.54249600	-0.01021000
Xe	-0.80956300	-0.03412300	0.00191500
O	1.67196900	1.13731100	-0.01909100

TS2

C	-0.06638400	-2.39499300	0.00000000
O	1.11776600	-2.25362400	0.00000000
H	-0.61422600	-3.37262500	0.00000000
H	0.91612400	3.65082000	0.00000000
Xe	0.00000000	0.82662400	0.00000000
O	-1.10571500	-1.56461600	0.00000000

TS3

C	-2.09081500	-0.09670200	0.00020100
O	-3.26588200	-0.45185500	-0.00022900
H	-1.33830700	-0.99761700	0.00086500
O	-1.51732300	1.02814000	0.00008900
Xe	0.93510000	-0.08095500	-0.00000900
H	1.65344600	1.33909400	-0.00046000

TS4

C	-0.38779700	-2.28511100	0.00000000
O	-0.23514900	-3.47870600	0.00000000
H	-1.31050300	-1.70555200	0.00000000
O	0.77499200	-1.58279300	0.00000000
Xe	0.00000000	0.96865500	0.00000000
H	-0.68146000	3.60083100	0.00000000

TS5

C	0.10164600	-2.71944100	0.00000000
O	0.53273600	-3.84564800	0.00000000
H	0.70728000	-1.78839800	0.00000000
O	-1.05643900	-2.12997900	0.00000000
H	2.87246500	-0.92036900	0.00000000
Xe	0.00000000	1.23760000	0.00000000