Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information

A density functional theory study of water gas shift reaction on Ag(111): potassium effect

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Content

Section 1: Figures

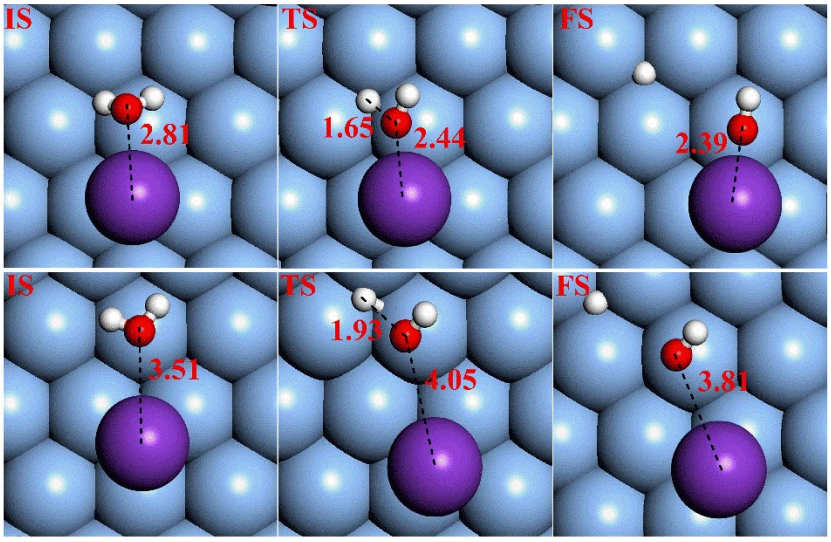

Figure S1. The IS, TS and FS optimized structures for H_2O dissociation on K/Ag(111) surfaces with short-range K-O distances (top) and long-range K-O distances (bottom).

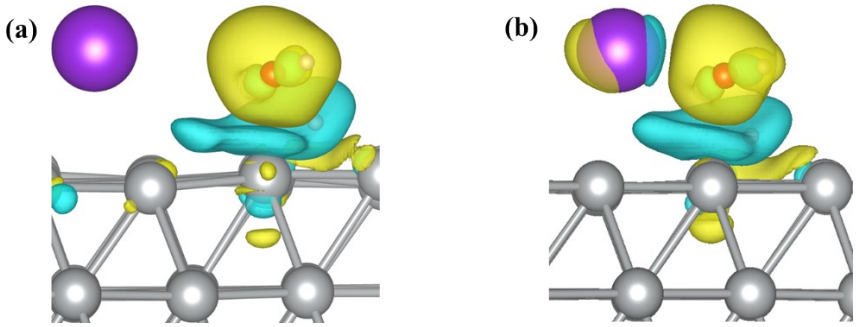

Figure S2. The charge density difference as to OH adsorption at the (a) long-range TS geometry and (b) short-range TS structure.

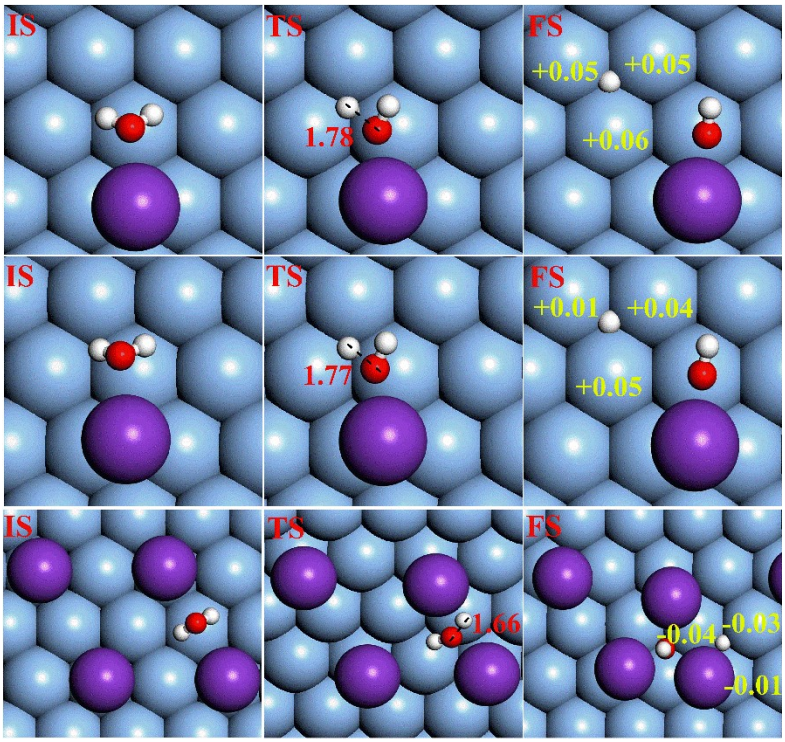

Figure S3. The IS, TS and FS optimized structures for H_2O dissociation on Ag(111) surfaces with different coverages of K (6.25%, 11.1% and 25% from top to bottom). Bader charges are marked with yellow typeface on Ag atoms connected with H atoms.

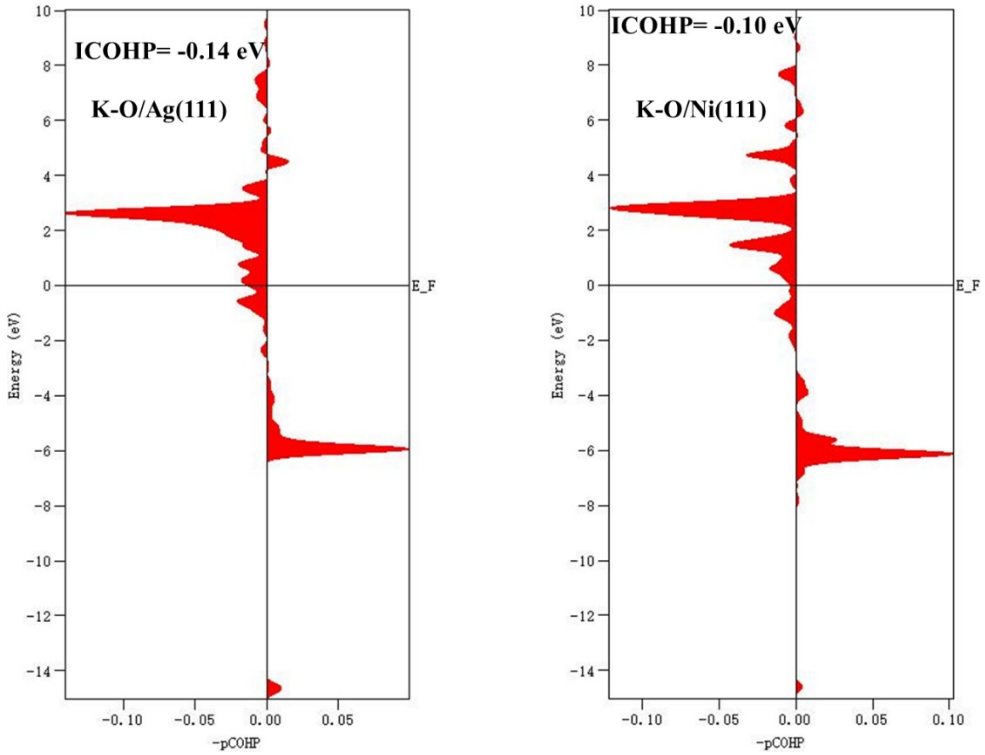

Figure S4. pCOHP bonding analysis between K-O bonding at TSs for H_2O dissociation on (a) Ag(111) and (b) Ni(111) surfaces.

Section 2: Tables

Table S1 The stabilization energy of OH by Ag(111) surfaces with different coverage of K

coverage of K	0	6.25%	11.1%	25%
stabilization energy	-4.45	-4.51	-4.43	-5.07

Section 3: Coordinates of TS structures for WGS reactions on Ag (111) and K/Ag(111)

R1.H_2O*+*=OH*+H* on Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.00246208	0.00267997	0.41777236
3	Ag	0.21556626	0.10645743	0.30668016
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333000	0.00000000	0.09024000
6	Ag	0.32605934	0.99677283	0.41341021
7	Ag	0.55241010	0.10831917	0.30459210
8	Ag	0.44444000	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.65763684	0.00788329	0.41290710
11	Ag	0.88624500	0.10798216	0.30686614
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333000	0.09024000
14	Ag	1.00057092	0.33446203	0.41235589
15	Ag	0.22166514	0.44489198	0.30600967
16	Ag	0.11111000	0.55555999	0.19797000
17	Ag	0.33333000	0.33333000	0.09024000
18	Ag	0.32598571	0.32588147	0.41316742
19	Ag	0.55273888	0.44253846	0.30505888
20	Ag	0.44444000	0.55555999	0.19797000
21	Ag	0.66667002	0.33333000	0.09024000
22	Ag	0.66462847	0.32975910	0.41186681
23	Ag	0.88749141	0.44267530	0.30505698
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	1.00153268	0.66223182	0.41222090
27	Ag	0.22143297	0.77503335	0.30575591
28	Ag	0.11111000	0.88889002	0.19797000
29	Ag	0.33333000	0.66667002	0.09024000
30	Ag	0.34056792	0.66929665	0.41705676
31	Ag	0.55576385	0.77647086	0.30583549
32	Ag	0.44444000	0.88889002	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.65875606	0.64480154	0.41281655
35	Ag	0.88663927	0.77609404	0.30678524
36	Ag	0.77777999	0.88889002	0.19797000
37	O	0.75827591	0.86368133	0.49022353

38	H	0.56098477	0.78813867	0.46058250
39	H	0.75854047	0.84487118	0.53383208

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R1.H_2O*+*=OH*+H* on K/Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.00439855	0.99798114	0.41308616
3	Ag	0.22267740	0.10687843	0.30434227
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.33503374	0.00195156	0.41384325
7	Ag	0.55658063	0.10672735	0.30529182
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.66494381	0.99297827	0.41649655
11	Ag	0.88783798	0.10742997	0.30662411
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	1.00209754	0.32908920	0.41342927
15	Ag	0.22399365	0.44451646	0.30582802
16	Ag	0.11111001	0.55556002	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000
18	Ag	0.33215767	0.32627803	0.41016192
19	Ag	0.55847541	0.44493336	0.30604654
20	Ag	0.44444001	0.55556002	0.19797000
21	Ag	0.66667002	0.33333000	0.09024000
22	Ag	0.66923136	0.32617585	0.41138745
23	Ag	0.89088851	0.44189695	0.30521366
24	Ag	0.77778000	0.55556002	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	1.00475643	0.66216807	0.41282522
27	Ag	0.22485770	0.77544036	0.30609704
28	Ag	0.11110999	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.33812491	0.66511970	0.41627603
31	Ag	0.55780622	0.77439729	0.30619075
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.67299428	0.65962570	0.41738314
35	Ag	0.88803665	0.77421391	0.30704132

36	Ag	0.77778000	0.88889003	0.19797000
37	O	0.62811230	0.69762223	0.52536320
38	H	0.55387320	0.77583646	0.46508487
39	H	0.73005426	0.81223962	0.53424998
40	K	0.50546238	0.38695049	0.55068891

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R2.OH*+*=O*+H* on Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.01014834	0.00790425	0.41779751
3	Ag	0.21767759	0.11027062	0.30634991
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.33204109	0.00329955	0.41232534
7	Ag	0.55666900	0.11170558	0.30524541
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.66528135	0.01824905	0.41597191
11	Ag	0.88846742	0.11243860	0.30659358
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	0.00443358	0.34183438	0.41189111
15	Ag	0.22377103	0.44779356	0.30569963
16	Ag	0.11111000	0.55555999	0.19797000
17	Ag	0.33333001	0.33333000	0.09024000
18	Ag	0.33214635	0.33409742	0.41201536
19	Ag	0.55628110	0.44902241	0.30558394
20	Ag	0.44444001	0.55555999	0.19797000
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.66862812	0.33785428	0.41132689
23	Ag	0.88965775	0.44655474	0.30533102
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	0.00370244	0.66879070	0.41232724
27	Ag	0.22242373	0.77935968	0.30532453
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.33624406	0.67143148	0.41535918
31	Ag	0.55667935	0.77987964	0.30576358

32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.66278265	0.65281133	0.41544618
35	Ag	0.88889054	0.77987462	0.30673379
36	Ag	0.77778000	0.88889003	0.19797000
37	O	0.77617135	0.88716135	0.47322055
38	H	0.53807558	0.81220205	0.45679524

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R2.OH*+*=O*+H* on K/Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.01796843	1.00585709	0.41798951
3	Ag	0.22011024	0.11216187	0.30645348
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.33375700	0.99993358	0.41233493
7	Ag	0.55761918	0.11229016	0.30534421
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.65615706	1.00658221	0.41461981
11	Ag	0.88946852	0.11158576	0.30612622
12	Ag	0.77777800	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	-0.00154350	0.32911111	0.41695905
15	Ag	0.22059527	0.44440318	0.30539174
16	Ag	0.11111000	0.55555999	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000
18	Ag	0.33732872	0.33918113	0.41326693
19	Ag	0.55835882	0.45016615	0.30616290
20	Ag	0.44444001	0.55555999	0.19797000
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.66770362	0.33784767	0.41275953
23	Ag	0.89074480	0.44539711	0.30606312
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	0.00313864	0.66526371	0.41264153
27	Ag	0.22188557	0.77865102	0.30469740
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000

30	Ag	0.32859462	0.66465000	0.41102407
31	Ag	0.55699862	0.78045447	0.30578685
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.66712629	0.66334622	0.41546881
35	Ag	0.89081877	0.78091045	0.30672499
36	Ag	0.77778000	0.88889003	0.19797000
37	O	0.77785898	0.89000679	0.48130278
38	H	0.88391366	0.11160824	0.45783398
39	K	0.53424167	0.74286386	0.55141356

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R3.OH*+OH*=H_2O*+O* on Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.00579465	0.00336109	0.41749651
3	Ag	0.21651229	0.10851149	0.30603639
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.33104794	1.00193901	0.41175903
7	Ag	0.55567839	0.10917078	0.30486859
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.66585622	0.01312152	0.41155042
11	Ag	0.88964777	0.11058341	0.30561304
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	1.00135267	0.33684302	0.41183305
15	Ag	0.22449642	0.44805840	0.30715163
16	Ag	0.11111000	0.55555999	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000
18	Ag	0.33100983	0.33011778	0.41226840
19	Ag	0.55563717	0.44639747	0.30503986
20	Ag	0.44444001	0.55555999	0.19797000
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.66569931	0.33248027	0.41123197
23	Ag	0.88808761	0.44412755	0.30477471
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	1.00087109	0.66489227	0.41160329

27	Ag	0.22387817	0.77680610	0.30668601
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.32947065	0.66617236	0.41826375
31	Ag	0.55459970	0.77714733	0.30712266
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.66502270	0.65147003	0.41174643
35	Ag	0.88972045	0.77919063	0.30568193
36	Ag	0.77778000	0.88889003	0.19797000
37	O	0.75426265	0.87460060	0.47482493
38	O	0.45073447	0.73470900	0.51048530
39	H	0.61890105	0.81532612	0.49814729
40	H	0.42018853	0.80829364	0.53466157

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R3.OH*+OH*=H_2O*+O* on K/Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.01065035	0.00553760	0.41856667
3	Ag	0.22083688	0.10994588	0.30648241
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.33701781	1.00234668	0.41260817
7	Ag	0.55979643	0.11064878	0.30563049
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.67260320	0.01327341	0.41333345
11	Ag	0.89353329	0.11286635	0.30622017
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	1.00791688	0.33988136	0.41247888
15	Ag	0.22735125	0.44876967	0.30669564
16	Ag	0.11111000	0.55555999	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000
18	Ag	0.33635430	0.33318710	0.41245079
19	Ag	0.55873051	0.44645360	0.30444834
20	Ag	0.44444001	0.55555999	0.19797000
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.67173914	0.33535461	0.41215075

23	Ag	0.89236270	0.44577583	0.30486151
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	0.00687216	0.66786605	0.41200132
27	Ag	0.22719105	0.77824411	0.30655236
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.33846394	0.66982878	0.41832315
31	Ag	0.55748835	0.77961895	0.30637464
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.66791090	0.65626323	0.40898863
35	Ag	0.89409864	0.78069224	0.30525142
36	Ag	0.77778000	0.88889003	0.19797000
37	O	0.76114693	0.86923930	0.47923558
38	O	0.47974995	0.75430478	0.53107164
39	H	0.61654563	0.82638934	0.50648010
40	H	0.45262630	0.84405421	0.54399983
41	K	0.66319330	0.60392694	0.55477190

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R4.H*+H*= H_2* on Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	1.00308719	1.00572252	0.41280407
3	Ag	0.22287586	0.11242814	0.30539490
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.33314782	1.00128324	0.41339182
7	Ag	0.55522382	0.11270939	0.30554665
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.66752690	1.00574145	0.412891780
11	Ag	0.88894949	0.11235463	0.305853364
12	Ag	0.77778000	0.22222000	0.197970003
13	Ag	1.00000000	0.33333001	0.090240002
14	Ag	1.00059576	0.33610729	0.413773416
15	Ag	0.22237297	0.44595246	0.306139437
16	Ag	0.11111000	0.55556000	0.197970003
17	Ag	0.33333001	0.33333001	0.090240002

18	Ag	0.33063955	0.33243898	0.413239443
19	Ag	0.55553756	0.44554238	0.305235430
20	Ag	0.44444000	0.55555999	0.197970003
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.66696408	0.33312526	0.41363105
23	Ag	0.88920638	0.44589778	0.30619350
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	-0.00119584	0.66805748	0.41597772
27	Ag	0.22147324	0.77753531	0.30677329
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.33357366	0.66829501	0.41560582
31	Ag	0.55638050	0.77833108	0.30626914
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.66810313	0.67332240	0.41256238
35	Ag	0.88739557	0.77816297	0.30636863
36	Ag	0.77778000	0.88889003	0.19797000
37	H	0.73235804	0.61501153	0.47659179
38	H	0.56152666	0.62366735	0.47944738

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R4.H*+H*= H_2* on K/Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	1.00535497	1.00556592	0.41131728
3	Ag	0.22422810	0.11298558	0.30538029
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.33398329	1.00172556	0.41447770
7	Ag	0.55491159	0.11333292	0.30490423
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.66559524	1.00545484	0.40979196
11	Ag	0.88999299	0.11282212	0.30449437
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	1.00016043	0.33388591	0.41514279
15	Ag	0.22220663	0.44496646	0.30698830

16	Ag	0.11111000	0.55555999	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000
18	Ag	0.33069721	0.33278674	0.41594320
19	Ag	0.55601360	0.44539991	0.30734381
20	Ag	0.44444001	0.55555999	0.19797000
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.66851802	0.33248360	0.41586107
23	Ag	0.88938312	0.44505100	0.30699257
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	0.00029239	0.66750078	0.41722006
27	Ag	0.22176903	0.77701444	0.30747511
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.33347519	0.66756717	0.41711997
31	Ag	0.55621236	0.77562103	0.30678650
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.67093939	0.67569459	0.41728530
35	Ag	0.88627846	0.77609648	0.30719046
36	Ag	0.77778000	0.88889003	0.19797000
37	H	0.71788552	0.60032882	0.48258417
38	H	0.54817859	0.59778042	0.48245693
39	K	0.82476957	1.01636600	0.54204421

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R5.CO*+OH*=cis-COOH* on Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.99103413	0.99299649	0.41164664
3	Ag	0.22096286	0.11155718	0.30602930
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.32837084	0.99491519	0.41217391
7	Ag	0.55469501	0.11309022	0.30648731
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.66181752	0.99685659	0.41294968
11	Ag	0.88695669	0.10967801	0.30472251
12	Ag	0.77778000	0.22222000	0.19797000

13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	0.99112991	0.32999021	0.41166836
15	Ag	0.22102108	0.44178092	0.30606339
16	Ag	0.11111000	0.55555999	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000
18	Ag	0.31283944	0.32235898	0.41527364
19	Ag	0.55164884	0.44196035	0.30831559
20	Ag	0.44444001	0.55555999	0.19797000
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.66360493	0.32512236	0.41658636
23	Ag	0.88390526	0.44264171	0.30571807
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	-0.00001188	0.66601439	0.41168289
27	Ag	0.22006958	0.77619691	0.30421250
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333000	0.66667002	0.09024000
30	Ag	0.32834337	0.66541362	0.41223779
31	Ag	0.55466243	0.77383456	0.30650778
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.66350997	0.67023559	0.41666483
35	Ag	0.88388962	0.77359771	0.30569892
36	Ag	0.77778000	0.88889003	0.19797000
37	C	0.35904142	0.34441032	0.51276190
38	O	0.62462700	0.47795331	0.49603968
39	O	0.32257321	0.32535726	0.56355126
40	H	0.70646406	0.51863060	0.53023371

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R5.CO*+OH*=cis-COOH* on K/Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	-0.00326429	-0.00365075	0.41076021
3	Ag	0.22421179	0.11425109	0.30690056
4	Ag	0.11111000	0.22222000	0.19796999
5	Ag	0.33333332	0.00000000	0.09024000
6	Ag	0.33248299	-0.00250121	0.41313811
7	Ag	0.55456598	0.10958230	0.30520295
8	Ag	0.44443998	0.22221999	0.19796999

9	Ag	0.66666664	0.00000000	0.09024000
10	Ag	0.66593508	-0.00239875	0.41341925
11	Ag	0.88821999	0.11093211	0.30473711
12	Ag	0.77777997	0.22221999	0.19796999
13	Ag	1.00000000	0.33333332	0.09024000
14	Ag	0.99565747	0.33046237	0.41328612
15	Ag	0.22278853	0.44201263	0.30749564
16	Ag	0.11111000	0.55555998	0.19796999
17	Ag	0.33333332	0.33333332	0.09024000
18	Ag	0.32811120	0.32980826	0.41981616
19	Ag	0.55282789	0.44327879	0.30815648
20	Ag	0.44443998	0.55555998	0.19796999
21	Ag	0.66666664	0.33333332	0.09024000
22	Ag	0.66749243	0.32822701	0.41240120
23	Ag	0.88845316	0.44399456	0.30516093
24	Ag	0.77777997	0.55555998	0.19797000
25	Ag	0.00000000	0.66666664	0.09024000
26	Ag	-0.00059527	0.66522140	0.41335774
27	Ag	0.22119102	0.77719051	0.30490631
28	Ag	0.11111000	0.88888997	0.19796999
29	Ag	0.33333332	0.66666664	0.09024000
30	Ag	0.33109124	0.66807793	0.41283503
31	Ag	0.55553045	0.77487894	0.30684666
32	Ag	0.44443998	0.88888997	0.19796999
33	Ag	0.66666664	0.66666664	0.09024000
34	Ag	0.66617654	0.66290188	0.41769754
35	Ag	0.88519629	0.77397471	0.30571554
36	Ag	0.77777997	0.88888997	0.19796999
37	C	0.36103961	0.36879741	0.51844757
38	O	0.59425415	0.56193835	0.53016188
39	O	0.29450252	0.30887513	0.56518522
40	H	0.64895359	0.48944836	0.53632691
41	K	0.82753034	0.88491009	0.55294146

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R6. cis-COOH*=trans-COOH* on Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.99902256	0.99738100	0.41254913
3	Ag	0.22401462	0.11383989	0.30676959

4	Ag	0.11111000	0.22221999	0.19797000
5	Ag	0.33333332	0.00000000	0.09024000
6	Ag	0.33446992	0.99903949	0.41287883
7	Ag	0.55532585	0.11098922	0.30520769
8	Ag	0.44443998	0.22221999	0.19797000
9	Ag	0.66666664	0.00000000	0.09024000
10	Ag	0.66690891	0.99903350	0.41293800
11	Ag	0.89024930	0.11153692	0.30566574
12	Ag	0.77777997	0.22221999	0.19796999
13	Ag	1.00000000	0.33333332	0.09024000
14	Ag	0.99765351	0.33195262	0.41302831
15	Ag	0.22280638	0.44329557	0.30636973
16	Ag	0.11111000	0.55555998	0.19796999
17	Ag	0.33333332	0.33333332	0.09024000
18	Ag	0.33536548	0.33348710	0.41801970
19	Ag	0.55383514	0.44326271	0.30644427
20	Ag	0.44443998	0.55555998	0.19796999
21	Ag	0.66666664	0.33333332	0.09024000
22	Ag	0.66875208	0.33207837	0.41232483
23	Ag	0.88981164	0.44436711	0.30548094
24	Ag	0.77777997	0.55555998	0.19796999
25	Ag	0.00000000	0.66666664	0.09024000
26	Ag	0.00088195	0.66606369	0.41294666
27	Ag	0.22255111	0.77740425	0.30554292
28	Ag	0.11111000	0.88888997	0.19796999
29	Ag	0.33333332	0.66666664	0.09024000
30	Ag	0.33441976	0.66790464	0.41289570
31	Ag	0.55539037	0.77643604	0.30560394
32	Ag	0.44443998	0.88888997	0.19797000
33	Ag	0.66666664	0.66666664	0.09024000
34	Ag	0.66955798	0.66802540	0.41318311
35	Ag	0.88893154	0.77704329	0.30538858
36	Ag	0.77777997	0.88888997	0.19796999
37	C	0.31137768	0.36592393	0.51432908
38	O	0.17297850	0.31716977	0.53994028
39	O	0.47190385	0.45728717	0.54559407
40	H	0.50542903	0.37373525	0.56117260

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R6. cis-COOH*=trans-COOH* on K/Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.99822531	0.99851787	0.41374076
3	Ag	0.22474235	0.11499885	0.30844402
4	Ag	0.11111000	0.22221999	0.19797000
5	Ag	0.33333332	0.00000000	0.09024000
6	Ag	0.33446667	0.99791029	0.41402493
7	Ag	0.55562742	0.11163918	0.30589760
8	Ag	0.44443998	0.22221999	0.19797000
9	Ag	0.66666664	0.00000000	0.09024000
10	Ag	0.66812131	0.00053954	0.41371086
11	Ag	0.88961338	0.11021049	0.30458461
12	Ag	0.77777997	0.22221999	0.19796999
13	Ag	1.00000000	0.33333332	0.09024000
14	Ag	0.99959237	0.33399521	0.40895877
15	Ag	0.22665854	0.44380870	0.30697526
16	Ag	0.11111000	0.55555998	0.19796999
17	Ag	0.33333332	0.33333332	0.09024000
18	Ag	0.33393746	0.33185959	0.42533589
19	Ag	0.55288642	0.44278510	0.30846869
20	Ag	0.44443998	0.55555998	0.19796999
21	Ag	0.66666664	0.33333332	0.09024000
22	Ag	0.67049878	0.33326204	0.41395805
23	Ag	0.88861715	0.44594451	0.30429293
24	Ag	0.77777997	0.55555998	0.19796999
25	Ag	0.00000000	0.66666664	0.09024000
26	Ag	1.00034969	0.66601621	0.41410840
27	Ag	0.22238520	0.77788673	0.30579624
28	Ag	0.11111000	0.88888997	0.19796999
29	Ag	0.33333332	0.66666664	0.09024000
30	Ag	0.33463846	0.66782983	0.41366823
31	Ag	0.55618229	0.77770092	0.30579726
32	Ag	0.44443998	0.88888997	0.19796999
33	Ag	0.66666664	0.66666664	0.09024000
34	Ag	0.66900162	0.66901785	0.41400210
35	Ag	0.88984880	0.77789350	0.30569806
36	Ag	0.77777997	0.88888997	0.19796999
37	C	0.33159001	0.32553508	0.52481398
38	O	0.21597863	0.31268844	0.55895967
39	O	0.48551709	0.33847047	0.55369835
40	H	0.56592032	0.46363360	0.56136442
41	K	0.89541962	0.26401978	0.55145302

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R7.COOH*=CO_2*+ H* on Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.99911259	0.99959037	0.41321423
3	Ag	0.22214645	0.11151731	0.30505406
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.33213994	0.99979418	0.41337260
7	Ag	0.55585804	0.11267547	0.30631918
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.66638350	1.00097071	0.41314926
11	Ag	0.88924633	0.11206487	0.30579991
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	0.99921052	0.33397084	0.41337845
15	Ag	0.22216235	0.44516036	0.30497047
16	Ag	0.11111000	0.55555999	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000
18	Ag	0.33200147	0.33378644	0.41163818
19	Ag	0.55556480	0.44515500	0.30503572
20	Ag	0.44444001	0.55555999	0.19797000
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.66171481	0.33475256	0.41662231
23	Ag	0.88732303	0.44389685	0.30679422
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	-0.00067113	0.66688566	0.41355068
27	Ag	0.22252216	0.77835386	0.30606083
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.33256897	0.66701230	0.41361193
31	Ag	0.55553314	0.77768108	0.30625330
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.66438481	0.66502877	0.41473061
35	Ag	0.88800994	0.77788792	0.30624753
36	Ag	0.77778000	0.88889003	0.19797000

37	C	0.24296023	0.36137624	0.53581406
38	O	0.11388361	0.34479683	0.55870122
39	O	0.39373481	0.38289813	0.54067439
40	H	0.45573938	0.38779729	0.48726697

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R7. COOH*=CO_2*+ H* on K/Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.99266166	0.99481603	0.41333027
3	Ag	0.22119262	0.11236273	0.30739489
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.33069075	-0.00118604	0.41382900
7	Ag	0.55406272	0.11192894	0.30642747
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.66410370	0.99795040	0.41285255
11	Ag	0.88694940	0.10924943	0.30456759
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	0.99367017	0.33246570	0.40894172
15	Ag	0.22240162	0.44309170	0.30594430
16	Ag	0.11111000	0.55555999	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000
18	Ag	0.31686067	0.32665227	0.42168542
19	Ag	0.55002978	0.44135591	0.30725784
20	Ag	0.44444001	0.55555999	0.19797000
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.66683614	0.33555751	0.41578485
23	Ag	0.88620362	0.44425101	0.30427899
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	-0.00112658	0.66552909	0.41423769
27	Ag	0.22046007	0.77684604	0.30648163
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.33089894	0.66534951	0.41382519
31	Ag	0.55418282	0.77466300	0.30674200
32	Ag	0.44444001	0.88889003	0.19797000

33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.66506027	0.66043574	0.41679682
35	Ag	0.88656002	0.77641652	0.30592220
36	Ag	0.77778000	0.88889003	0.19797000
37	C	0.35054260	0.35345019	0.52344542
38	O	0.22474960	0.30991957	0.55821245
39	O	0.51241658	0.41494040	0.53531708
40	H	0.61229059	0.45794418	0.47547502
41	K	0.90514248	0.24107415	0.55291931

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R10.CO*+O*= CO_2* on Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.99759970	1.00100769	0.41201654
3	Ag	0.22291513	0.11403343	0.30702028
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.32302454	0.99122631	0.41243232
7	Ag	0.55400169	0.11245608	0.30539237
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.66225631	0.99830224	0.41078605
11	Ag	0.88694575	0.11041425	0.30485752
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	0.99761290	0.33101815	0.41201917
15	Ag	0.22291030	0.44283802	0.30702481
16	Ag	0.11111000	0.55555999	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000
18	Ag	0.32614300	0.33022219	0.41902234
19	Ag	0.55374234	0.44382049	0.30763655
20	Ag	0.44444001	0.55555999	0.19797000
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.66029557	0.31481842	0.41337690
23	Ag	0.88738021	0.44479418	0.30634481
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	-0.01382103	0.66032232	0.41983229
27	Ag	0.21441930	0.77420776	0.30622709

28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.32301662	0.66620228	0.41245002
31	Ag	0.55393566	0.77549353	0.30537277
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.66027835	0.67986315	0.41329106
35	Ag	0.88740076	0.77653924	0.30634237
36	Ag	0.77778000	0.88889003	0.19797000
37	O	0.69649049	0.51557080	0.47617901
38	O	0.42648017	0.38058083	0.56388888
39	C	0.42807542	0.38136271	0.51170509

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R10.CO*+O*=CO_2* on K/Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.99984173	0.00138366	0.41082542
3	Ag	0.22409059	0.11389312	0.30647361
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.32817363	-0.00599556	0.41247266
7	Ag	0.55562280	0.11339389	0.30609094
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.66519829	-0.00186849	0.41204451
11	Ag	0.88739495	0.11028605	0.30442584
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	0.99974206	0.32916481	0.41210516
15	Ag	0.22342427	0.44175329	0.30708186
16	Ag	0.11111000	0.55556000	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000
18	Ag	0.33001778	0.32998531	0.41826456
19	Ag	0.55382995	0.44234339	0.30727186
20	Ag	0.44444001	0.55556000	0.19797000
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.66349815	0.31616796	0.41542104
23	Ag	0.88792990	0.44311590	0.30591641
24	Ag	0.77778000	0.55556000	0.19797000

25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	0.00194036	0.66526358	0.41540995
27	Ag	0.21640993	0.77426091	0.30557848
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.32863624	0.66576984	0.41213385
31	Ag	0.55500235	0.77517769	0.30504284
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.66134000	0.67708225	0.41204198
35	Ag	0.88829466	0.77660443	0.30502394
36	Ag	0.77778000	0.88889003	0.19797000
37	O	0.75415585	0.54591587	0.47558455
38	O	0.44644221	0.38712785	0.56349680
39	C	0.43716567	0.38153026	0.51121192
40	K	0.88067640	0.77627453	0.55115515

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R11.CO*+H*=CHO* on Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.98506124	0.98979491	0.41310092
3	Ag	0.21725191	0.11018471	0.30621088
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.32520933	0.99581533	0.41261314
7	Ag	0.55196532	0.11172724	0.30678848
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.65688785	0.99570756	0.41372445
11	Ag	0.88359545	0.10900368	0.30538240
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	0.98489132	0.32984599	0.41309601
15	Ag	0.21722052	0.44152674	0.30611074
16	Ag	0.11111000	0.55555999	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000
18	Ag	0.29798083	0.31683224	0.41506565
19	Ag	0.54704693	0.44064962	0.30704589
20	Ag	0.44444001	0.55555999	0.19797000

21	Ag	0.66667002	0.33333000	0.09024000
22	Ag	0.66457623	0.33403931	0.41554778
23	Ag	0.88346907	0.44282712	0.30531461
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	-0.00343309	0.66562587	0.41299895
27	Ag	0.21817448	0.77620923	0.30493080
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.32539188	0.66417494	0.41264387
31	Ag	0.55191930	0.77462657	0.30670074
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.66432506	0.66476777	0.41524439
35	Ag	0.88355944	0.77493949	0.30526802
36	Ag	0.77778000	0.88889003	0.19797000
37	O	0.40858269	0.37903754	0.55765079
38	C	0.41086492	0.37510503	0.50451166
39	H	0.58244087	0.45408781	0.47588624

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R11.CO*+H*=CHO* on K/Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.98933964	-0.00557670	0.41283449
3	Ag	0.22053353	0.11266121	0.30669578
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.32893983	-0.00113557	0.41326968
7	Ag	0.55526414	0.11444671	0.30771702
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.66162066	0.00052836	0.41390214
11	Ag	0.88580193	0.10997837	0.30432507
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	0.98752076	0.33542659	0.40928874
15	Ag	0.22130305	0.44408682	0.30543364
16	Ag	0.11111000	0.55555999	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000

18	Ag	0.30706475	0.32747810	0.41544506
19	Ag	0.55071767	0.44187235	0.31009787
20	Ag	0.44444001	0.55555999	0.19797000
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.66358075	0.33793664	0.42577298
23	Ag	0.88153668	0.44466456	0.30583919
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	-0.00172923	0.66944631	0.41406461
27	Ag	0.22039957	0.77795358	0.30513566
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.32995331	0.67001615	0.41304191
31	Ag	0.55417816	0.77700948	0.30634502
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.66434362	0.66922328	0.41677466
35	Ag	0.88480810	0.77597924	0.30570599
36	Ag	0.77778000	0.88889003	0.19797000
37	O	0.31360061	0.32886655	0.56359753
38	C	0.34947063	0.34222601	0.51180619
39	H	0.57086421	0.39698265	0.48939703
40	K	0.91027537	0.18290655	0.54649656

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R12.CHO*+O*=HCOO* on /Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.01062369	0.00629876	0.41571014
3	Ag	0.21593662	0.10928641	0.30597431
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.32971511	-0.00075817	0.41150754
7	Ag	0.55424423	0.10769112	0.30562492
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.65652751	0.00518107	0.41546551
11	Ag	0.88591838	0.10910357	0.30602292
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000

14	Ag	-0.00380664	0.33336301	0.41116110
15	Ag	0.22032815	0.44294801	0.30554364
16	Ag	0.11111000	0.55556000	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000
18	Ag	0.33153532	0.33021623	0.41293130
19	Ag	0.55484188	0.44728698	0.30554496
20	Ag	0.44444001	0.55555999	0.19797000
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.66405225	0.33028361	0.41093284
23	Ag	0.88553150	0.44321985	0.30487831
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	0.99442790	0.66336139	0.41111539
27	Ag	0.21948320	0.77785678	0.30451061
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.32017115	0.66724623	0.41053878
31	Ag	0.55288457	0.77585808	0.30715779
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.65138450	0.64661802	0.42122496
35	Ag	0.88183996	0.77565976	0.30721873
36	Ag	0.77778000	0.88889003	0.19797000
37	C	0.51007924	0.57082593	0.50746279
38	O	0.39857699	0.60612587	0.52237066
39	O	0.77863236	0.89391297	0.47058555
40	H	0.58412334	0.53970214	0.54148295

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R12.CHO*+O*=HCOO* on K/Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.00219798	0.00032392	0.41276533
3	Ag	0.22393815	0.11317292	0.30672523
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.32944699	-0.00653449	0.41204029
7	Ag	0.55616619	0.11108886	0.30564055
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000

10	Ag	0.66728459	-0.00509545	0.41172657
11	Ag	0.88984263	0.10906595	0.30444197
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	1.00277900	0.32876738	0.41055799
15	Ag	0.22486153	0.44141418	0.30575957
16	Ag	0.11111000	0.55555999	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000
18	Ag	0.33396341	0.33275284	0.42117981
19	Ag	0.55555292	0.44231508	0.30805936
20	Ag	0.44444001	0.55555999	0.19797000
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.66581416	0.31511902	0.41383597
23	Ag	0.88872971	0.44217461	0.30518424
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	-0.00188350	0.66482482	0.41299243
27	Ag	0.21931711	0.77462628	0.30503908
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.32877572	0.66456941	0.41208375
31	Ag	0.55637961	0.77186058	0.30671683
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.66597769	0.67135823	0.41794197
35	Ag	0.88773059	0.77630476	0.30607319
36	Ag	0.77778000	0.88889003	0.19797000
37	C	0.43695077	0.39367845	0.51532800
38	O	0.41556935	0.48942502	0.54949555
39	O	0.72181220	0.51395258	0.48425029
40	H	0.46814520	0.29168398	0.53033318
41	K	-0.060711833	0.488814471	0.54927842

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R13.HCOO*=CO_2*+ H* on Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.00159770	0.00100819	0.41350296
3	Ag	0.22284482	0.11154075	0.30565528

4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333000	0.00000000	0.09024000
6	Ag	0.33378156	0.00088421	0.41353533
7	Ag	0.55604972	0.11031111	0.30600731
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.66727817	0.00050968	0.41528932
11	Ag	0.88830672	0.11020441	0.30605628
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	0.99992469	0.33252376	0.41344515
15	Ag	0.22341525	0.44533135	0.30632199
16	Ag	0.11111001	0.55556001	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000
18	Ag	0.33351990	0.33326068	0.41439746
19	Ag	0.55644536	0.44577499	0.30684168
20	Ag	0.44444001	0.55556001	0.19797000
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.66723009	0.33213010	0.41355592
23	Ag	0.88910729	0.44426126	0.30560911
24	Ag	0.77778000	0.55556001	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	0.00096451	0.66613455	0.41310658
27	Ag	0.22351479	0.77758067	0.30603041
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.33149355	0.66728609	0.41552148
31	Ag	0.55615043	0.77695962	0.30756918
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.67087399	0.66615209	0.41765139
35	Ag	0.88755124	0.77707255	0.30657093
36	Ag	0.77778000	0.88889003	0.19797000
37	C	0.51174561	0.66736218	0.53588995
38	H	0.41321378	0.51734506	0.53186282
39	O	0.41237982	0.73078058	0.53761910
40	O	0.67482590	0.72523166	0.53152714

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092

R13.HCOO*=CO_2*+ H* on K/Ag (111)

n°	atom	Relaxed atomic coordinates (cartesian) [Å]		
1	Ag	0.00000000	0.00000000	0.09024000
2	Ag	0.00075077	0.00119389	0.41398311
3	Ag	0.22281805	0.11129938	0.30520982
4	Ag	0.11111000	0.22222000	0.19797000
5	Ag	0.33333001	0.00000000	0.09024000
6	Ag	0.33294162	0.00027330	0.41302933
7	Ag	0.55680974	0.11272167	0.30632802
8	Ag	0.44444001	0.22222000	0.19797000
9	Ag	0.66667002	0.00000000	0.09024000
10	Ag	0.66780992	1.00046020	0.41325240
11	Ag	0.88939830	0.11074532	0.30517059
12	Ag	0.77778000	0.22222000	0.19797000
13	Ag	1.00000000	0.33333001	0.09024000
14	Ag	0.00074138	0.33414861	0.41153755
15	Ag	0.22348739	0.44543728	0.30443173
16	Ag	0.11111000	0.55555999	0.19797000
17	Ag	0.33333001	0.33333001	0.09024000
18	Ag	0.32961472	0.33349324	0.41190891
19	Ag	0.55640558	0.44455412	0.30598027
20	Ag	0.44444001	0.55555999	0.19797000
21	Ag	0.66667002	0.33333001	0.09024000
22	Ag	0.67112100	0.33632742	0.41424981
23	Ag	0.88826076	0.44512481	0.30565709
24	Ag	0.77778000	0.55555999	0.19797000
25	Ag	1.00000000	0.66667002	0.09024000
26	Ag	0.00268255	0.66850290	0.41353875
27	Ag	0.22334445	0.77875478	0.30526811
28	Ag	0.11111000	0.88889003	0.19797000
29	Ag	0.33333001	0.66667002	0.09024000
30	Ag	0.33400850	0.66751094	0.41301292
31	Ag	0.55640478	0.77826500	0.30548523
32	Ag	0.44444001	0.88889003	0.19797000
33	Ag	0.66667002	0.66667002	0.09024000
34	Ag	0.66761647	0.66874283	0.41304324
35	Ag	0.88973938	0.77832643	0.30601265
36	Ag	0.77778000	0.88889003	0.19797000
37	C	0.57189090	0.41365816	0.57435792
38	H	0.41529347	0.25269795	0.50964072
39	O	0.44451949	0.42272477	0.59365102
40	O	0.54317600	0.30852237	0.52368978
41	K	0.15441749	0.40713858	0.56071167

Lattice vector 1[Å]	8.77270031	0.00000000	0.00000000
Lattice vector 2[Å]	-4.38635015	7.59738133	0.00000000
Lattice vector 3[Å]	0.00000000	0.00000000	22.16290092