Electronic Supplementary Material (ESI) for Catalysis Science & Technology.
This journal is © The Royal Society of Chemistry 2024

Electronic Supplementary Information for:

Synergistic effect and coordination environment tuned water-gas shift reaction on MoS_2 catalyst

Hai-Yan Su,[a] Wenbo Liao,[a,*] Keju Sun[b,*]

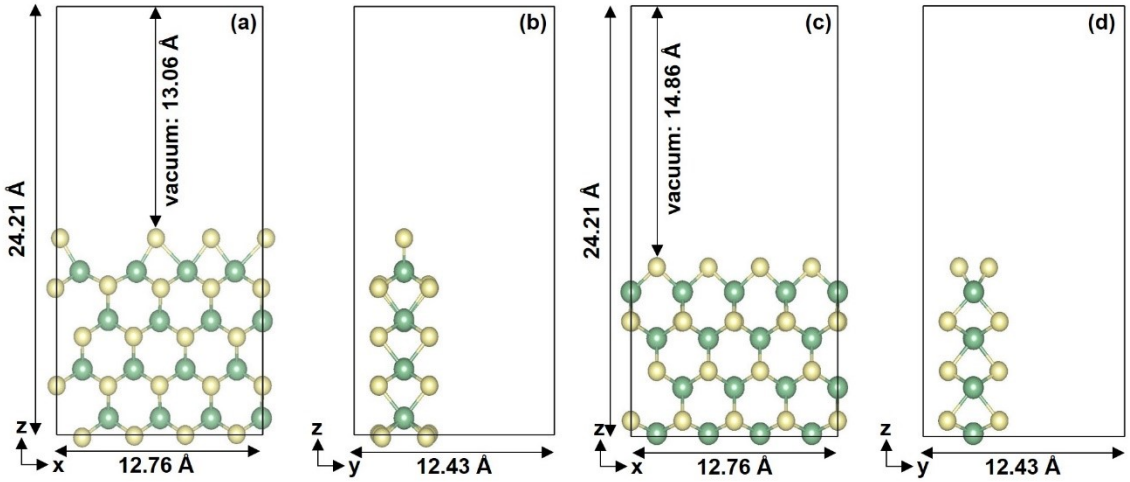
[a]*Guangdong Provincial Key Laboratory of Distributed Energy Systems, School of Chemical Engineering and Energy Technology, Dongguan University of Technology, 1 Daxue Road, Dongguan 523808, China.*

[b]*Hebei Key Laboratory of Applied Chemistry, School of Environmental and Chemical Engineering, Yanshan University, 438 Hebei Avenue, Qinhuangdao 066004, China.*

**E-mail: liaowenbo110@163.com (Wenbo Liao); kjsun@ysu.edu.cn (Keju Sun)*

S1. Calculation models for MoS_2 edges

Figure S1. The calculation models for (a, b) Mo edge and (c, d) S edge. Green and yellow spheres represent Mo and S atoms, respectively.



S2. Effect of force convergence on adsorption energies of species

Table S1. Effect of force convergence (F, in eV/Å) on adsorption energies (ΔE_{Ads}, in eV) of selected species at favorable adsorption sites on MoS_{2-v}(001), Cu/MoS_{2-v}(001), Mo and S edges, with 13%, 13%, 62.5% and 50% S vacancy, respectively. ZPE corrections are not included.

Species	MoS_{2-v}(001)		Cu/MoS_{2-v}(001)		Mo edge		S edge	
	F=0.03	F=0.02	F=0.03	F=0.02	F=0.03	F=0.02	F=0.03	F=0.02
H_2O	-0.11	-0.11	-0.42	-0.42	-0.84	-0.73	-0.22	-0.22
CO	-0.89	-0.89	-0.80	-0.80	-1.24	-1.11	-0.67	-0.67
OH	-4.25	-4.25	-4.03	-4.03	-4.27	-4.15	-3.41	-3.41
H	-0.33	-0.33	-0.35	-0.35	-0.31	-0.19	-0.19	-0.19
O	-7.29	-7.29	-5.70	-5.70	-5.56	-5.44	-5.41	-5.41
HCOO	-2.80	-2.80	-2.79	-2.79	-3.15	-3.03	-2.74	-2.74
COOH	-1.93	-1.93	-1.72	-1.73	-2.54	-2.42	-2.02	-2.02

S3. Imaginary frequency analysis of the transition states

Table S2. Imaginary frequency (in cm^{-1}) at the transition states of various elementary reactions on $MoS_{2-v}(001)$, $Cu/MoS_{2-v}(001)$, Mo and S edge. * and # denote the S vacancy and S site, respectively. Adsorbed and gaseous CH_4 are used for $MoS_{2-v}(001)$ and $Cu/MoS_{2-v}(001)$, respectively. Adsorbed and gaseous CO_2 are used for the Mo and S edge, respectively.

Elementary reactions	$MoS_{2-v}(001)$	$Cu/MoS_{2-v}(001)$
$H_2O^* + * = OH^* + H^*$	-1043.86	-861.78
$OH^* + * = O^* + H^*$	-1377.42	-1310.65
$2OH^* = H_2O^* + O^*$	-933.79	-760.65
$CO^* + O^* = CO_2^* + *$	-299.89	-105.12
$CO^* + OH^* = COOH^* + *$	-354.11	-195.28
$CO^* + H^* = CHO^* + *$	-403.95	-118.73
$CO^* + H^* = COH^* + *$	-1372.31	-551.52
$CHO^* + O^* = HCOO^* + *$	-371.78	-239.77
$COH^* + O^* = COOH^* + *$	-44.55	- 348.71
$HCOO^* + * = CO_2^* + H^*$	-424.98	-409.41
$COOH^* + * = CO_2^* + H^*$	-1477.39	-1344.90
$2H^* = H_2 + 2^*$	-370.81	- 373.24
$CHO^* + * = CH^* + O^*$	-456.48	-502.07
$CHO^* + H^* = CH_2O^* + *$	-814.00	-880.31
$CHO^* + H^* = CHOH^* + *$	-1376.11	-1328.97
$COH^* + H^* = CHOH^* + *$	-850.03	-828.04
$CH_2O^* + * = CH_2^* + O^*$	-513.39	-420.62
$CHOH^* + * = CH^* + OH^*$	-308.20	-302.52
$CH_2O^* + H^* = CH_3O^* + *$	-966.42	-583.72
$CH_2O^* + H^* = CH_2OH^* + *$	-1376.13	-1377.29
$CHOH^* + H^* = CH_2OH^* + *$	-862.06	-846.00
$CH_3O^* + * = CH_3^* + O^*$	-324.81	-149.43
$CH_2OH^* + * = CH_2^* + OH^*$	-423.19	-418.76
$CH^* + H^* = CH_2^* + *$	-940.01	-602.79
$CH_2^* + H^* = CH_3^* + *$	-941.57	-892.61
$CH_3^* + H^* = CH_4^* + */CH_4 + 2^*$	-874.58	-456.44

Elementary reactions	Mo edge	S edge
$H_2O^* + \# = OH^* + H^\#$	-696.26	-1075.45
$OH^* + \# = O^* + H^\#$	-307.62	-1254.70
$CO^* + O^* = CO_2^* + */CO_2 + 2^*$	-277.35	-202.53
$CO^* + OH^* = COOH^* + *$	-42.05	-188.13
$CO^* + H^\# = CHO^* + \#$	-183.18	-131.20
$CO^* + H^\# = COH^* + \#$	-1139.51	-1043.27
$CHO^* + O^* = HCOO^* + *$	-317.14	-218.93
$COH^* + O^* = COOH^* + *$	-469.28	-231.69
$HCOO^* + \# = CO_2^* + H^\#/CO_2 + * + H^\#$	-594.75	-841.71
$COOH^* + \# = CO_2^* + H^\#/CO_2 + * + H^\#$	-519.47	-825.55
$H^\# + * = H^* + \#$	-292.05	-706.52
$H^* + H^\# = H_2^* + \#$	-377.20	
$2H^* = H_2 + 2^*$		-718.18
$CHO^* + * = CH^* + O^*$	-27.31	-431.27
$CHO^* + H^\# = CH_2O^* + \#$	-1067.27	-689.04
$CHO + H^\# = CHOH^* + \#$	-1025.92	-899.70
$CH_2O^* + * = CH_2^* + O^*$	-371.15	-429.90
$CHOH^* + * = CH^* + OH^*$	-288.58	-136.32
$CH_2O^* + H^\# = CH_3O^* + \#$	-792.54	-742.54
$CH_2O^* + H^\# = CH_2OH^* + \#$	-845.44	-1042.98
$CHOH^* + H^\# = CH_2OH^* + \#$	-294.85	-773.74
$CH_2OH^* + * = CH_2^* + OH^*$	-278.20	-362.96
$CH^* + H^\# = CH_2^* + \#$	-646.40	-230.98
$CH_2^* + H^\# = CH_3^* + \#$	-389.77	-441.81
$CH_3^* + H^\# = CH_4^* + \#$	-510.94	-956.58

S4. Zero-point energy of adsorbed species and transition states

Table S3. Zero-point energy (ZPE, in eV) of adsorbed species on $MoS_{2-v}(001)$, $Cu/MoS_{2-v}(001)$, Mo and S edge. * and # denote the S vacancy and S site, respectively.

Species	$MoS_{2-v}(001)$	$Cu/MoS_{2-v}(001)$	Mo edge	S edge
H_2O*	0.65	0.66	0.65	0.65
OH*	0.39	0.38	0.36	0.38
H*	0.16	0.19	0.14	0.19
$H^{\#}$			0.21	0.21
O*	0.09	0.08	0.07	0.08
CO*	0.18	0.20	0.20	0.20
CO_2*	0.31	0.31	0.32	
HCOO*	0.61	0.62	0.64	0.64
COOH*	0.64	0.65	0.64	0.64
CHO*	0.49	0.51	0.49	0.51
COH*	0.49	0.51	0.50	0.50
CH_2O*	0.82	0.82	0.79	0.77
CHOH*	0.75	0.79	0.80	0.83
CH_3O*	1.14	1.12		
CH_2OH*	1.13	1.14	1.11	1.12
CH*	0.38	0.38	0.39	0.39
CH_2*	0.63	0.68	0.64	0.67
CH_3*	0.91	0.95	0.93	0.94
CH_4*	1.19		1.23	1.20

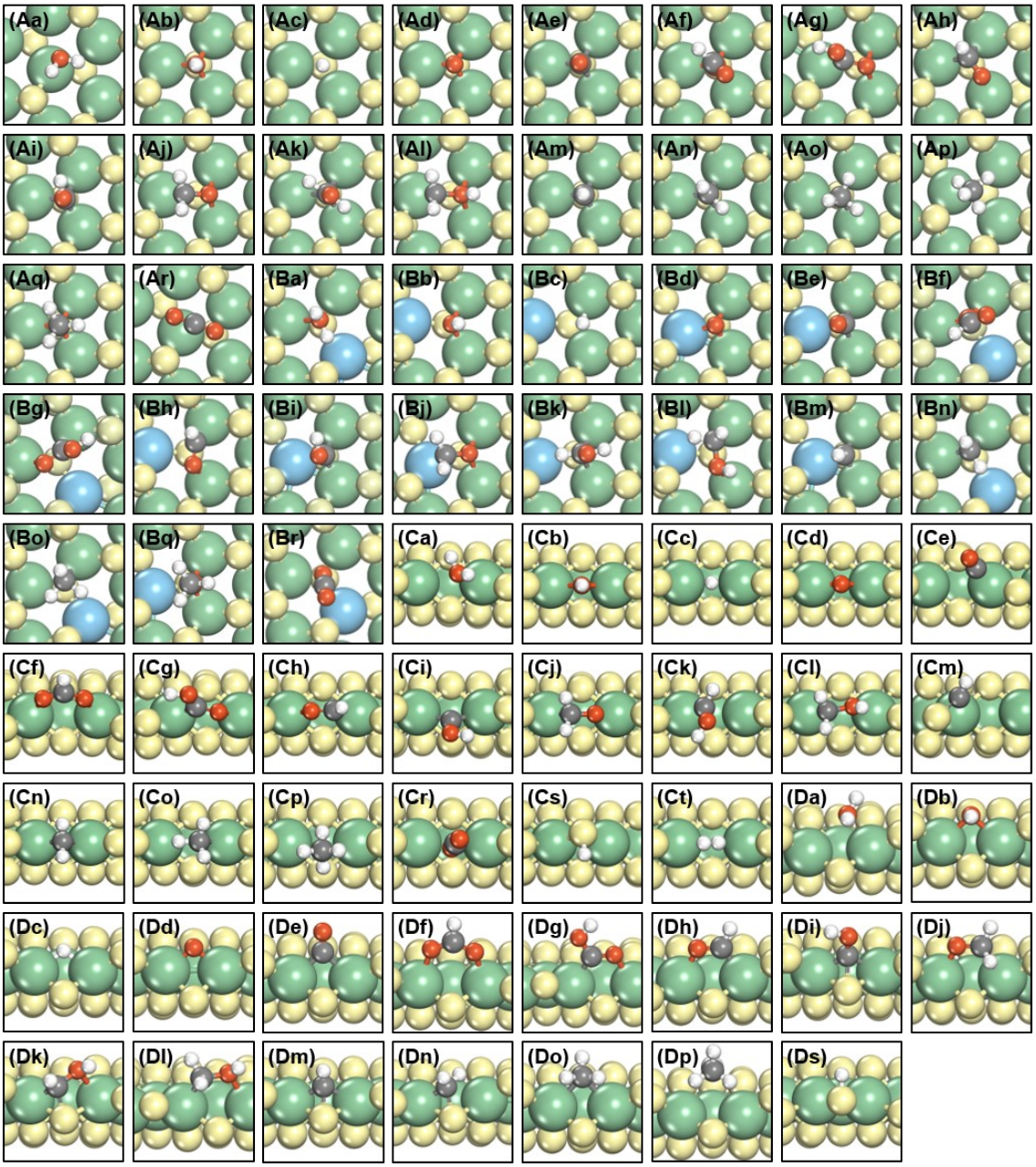
Table S4. The zero-point energy (ZPE, in eV) at the transition states of various elementary reactions on MoS_{2-v}(001), Cu/MoS_{2-v}(001), Mo and S edge. * and # denote the S vacancy and S site, respectively. Adsorbed and gaseous CH_4 are used for MoS_{2-v}(001) and Cu/MoS_{2-v}(001), respectively. Adsorbed and gaseous CO_2 are used for the Mo and S edge, respectively.

Elementary reactions	MoS_{2-v}(001)	Cu/MoS_{2-v}(001)
$H_2O^* + * = OH^* + H^*$	0.48	0.50
$OH^* + * = O^* + H^*$	0.21	0.20
$2OH^* = H_2O^* + O^*$	0.63	0.85
$CO^* + O^* = CO_2^* + *$	0.27	0.26
$CO^* + OH^* = COOH^* + *$	0.54	0.57
$CO^* + H^* = CHO^* + *$	0.42	0.43
$CO^* + H^* = COH^* + *$	0.34	0.38
$CHO^* + O^* = HCOO^* + *$	0.57	0.57
$COH^* + O^* = COOH^* + *$	0.60	0.56
$HCOO^* + * = CO_2^* + H^*$	0.47	0.49
$COOH^* + * = CO_2^* + H^*$	0.42	0.43
$2H^* = H_2 + 2*$	0.34	0.35
$CHO^* + * = CH^* + O^*$	0.44	0.43
$CHO^* + H^* = CH_2O^* + *$	0.64	0.63
$CHO^* + H^* = CHOH^* + *$	0.63	0.60
$COH^* + H^* = CHOH^* + *$	0.63	0.65
$CH_2O^* + * = CH_2^* + O^*$	0.74	0.74
$CHOH^* + * = CH^* + OH^*$	0.73	0.72
$CH_2O^* + H^* = CH_3O^* + *$	0.99	0.92
$CH_2O^* + H^* = CH_2OH^* + *$	0.95	0.90
$CHOH^* + H^* = CH_2OH^* + *$	0.99	0.94
$CH_3O^* + * = CH_3^* + O^*$	0.98	0.93
$CH_2OH^* + * = CH_2^* + OH^*$	0.99	1.03
$CH^* + H^* = CH_2^* + *$	0.52	0.50
$CH_2^* + H^* = CH_3^* + *$	0.81	0.84
$CH_3^* + H^* = CH_4^* + */CH_4 + 2*$	1.10	1.01

Elementary reactions	Mo edge	S edge
$H_2O^* + \# = OH^* + H^\#$	0.49	0.51
$OH^* + \# = O^* + H^\#$	0.21	0.21
$CO^* + O^* = CO_2^* + */CO_2 + 2^*$	0.27	0.28
$CO^* + OH^* = COOH^* + *$	0.60	0.55
$CO^* + H^\# = CHO^* + \#$	0.41	0.24
$CO^* + H^\# = COH^* + \#$	0.33	0.33
$CHO^* + O^* = HCOO^* + *$	0.55	0.56
$COH^* + O^* = COOH^* + *$	0.54	0.54
$HCOO^* + \# = CO_2^* + H^\#/CO_2 + * + H^\#$	0.51	0.46
$COOH^* + \# = CO_2^* + H^\#/CO_2 + * + H^\#$	0.48	0.45
$H^\# + * = H^* + \#$	0.13	0.13
$H^* + H^\# = H_2^* + \#$	0.32	
$2H^* = H_2 + 2^*$		0.34
$CHO^* + * = CH^* + O^*$	0.48	0.42
$CHO^* + H^\# = CH_2O^* + \#$	0.64	0.65
$CHO^* + H^\# = CHOH^* + \#$	0.60	0.66
$CH_2O^* + * = CH_2^* + O^*$	0.74	0.74
$CHOH^* + * = CH^* + OH^*$	0.74	0.74
$CH_2O^* + H^\# = CH_3O^* + \#$	0.91	0.94
$CH_2O^* + H^\# = CH_2OH^* + \#$	0.93	0.96
$CHOH^* + H^\# = CH_2OH^* + \#$	0.98	0.95
$CH_2OH^* + * = CH_2^* + OH^*$	1.03	1.02
$CH^* + H^\# = CH_2^* + \#$	0.49	0.54
$CH_2^* + H^\# = CH_3^* + \#$	0.81	0.84
$CH_3^* + H^\# = CH_4^* + \#$	1.10	1.08

S5. Structures for intermediates adsorption on various surfaces

Figure S2. Optimized configurations for (a) H_2O (b) OH (c) H (at Mo) (d) O (e) CO (f) HCOO (g) COOH (h) CHO (i) COH (j) CH_2O (k) CHOH (l) CH_2OH (m) CH (n) CH_2 (o) CH_3 (p) CH_4 (q) CH_3O (r) CO_2 (s) H (at S) (t) H_2 adsorption on (A) $MoS_{2-v}(001)$, (B) $Cu/MoS_{2-v}(001)$, (C) Mo edge and (D) S edge. The green, blue, yellow, grey, red and white balls represent Mo, Cu, S, C, O and H atoms, respectively. The notation is used throughout the paper.



S6. Structures at transition states of elementary reactions on various surfaces

Figure S3. Optimized configurations at the transition states of (a) $H_2O^* + * = OH^* + H^*$ (b) $OH^* + * = O^* + H^*$ (c) $CO^* + O^* = CO_2^* + *$ (d) $CO^* + OH^* = COOH^* + *$ (e) $CO^* + H^* = CHO^* + *$ (f) $CO^* + H^* = COH^* + *$ (g) $CHO^* + O^* = HCOO^* + *$ (h) $COH^* + O^* = COOH^* + *$ (i) $HCOO^* + * = CO_2^* + H^*$ (j) $COOH^* + * = CO_2^* + H^*$ (k) $2H^* = H_2 + 2^*$ (l) $2OH^* = H_2O^* + O^*$ (m) $CHO^* + * = CH^* + O^*$ (n) $CHO^* + H^* = CH_2O^* + *$ (o) $CHO^* + H^* = CHOH^* + *$ (p) $CH_2O^* + * = CH_2^* + O^*$ (q) $CHOH^* + * = CH^* + OH^*$ (r) $CH_2O^* + H^* = CH_3O^* + *$ (s) $CH_2O^* + H^* = CH_2OH^* + *$ (t) $CHOH^* + H^* = CH_2OH^* + *$ (u) $CH_3O^* + * = CH_3^* + O^*$ (v) $CH_2OH^* + * = CH_2^* + OH^*$ (w) $CH^* + H^* = CH_2^* + *$ (x) $CH_2^* + H^* = CH_3^* + *$ (y) $CH_3^* + H^* = CH_4^* + */CH_4 + 2^*$ (z) $COH^* + H^* = CHOH^* + *$ on (A) $MoS_{2-v}(001)$ and (B) $Cu/MoS_{2-v}(001)$. * denotes the S vacancy. Adsorbed and gaseous CH_4 are used for $MoS_{2-v}(001)$ and $Cu/MoS_{2-v}(001)$, respectively.

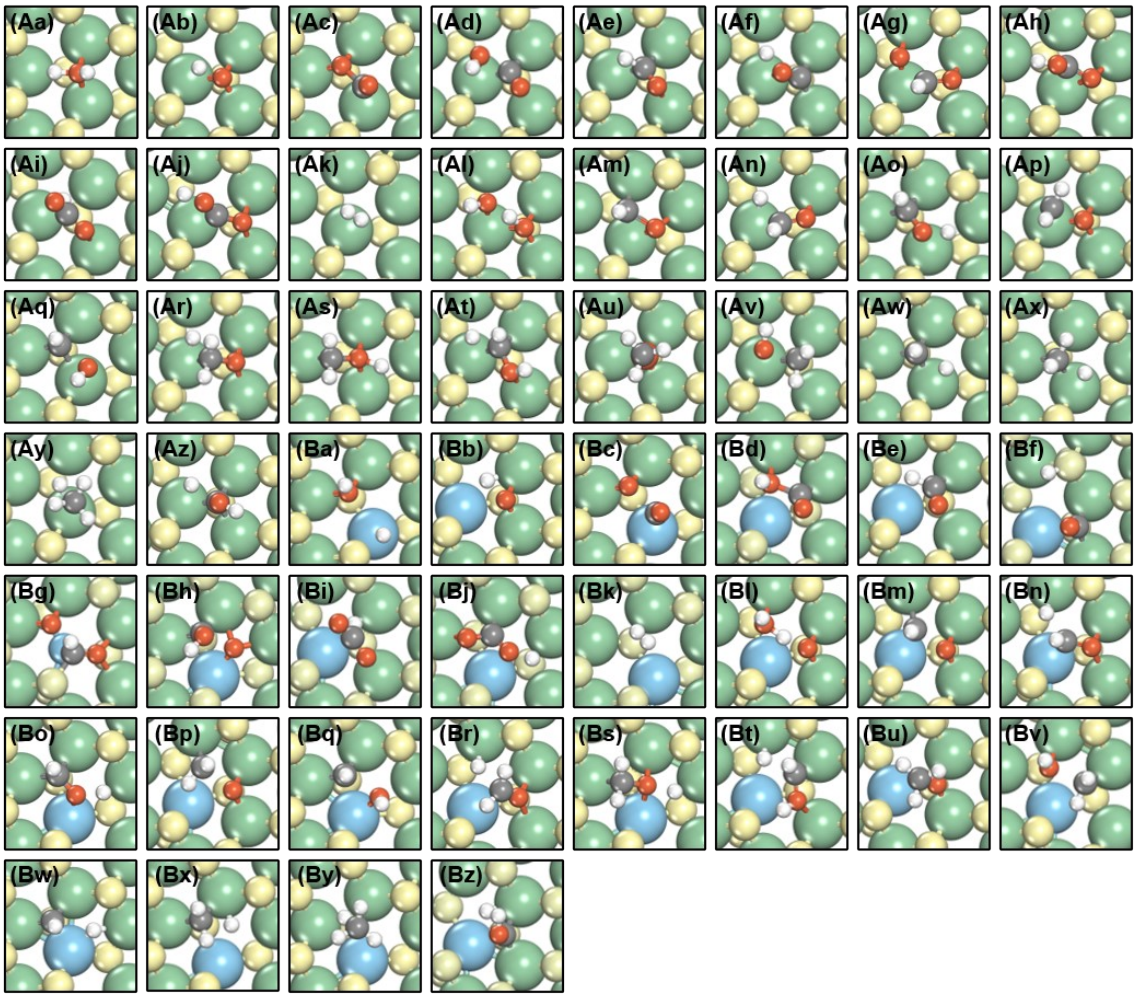


Figure S4. Optimized configurations at the transition states of (a) $H_2O^* + \# = OH^* + H^\#$ (b) $OH^* + \# = O^* + H^\#$ (c) $CO^* + O^* = CO_2^* + */CO_2 + 2^*$ (d) $CO^* + OH^* = COOH^* + *$ (e) $CO^* + H^\# = CHO^* + \#$ (f) $CO^* + H^\# = COH^* + \#$ (g) $CHO^* + O^* = HCOO^* + *$ (h) $COH^* + O^* = COOH^* + *$ (i) $HCOO^* + \# = CO_2^* + H^\#/CO_2 + * + H^\#$ (j) $COOH^* + \# = CO_2^* + H^\#/CO_2 + * + H^\#$ (k) $H^* + H^\# = H_2 + * + \#$ (l) $H^\# + * = H^* + \#$ (m) $CHO^* + * = CH^* + O^*$ (n) $CHO^* + H^\# = CH_2O^* + \#$ (o) $CHO^* + H^\# = CHOH^* + \#$ (p) $CH_2O^* + * = CH_2^* + O^*$ (q) $CHOH^* + * = CH^* + OH^*$ (r) $CH_2O^* + H^\# = CH_3O^* + \#$ (s) $CH_2O^* + H^\# = CH_2OH^* + \#$ (t) $CHOH^* + H^\# = CH_2OH^* + \#$ (u) $CH_2OH^* + * = CH_2^* + OH^*$ (v) $CH^* + H^\# = CH_2^* + \#$ (w) $CH_2^* + H^\# = CH_3^* + \#$ (x) $CH_3^* + H^\# = CH_4^* + \#$ on (A) Mo edge and (B) S edge. * and # denote the S vacancy and S site on the MoS_2 edges, respectively. Adsorbed and gaseous CO_2 are used for the Mo and S edge, respectively.

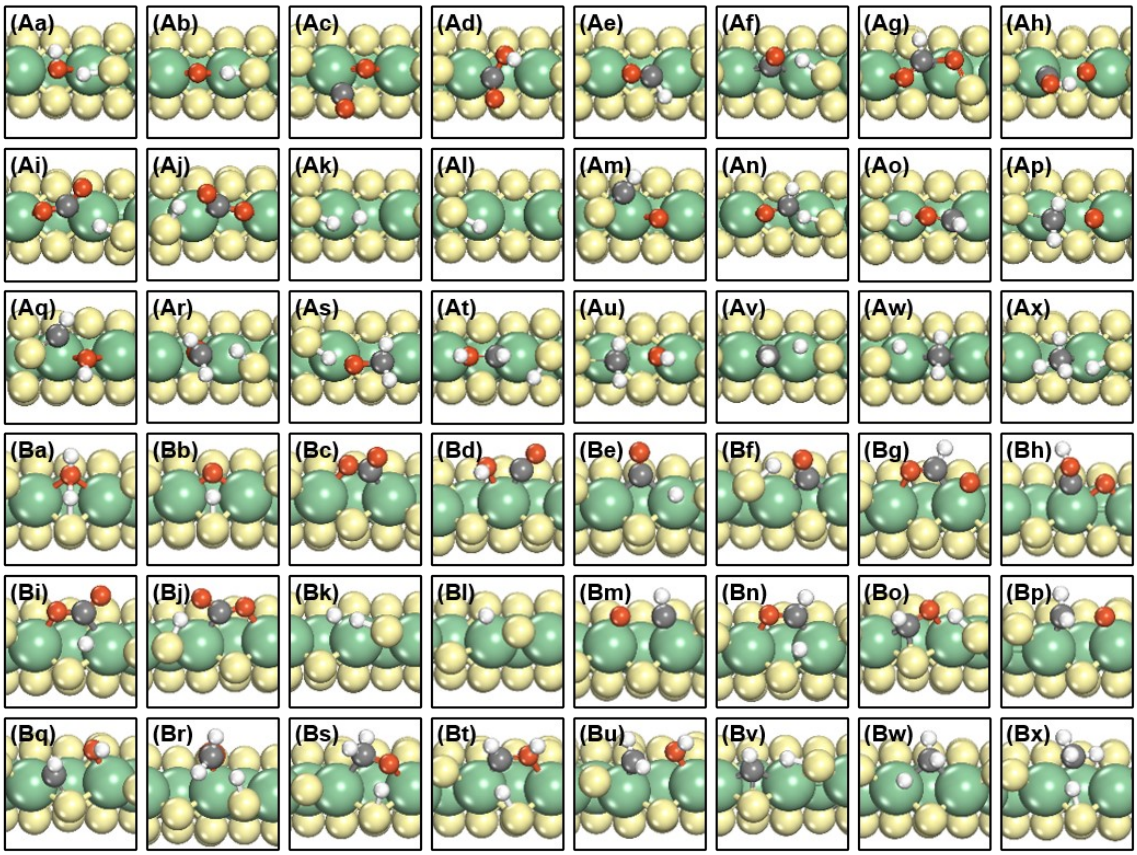


Table S5. The distance (in Å) between the atoms involved in bond formation and scission at the transition states of various elementary reactions on $MoS_{2-v}(001)$, $Cu/MoS_{2-v}(001)$, Mo and S edge. * and # denote the S vacancy and S site, respectively. Adsorbed and gaseous CH_4 are used for $MoS_{2-v}(001)$ and $Cu/MoS_{2-v}(001)$, respectively. Adsorbed and gaseous CO_2 are used for the Mo and S edge, respectively.

Elementary reactions	$MoS_{2-v}(001)$	$Cu/MoS_{2-v}(001)$
$H_2O^* + * = OH^* + H^*$	1.19	1.62
$OH^* + * = O^* + H^*$	1.32	1.49
$2OH^* = H_2O^* + O^*$	1.32	1.18
$CO^* + O^* = CO_2^* + *$	1.59	2.04
$CO^* + OH^* = COOH^* + *$	1.79	1.62
$CO^* + H^* = CHO^* + *$	1.16	1.18
$CO^* + H^* = COH^* + *$	1.35	1.38
$CHO^* + O^* = HCOO^* + *$	1.82	1.92
$COH^* + O^* = COOH^* + *$	1.37	1.87
$HCOO^* + * = CO_2^* + H^*$	1.59	1.65
$COOH^* + * = CO_2^* + H^*$	1.43	1.39
$2H^* = H_2 + 2^*$	0.76	0.77
$CHO^* + * = CH^* + O^*$	1.68	1.87
$CHO^* + H^* = CH_2O^* + *$	1.65	1.69
$CHO^* + H^* = CHOH^* + *$	1.39	1.37
$COH^* + H^* = CHOH^* + *$	1.57	1.59
$CH_2O^* + * = CH_2^* + O^*$	1.88	1.90
$CHOH^* + * = CH^* + OH^*$	1.99	2.04
$CH_2O^* + H^* = CH_3O^* + *$	1.53	1.94
$CH_2O^* + H^* = CH_2OH^* + *$	1.23	1.45
$CHOH^* + H^* = CH_2OH^* + *$	1.43	1.76
$CH_3O^* + * = CH_3^* + O^*$	2.13	2.49
$CH_2OH^* + * = CH_2^* + OH^*$	1.87	1.97
$CH^* + H^* = CH_2^* + *$	1.67	2.14
$CH_2^* + H^* = CH_3^* + *$	1.53	1.73

CH_3* + H* = CH_4* + */CH_4 + 2*	1.66	2.01

Elementary reactions	Mo edge	S edge
H_2O* + # = OH* + $H^{\#}$	1.45	1.27
OH* + # = O* + $H^{\#}$	1.93	1.40
CO* + O* = CO_2* + */CO_2 + 2*	1.77	1.35
CO* + OH* = COOH* + *	1.38	1.72
CO*+ $H^{\#}$ = CHO* + #	1.22	2.26
CO* + $H^{\#}$ = COH* + #	1.40	1.46
CHO* + O* = HCOO* + *	1.68	1.96
COH* + O* = COOH* + *	2.01	1.87
HCOO* + # = CO_2* + $H^{\#}$/CO_2 + * + $H^{\#}$	2.02	1.55
COOH*+ # = CO_2* + $H^{\#}$/CO_2 + * + $H^{\#}$	1.57	1.50
$H^{\#}$ + * = H* + #	1.56	1.82
H* + $H^{\#}$ = H_2* + #	1.52	
2H* = H_2 + 2*		1.51
CHO* + * = CH* + O*	2.20	2.08
CHO* + $H^{\#}$ = CH_2O* + #	1.44	1.75
CHO* + $H^{\#}$ = CHOH* + #	1.28	1.46
CH_2O* + * = CH_2* + O*	2.09	2.05
CHOH* + * = CH* + OH*	1.87	2.29
CH_2O* + $H^{\#}$ = CH_3O* + #	1.82	1.61
CH_2O* + $H^{\#}$ = CH_2OH* + #	1.47	1.35
CHOH* + $H^{\#}$ = CH_2OH* + #	2.18	1.64
CH_2OH* + * = CH_2* + OH*	2.12	2.14
CH* + $H^{\#}$ = CH_2* + #	1.74	1.81
CH_2* + $H^{\#}$ = CH_3* + #	2.10	1.87
CH_3* + $H^{\#}$ = CH_4* + #	1.69	1.57

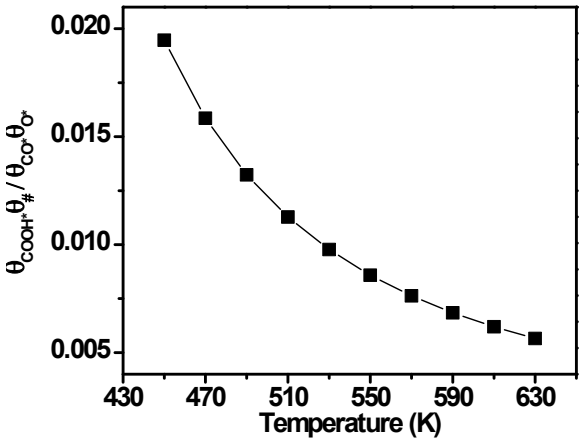
S7. Coverage of species via microkinetic modeling

Table S6. Coverage (in ML) of species on Cu/MoS_{2-v}(001), Mo edge, and S edge at 550 K, 1 bar and CO/H_2O ratio of 1 calculated via microkinetic modeling. * and # denote the S vacancy and S site, respectively.

Species	Cu/MoS_{2-v}(001)	Mo edge	S edge
H_2O*	2.59×10^{-7}	1.81×10^{-7}	4.57×10^{-5}
CO*	6.95×10^{-4}	3.50×10^{-4}	2.12×10^{-2}
OH*	9.87×10^{-1}	5.00×10^{-1}	2.55×10^{-3}
H*	7.09×10^{-4}	2.66×10^{-10}	3.61×10^{-3}
O*	5.23×10^{-5}	6.78×10^{-8}	1.45×10^{-4}
H_2*		7.05×10^{-14}	
CO_2*	2.88×10^{-16}	1.76×10^{-14}	
HCOO*	5.44×10^{-4}	7.86×10^{-19}	1.36×10^{-8}
COOH*	3.60×10^{-11}	4.07×10^{-13}	3.16×10^{-5}
CHO*	7.97×10^{-11}	9.16×10^{-13}	3.27×10^{-7}
COH*	9.78×10^{-9}	4.34×10^{-19}	7.73×10^{-8}
CH_2O*	3.21×10^{-15}	6.95×10^{-14}	7.34×10^{-11}
CHOH*	2.78×10^{-14}	2.88×10^{-19}	3.97×10^{-10}
CH_3O*	9.61×10^{-3}		
CH_2OH*	1.00×10^{-18}	5.42×10^{-16}	3.93×10^{-12}
CH*	1.86×10^{-7}	1.11×10^{-19}	2.74×10^{-5}
CH_2*	4.24×10^{-8}	1.02×10^{-20}	1.53×10^{-6}
CH_3*	1.38×10^{-6}	5.92×10^{-19}	7.45×10^{-7}
CH_4*		1.52×10^{-25}	1.65×10^{-13}
H#		2.56×10^{-6}	1.33×10^{-5}

S8. Ratio of coverage of intermediates and vacant sites as a function of temperature

Figure S5. Ratio of coverage of intermediates and vacant sites as a function of temperature on the Mo edge.



S9. Converged Cartesian coordinates for species adsorption and transition state

1. Adsorption of species on $MoS_{2-v}(001)$

H_2O*			
Mo	1.865918	-0.024101	1.536531
Mo	1.872142	3.175100	1.547184
Mo	1.852586	6.362945	1.508979
Mo	4.653085	-1.604457	1.531009
Mo	4.653906	1.568441	1.536973
Mo	4.645913	4.760103	1.524218
Mo	7.409243	-3.191099	1.505933
Mo	7.456942	-0.004055	1.488787
Mo	7.431788	3.144566	1.486572
Mo	10.189602	-4.806786	1.512377
Mo	10.201507	-1.553087	1.584649
Mo	10.162238	1.531707	1.434052
Mo	12.924484	-6.387918	1.528424
Mo	12.927818	-3.157791	1.503362
Mo	12.903257	-0.037811	1.436381
S	0.958710	1.582361	-0.013340
S	0.939681	4.751450	-0.045592
S	0.953541	7.968912	-0.071056
S	3.717102	-0.015794	-0.017943
S	3.714412	3.160801	-0.019736
S	3.724124	6.365706	-0.029981
S	6.493897	-1.583756	-0.049955
S	6.485120	1.543606	-0.060701
S	6.488451	4.767370	-0.046834
S	9.298948	-3.139284	-0.011907
S	9.278821	-0.086610	-0.043196
S	9.277287	3.168831	-0.084686
S	12.035040	-4.776633	-0.037775
S	11.948989	-1.620871	-0.029539
S	12.020622	1.602064	-0.089468
S	0.946870	1.569630	3.102952
S	0.916860	4.813105	3.088857
S	0.875460	7.914354	3.061835
S	3.718320	-0.025616	3.096413
S	3.731566	3.171538	3.097343
S	3.712469	6.361114	3.073801
S	6.548595	-1.580704	3.066414
S	6.559637	1.557074	3.067865
S	6.508057	4.748072	3.055198
S	9.233348	-3.226682	3.045250
S	12.006251	-4.742670	3.077897
S	11.949580	1.494528	3.025585
S	9.264356	3.082051	3.037223
O	10.724178	-0.991902	3.883424
H	11.688120	-1.150912	3.970969
H	10.275734	-1.680565	4.424652

CO*			
Mo	1.832724	0.001286	1.597303
Mo	1.838792	3.194391	1.604981
Mo	1.833130	6.383954	1.583372
Mo	4.622876	-1.582429	1.585383
Mo	4.622064	1.595246	1.589651
Mo	4.617540	4.791118	1.585383
Mo	7.403236	-3.151433	1.535964
Mo	7.417106	0.008455	1.499906
Mo	7.395721	3.173582	1.536217
Mo	10.140910	-4.765739	1.563392
Mo	10.127045	-1.563564	1.496643
Mo	10.120327	1.556455	1.488628
Mo	12.874258	-6.386640	1.590344
Mo	12.884964	-3.173858	1.558261
Mo	12.851521	-0.010504	1.524102
S	0.918770	1.600569	0.043469
S	0.932345	4.779879	0.019338
S	0.929717	7.980191	0.009251
S	3.680660	0.007912	0.038964
S	3.681966	3.190322	0.040055
S	3.687709	6.388040	0.031319
S	6.443406	-1.565857	-0.020555
S	6.439295	1.582415	-0.019211
S	6.449787	4.794632	0.004684
S	9.244659	-3.171438	-0.035300
S	9.216217	0.000402	-0.060482
S	9.240698	3.197525	-0.028186
S	11.983468	-4.789368	0.015935
S	11.963993	-1.610292	-0.042306
S	11.965069	1.617565	-0.030745
S	0.904717	1.589720	3.162452
S	0.892232	4.806887	3.147400
S	0.861127	7.963025	3.126062
S	3.692669	0.001753	3.151901
S	3.705642	3.195510	3.154181
S	3.692948	6.388641	3.143954
S	6.534672	-1.551327	3.102350
S	6.536131	1.567728	3.103255
S	6.497973	4.794781	3.101296
S	9.235179	-3.094295	3.098617
S	11.961440	-4.757614	3.136722
S	11.888094	1.517903	3.107062
S	9.223594	3.126068	3.085976
C	11.905846	-1.576384	2.873627
O	11.857421	-1.548399	4.080295

OH*			
Mo	1.840696	0.001918	1.619882
Mo	1.840710	3.189834	1.624426
Mo	1.829084	6.385038	1.591172
Mo	4.623671	-1.576914	1.605470
Mo	4.626689	1.595586	1.610674
Mo	4.609591	4.795263	1.600915
Mo	7.395628	-3.156706	1.546973
Mo	7.450771	0.025838	1.523337
Mo	7.387868	3.191764	1.537918
Mo	10.134727	-4.761990	1.533069
Mo	10.106569	-1.605490	1.426198
Mo	10.088291	1.590150	1.456268
Mo	12.875798	-6.391068	1.595682
Mo	12.882245	-3.179383	1.536913
Mo	12.854389	-0.005883	1.518833
S	0.927960	1.595112	0.060363
S	0.935795	4.764842	0.030349
S	0.925802	7.996402	0.025813
S	3.686909	0.010680	0.060722
S	3.682777	3.186740	0.059633
S	3.688237	6.396273	0.046069
S	6.445677	-1.554400	0.005504
S	6.441040	1.581213	-0.000761
S	6.430905	4.804764	0.010599
S	9.204514	-3.186069	-0.069343
S	9.209887	-0.009556	-0.086930
S	9.216970	3.214343	-0.055494
S	12.002016	-4.796956	0.009380
S	11.992515	-1.601319	-0.076750
S	11.989913	1.607882	-0.025641
S	0.900061	1.587028	3.178668
S	0.877592	4.805243	3.147852
S	0.853110	7.962690	3.132768
S	3.701469	0.004076	3.176575
S	3.706097	3.196014	3.173524
S	3.685455	6.392424	3.160023
S	6.548576	-1.542708	3.116504
S	6.553596	1.582655	3.120711
S	6.489189	4.800071	3.111401
S	9.242912	-3.085469	3.088666
S	11.949515	-4.752743	3.118036
S	11.854091	1.510308	3.092758
S	9.217289	3.144012	3.082176
O	11.908138	-1.584424	2.682342
H	11.893127	-1.596280	3.659289

H*			
Mo	1.820178	-0.011923	1.609836
Mo	1.826803	3.186094	1.621377
Mo	1.808693	6.372983	1.586255
Mo	4.618352	-1.584451	1.612328
Mo	4.617472	1.589846	1.616900
Mo	4.613729	4.793394	1.612689
Mo	7.416240	-3.139862	1.560323
Mo	7.433120	0.006003	1.521312
Mo	7.393625	3.182855	1.547533
Mo	10.152182	-4.747273	1.531754
Mo	10.161815	-1.574092	1.465367
Mo	10.133022	1.550378	1.447326
Mo	12.861410	-6.394878	1.587175
Mo	12.843484	-3.183542	1.512836
Mo	12.804616	0.000758	1.454567
S	0.921199	1.590911	0.058106
S	0.925940	4.763130	0.020085
S	0.926659	7.974767	0.001203
S	3.679287	0.002551	0.064508
S	3.681611	3.186929	0.068572
S	3.684678	6.384943	0.055575
S	6.443115	-1.560636	0.007941
S	6.435245	1.579834	0.006949
S	6.444182	4.810483	0.029730
S	9.236263	-3.145035	-0.050945
S	9.213637	-0.023182	-0.075047
S	9.218832	3.208438	-0.044579
S	11.993771	-4.800845	-0.012230
S	11.964236	-1.617346	-0.112152
S	11.974849	1.631542	-0.071766
S	0.884443	1.575731	3.171089
S	0.834596	4.806330	3.132132
S	0.785872	7.940902	3.099026
S	3.676555	-0.006517	3.175775
S	3.693324	3.193777	3.177583
S	3.666698	6.386346	3.161173
S	6.540268	-1.547289	3.125881
S	6.544401	1.572134	3.118484
S	6.506931	4.801776	3.121010
S	9.292619	-3.060654	3.093999
S	11.943574	-4.739458	3.121314
S	11.855273	1.463907	3.096669
S	9.247247	3.130466	3.058674
H	11.946956	-1.606824	2.428011

O*			
Mo	1.822417	-0.006480	1.615513
Mo	1.828287	3.187995	1.622423
Mo	1.828425	6.378867	1.594933
Mo	4.618918	-1.582655	1.611921
Mo	4.618401	1.593059	1.616736
Mo	4.614971	4.794078	1.610411
Mo	7.408093	-3.137305	1.557476
Mo	7.432483	0.017784	1.523636
Mo	7.395565	3.184948	1.550183
Mo	10.143075	-4.761118	1.554627
Mo	10.200293	-1.556149	1.463324
Mo	10.104003	1.561317	1.487957
Mo	12.873078	-6.392336	1.593948
Mo	12.850142	-3.130515	1.529595
Mo	12.822751	-0.059308	1.494297
S	0.921220	1.592984	0.057301
S	0.924965	4.769270	0.034835
S	0.923780	7.978643	0.021593
S	3.678441	0.004625	0.065712
S	3.680663	3.188284	0.067131
S	3.691300	6.387233	0.051683
S	6.441984	-1.558635	0.008376
S	6.436367	1.582136	0.007323
S	6.446084	4.809261	0.027388
S	9.234858	-3.155769	-0.030478
S	9.211133	-0.009864	-0.057919
S	9.230164	3.203366	-0.032503
S	11.993755	-4.789112	0.017142
S	11.967422	-1.615505	-0.162642
S	11.967431	1.608672	-0.029310
S	0.888827	1.582242	3.176870
S	0.853065	4.811694	3.146218
S	0.822717	7.942811	3.127076
S	3.679806	-0.002637	3.177745
S	3.693961	3.195986	3.177621
S	3.681970	6.386868	3.167125
S	6.540885	-1.541738	3.125488
S	6.542306	1.578765	3.125512
S	6.504751	4.805530	3.120632
S	9.277531	-3.062672	3.086730
S	11.962386	-4.734703	3.125452
S	11.873795	1.476396	3.090828
S	9.229214	3.139501	3.089259
O	11.922179	-1.567164	2.586962

CO_2*			
Mo	1.865598	0.007151	1.455460
Mo	1.874110	3.203916	1.466838
Mo	1.858686	6.393608	1.417364
Mo	4.664326	-1.560594	1.441346
Mo	4.662990	1.614754	1.449063
Mo	4.663788	4.813216	1.441507
Mo	7.462100	-3.114021	1.392461
Mo	7.471978	0.040889	1.353176
Mo	7.447684	3.206250	1.383504
Mo	10.209051	-4.723084	1.388242
Mo	10.218463	-1.512250	1.291547
Mo	10.156160	1.551496	1.310372
Mo	12.910469	-6.388903	1.452085
Mo	12.920196	-3.139563	1.378574
Mo	12.876887	-0.043259	1.328477
S	0.953646	1.606162	-0.085645
S	0.961864	4.772878	-0.138660
S	0.960355	7.997995	-0.156707
S	3.718410	0.027470	-0.100694
S	3.721223	3.208030	-0.097888
S	3.734595	6.406283	-0.115960
S	6.490146	-1.539491	-0.159423
S	6.480200	1.607599	-0.162582
S	6.500142	4.831325	-0.138088
S	9.295228	-3.117625	-0.202627
S	9.246723	0.002490	-0.246575
S	9.286794	3.227176	-0.190010
S	12.058624	-4.778057	-0.140907
S	12.019164	-1.614397	-0.232295
S	12.025661	1.613994	-0.191158
S	0.937349	1.593006	3.025133
S	0.900992	4.842485	2.984641
S	0.855012	7.938815	2.956602
S	3.727871	0.015983	3.010094
S	3.745100	3.217957	3.012329
S	3.720455	6.405970	2.988694
S	6.583397	-1.521513	2.954734
S	6.587493	1.600785	2.953656
S	6.556526	4.825769	2.952802
S	9.361375	-3.014886	2.915449
S	12.003858	-4.706294	2.971953
S	11.886029	1.417939	2.939245
S	9.291922	3.153660	2.909697
C	10.966359	-1.031379	5.823473
O	12.071551	-1.433137	5.862251
O	9.860678	-0.631009	5.782981

HCOO*			
Mo	1.884326	-0.001407	1.610915
Mo	1.890507	3.185980	1.610180
Mo	1.870528	6.378436	1.593884
Mo	4.667097	-1.586145	1.590116
Mo	4.672400	1.586752	1.589907
Mo	4.653605	4.785703	1.582592
Mo	7.433359	-3.168886	1.526642
Mo	7.492831	-0.010893	1.506251
Mo	7.436148	3.178015	1.519265
Mo	10.181047	-4.759681	1.531059
Mo	10.118277	-1.600641	1.443163
Mo	10.163854	1.594418	1.433645
Mo	12.928045	-6.381206	1.590155
Mo	12.925473	-3.175264	1.571966
Mo	12.892240	0.008362	1.535679
S	0.973701	1.593512	0.048951
S	0.962633	4.769946	0.037043
S	0.956254	7.988325	0.032409
S	3.725444	0.001024	0.045146
S	3.726647	3.179800	0.038792
S	3.721000	6.388121	0.035250
S	6.484279	-1.566262	-0.018589
S	6.491116	1.567193	-0.017813
S	6.474234	4.788309	-0.009573
S	9.257248	-3.181979	-0.074056
S	9.263207	-0.007642	-0.094949
S	9.268297	3.219263	-0.069780
S	12.052514	-4.774467	0.017320
S	12.021727	-1.595544	-0.036181
S	12.055044	1.612231	-0.034303
S	0.954335	1.588844	3.172291
S	0.947471	4.785422	3.152094
S	0.904610	7.963931	3.136611
S	3.749000	-0.000847	3.160533
S	3.757538	3.187042	3.155874
S	3.737444	6.382994	3.148314
S	6.587366	-1.564272	3.105242
S	6.599268	1.561478	3.094544
S	6.531571	4.783489	3.092548
S	9.255591	-3.108149	3.090448

S	11.993963	-4.765335	3.125231
S	11.904822	1.549455	3.097064
S	9.267509	3.135763	3.062388
C	11.785342	-1.461095	4.173095
O	12.448207	-2.084926	4.949790
O	11.908753	-1.595577	2.767896
H	11.004441	-0.716695	4.406509

COOH*

Mo	1.882032	-0.044832	1.621151
Mo	1.884155	3.136110	1.627886
Mo	1.870511	6.330521	1.615784
Mo	4.639892	-1.653252	1.561935
Mo	4.647890	1.526776	1.564898
Mo	4.629459	4.712690	1.560729
Mo	7.373224	-3.268734	1.496978
Mo	7.428794	-0.103801	1.476990
Mo	7.413046	3.095209	1.530945
Mo	10.156980	-4.823413	1.597293
Mo	9.918866	-1.615841	1.529588
Mo	10.181849	1.522378	1.514754
Mo	12.926853	-6.405527	1.650102
Mo	12.934986	-3.207207	1.677690
Mo	12.928642	-0.027225	1.654358
S	0.943597	1.554002	0.072677
S	0.916498	4.731261	0.082853
S	0.923078	7.932755	0.072775
S	3.692700	-0.055710	0.023492
S	3.687843	3.118598	0.020686
S	3.684652	6.319486	0.019479
S	6.441274	-1.647516	-0.058295
S	6.467881	1.513781	-0.037301
S	6.450203	4.679648	-0.031963
S	9.240423	-3.290907	-0.050467
S	9.236355	-0.000189	-0.072997
S	9.289400	3.140672	-0.001089
S	12.041246	-4.788772	0.098744
S	11.932720	-1.630853	0.166846
S	12.064098	1.552993	0.057602
S	0.973380	1.545973	3.199400
S	0.996012	4.728264	3.199140
S	0.981029	7.940323	3.186007
S	3.754857	-0.058760	3.145485
S	3.759439	3.121702	3.148473
S	3.746038	6.320684	3.139893
S	6.543205	-1.655696	3.082245
S	6.558561	1.469340	3.079011
S	6.486742	4.701108	3.082085
S	9.120081	-3.236289	3.119711
S	11.971401	-4.803228	3.198820
S	11.958498	1.554666	3.175844
S	9.232242	3.056801	3.110044
C	11.145003	-1.317903	3.223505
O	12.405963	-1.667738	3.192018
O	10.779271	-0.930525	4.444834
H	9.837972	-0.648354	4.393313

CHO*

Mo	1.819723	-0.016632	1.578047
Mo	1.820861	3.186878	1.566289
Mo	1.798054	6.372782	1.538774
Mo	4.608481	-1.591481	1.585313
Mo	4.587029	1.597868	1.577705
Mo	4.592355	4.788951	1.568749
Mo	7.386739	-3.177260	1.560807
Mo	7.387594	0.041707	1.573783
Mo	7.356610	3.195210	1.532782
Mo	10.143839	-4.801771	1.473893
Mo	10.226418	-1.674373	1.516970
Mo	10.092672	1.575458	1.500181
Mo	12.883067	-6.402239	1.539525
Mo	12.866503	-3.177760	1.470990
Mo	12.848384	-0.060915	1.497335
S	0.928722	1.577053	0.009037
S	0.914878	4.760532	-0.039138
S	0.893112	7.979793	-0.020521
S	3.673158	-0.008358	0.026658
S	3.670919	3.188361	0.012628
S	3.678652	6.390408	0.013669
S	6.450621	-1.573774	0.024603
S	6.423866	1.589720	0.000434
S	6.429486	4.808333	-0.002826
S	9.208014	-3.181321	-0.055944
S	9.218232	-0.073503	0.020193
S	9.182097	3.165150	-0.062121
S	12.011035	-4.809613	-0.070487
S	11.972538	-1.618372	-0.085871
S	11.985333	1.563040	-0.043064
S	0.892308	1.585614	3.127560
S	0.830636	4.814186	3.089269
S	0.828971	7.917593	3.102834
S	3.666553	-0.007104	3.142971
S	3.659494	3.201471	3.134009
S	3.646767	6.377783	3.120704
S	6.496543	-1.574238	3.131508
S	6.436340	1.624328	3.121454
S	6.457807	4.789377	3.111628
S	9.285368	-3.258488	3.060014
S	11.956211	-4.742679	3.054354
S	11.919635	1.512192	3.064561
S	9.224892	3.197013	3.050636
C	9.069621	0.356372	3.113415
O	9.829853	-0.687080	3.323333
H	8.770225	0.847730	4.056959

COH*

Mo	1.839405	-0.020802	1.585808
Mo	1.841692	3.170223	1.597262
Mo	1.855939	6.355964	1.583134
Mo	4.631405	-1.603399	1.583939
Mo	4.629205	1.574440	1.588681
Mo	4.629243	4.771363	1.588583
Mo	7.416755	-3.164264	1.536209
Mo	7.421351	-0.006052	1.493444
Mo	7.402730	3.157012	1.529957
Mo	10.150407	-4.793378	1.548945
Mo	10.168575	-1.563615	1.487365
Mo	10.125793	1.541566	1.460151
Mo	12.875000	-6.410619	1.577188
Mo	12.882170	-3.189830	1.537370
Mo	12.842429	-0.035743	1.486107
S	0.922296	1.577886	0.034324
S	0.956885	4.764130	0.012600
S	0.954085	7.949177	0.002051
S	3.691793	-0.012493	0.034294
S	3.691896	3.169871	0.041273
S	3.703931	6.363697	0.029828
S	6.451437	-1.586609	-0.022922
S	6.442790	1.564997	-0.024626
S	6.459822	4.782688	0.007252
S	9.254789	-3.174685	-0.033381
S	9.218710	-0.021060	-0.072643
S	9.235920	3.186184	-0.049405
S	11.974479	-4.822666	-0.003519
S	11.969813	-1.632118	-0.095445
S	11.962230	1.609128	-0.059480
S	0.903342	1.564827	3.150225
S	0.886034	4.782321	3.138979
S	0.855345	7.938618	3.104959
S	3.694489	-0.019653	3.146869
S	3.705959	3.172810	3.151689
S	3.707099	6.366596	3.147106
S	6.541595	-1.566862	3.098309
S	6.542546	1.550668	3.097964
S	6.512812	4.777054	3.102821
S	9.273339	-3.100608	3.077252
S	11.967357	-4.770730	3.127882
S	11.880464	1.470021	3.096747
S	9.235616	3.105153	3.067586
C	12.041003	-1.631625	2.697417
O	11.922156	-1.606983	4.044868
H	11.790943	-0.678139	4.353523

CH_2O*

Mo	1.863028	0.005476	1.578813
Mo	1.866399	3.181212	1.591564
Mo	1.866104	6.380343	1.569830
Mo	4.624914	-1.595140	1.511937
Mo	4.635129	1.580007	1.523103
Mo	4.613929	4.763935	1.517768
Mo	7.347886	-3.203946	1.470658
Mo	7.409883	-0.013179	1.445076
Mo	7.398721	3.149436	1.503239
Mo	10.138373	-4.774841	1.621963
Mo	9.956787	-1.560724	1.578559
Mo	10.112448	1.547475	1.559146
Mo	12.891142	-6.371911	1.648360
Mo	12.943608	-3.152063	1.674903
Mo	12.923532	-0.018958	1.631921
S	0.895265	1.601075	0.048106
S	0.898353	4.776757	0.049355
S	0.902809	7.980193	0.027356
S	3.673194	0.000955	-0.023104
S	3.666371	3.168578	-0.019958
S	3.676550	6.370815	-0.029845
S	6.441298	-1.580816	-0.093112
S	6.461281	1.572103	-0.078904
S	6.444328	4.737292	-0.065841
S	9.247369	-3.211289	-0.012167
S	9.241062	0.021049	-0.062616
S	9.296358	3.180447	0.007903
S	12.014766	-4.742558	0.109810
S	11.898139	-1.604295	0.154942
S	11.992410	1.595400	0.065120
S	0.958007	1.588432	3.168736
S	1.013974	4.781336	3.173151
S	0.990090	7.989977	3.149981
S	3.737413	-0.007296	3.099306
S	3.744625	3.170905	3.107006
S	3.738175	6.376613	3.092627
S	6.513698	-1.576489	3.038080
S	6.534050	1.536389	3.054594
S	6.461749	4.758649	3.049445
S	9.067553	-3.172836	3.100822
S	11.969892	-4.751289	3.206132
S	11.924809	1.544034	3.155932
S	9.184506	3.117452	3.121884
C	11.161106	-1.537126	3.455328
O	12.514777	-1.545529	3.053510
H	11.025493	-2.383021	4.146645
H	10.921390	-0.610719	4.004407

CHOH*

Mo	1.838437	0.031041	1.583115
Mo	1.837142	3.222424	1.589426
Mo	1.852192	6.418537	1.576139
Mo	4.634195	-1.559403	1.570311
Mo	4.626153	1.615265	1.572128
Mo	4.622731	4.811193	1.571594
Mo	7.409541	-3.134535	1.518069
Mo	7.429931	0.016310	1.484630
Mo	7.404192	3.185051	1.517469
Mo	10.132052	-4.754350	1.525851
Mo	10.141892	-1.563056	1.430067
Mo	10.138107	1.566668	1.474511
Mo	12.874375	-6.342851	1.568617
Mo	12.839221	-3.106766	1.537138
Mo	12.869923	0.023338	1.499619
S	0.921824	1.633289	0.027046
S	0.928438	4.821702	0.020267
S	0.950289	8.003931	0.001883
S	3.684895	0.030014	0.022769
S	3.681089	3.214108	0.026198
S	3.698173	6.409554	0.016870
S	6.452025	-1.543163	-0.040619
S	6.446516	1.593115	-0.034829
S	6.453997	4.807207	-0.008258
S	9.227468	-3.173367	-0.082857
S	9.225665	0.021563	-0.095338
S	9.243261	3.194265	-0.052666
S	11.980408	-4.747463	-0.004723
S	11.976557	-1.559731	-0.095122
S	11.969361	1.656212	-0.045028
S	0.902209	1.623334	3.143371
S	0.878554	4.840878	3.121203
S	0.871865	7.996912	3.115151
S	3.699052	0.026138	3.135281
S	3.706486	3.216322	3.136841
S	3.711134	6.413709	3.131731
S	6.545566	-1.536274	3.085724
S	6.540709	1.580287	3.079907
S	6.506149	4.811034	3.083122
S	9.249391	-3.084679	3.058207
S	11.942086	-4.714077	3.111371
S	11.917183	1.558725	3.094065
S	9.234781	3.142657	3.061594
C	12.006909	-1.523663	2.869936
O	12.163240	-1.631162	4.238792
H	12.907186	-2.243890	4.426702
H	10.994194	-0.887259	2.935032

CH_3O*

Mo	1.861844	0.006092	1.603267
Mo	1.864505	3.190667	1.606564
Mo	1.850410	6.387325	1.585520
Mo	4.642973	-1.575630	1.588571
Mo	4.649276	1.596110	1.589043
Mo	4.628771	4.796157	1.581291
Mo	7.409893	-3.157101	1.531850
Mo	7.472639	0.021911	1.513723
Mo	7.410229	3.193133	1.520021
Mo	10.154141	-4.758224	1.527445
Mo	10.132924	-1.600936	1.451756
Mo	10.112338	1.600248	1.448893
Mo	12.902019	-6.382409	1.578604
Mo	12.898386	-3.166762	1.553228
Mo	12.870302	-0.006935	1.533357
S	0.950129	1.598799	0.039497
S	0.944344	4.774117	0.029466
S	0.934830	7.992924	0.024137
S	3.705446	0.009576	0.041563
S	3.703512	3.188611	0.037614
S	3.701735	6.397993	0.030911
S	6.467253	-1.552669	-0.010635
S	6.468833	1.578748	-0.017627
S	6.451124	4.805016	-0.008876
S	9.234688	-3.172184	-0.065292
S	9.243753	-0.014320	-0.079820
S	9.243789	3.220301	-0.068792
S	12.024047	-4.777659	0.006568
S	12.006532	-1.596388	-0.051362
S	12.015694	1.604287	-0.030359
S	0.925821	1.592266	3.163002
S	0.913986	4.798154	3.140944
S	0.885486	7.974231	3.126421
S	3.724040	0.008473	3.157176
S	3.730971	3.194301	3.152452
S	3.711436	6.392891	3.146126
S	6.564737	-1.544029	3.103164
S	6.574865	1.584447	3.102321
S	6.503389	4.796733	3.094478
S	9.237755	-3.098863	3.082709
S	11.971423	-4.761546	3.110201
S	11.880158	1.538962	3.081531
S	9.233487	3.149504	3.073089
C	11.911054	-1.569425	4.214672
O	11.928616	-1.578127	2.757039
H	12.947445	-1.580449	4.577261
H	11.396689	-0.660391	4.548983
H	11.378423	-2.461558	4.566517

CH_2OH*

Mo	1.866300	-0.003285	1.572169
Mo	1.860269	3.166322	1.588153
Mo	1.843564	6.364998	1.565697
Mo	4.607906	-1.618581	1.509647
Mo	4.627517	1.557574	1.514266
Mo	4.595350	4.739098	1.506208
Mo	7.316558	-3.245458	1.470877
Mo	7.405207	-0.066545	1.462044
Mo	7.382299	3.125123	1.496713
Mo	10.119794	-4.795795	1.608791
Mo	9.878309	-1.592544	1.642810
Mo	10.149927	1.559995	1.511139
Mo	12.893334	-6.371638	1.637908
Mo	12.921104	-3.192505	1.669767
Mo	12.916801	0.043292	1.616679
S	0.900583	1.593627	0.040541
S	0.875610	4.759978	0.046550
S	0.897455	7.976943	0.020301
S	3.670553	-0.018437	-0.032967

S	3.654585	3.145016	-0.031486
S	3.652821	6.351084	-0.033792
S	6.425754	-1.609674	-0.090296
S	6.461166	1.538955	-0.075395
S	6.424325	4.706283	-0.078210
S	9.230065	-3.218766	0.002628
S	9.242758	-0.017708	-0.041306
S	9.268976	3.177686	-0.015990
S	12.000187	-4.749174	0.095614
S	11.863235	-1.590387	0.241099
S	12.024889	1.606922	0.032033
S	0.959081	1.577070	3.162185
S	0.992453	4.762000	3.167770
S	0.983466	7.988551	3.142090
S	3.737340	-0.022206	3.094748
S	3.739780	3.147308	3.098487
S	3.719644	6.351229	3.084880
S	6.491638	-1.619993	3.049062
S	6.525346	1.506720	3.048998
S	6.431066	4.718842	3.044449
S	9.002363	-3.247456	3.125711
S	11.943301	-4.773999	3.197661
S	11.917415	1.574224	3.158610
S	9.182484	3.082016	3.102817
C	10.982569	-1.502925	3.575980
O	12.411633	-1.535827	3.188492
H	10.787069	-0.552679	4.093243
H	10.866373	-2.328386	4.290249
H	13.035893	-1.512150	3.956325

CH*

Mo	1.822237	-0.004565	1.600484
Mo	1.830267	3.193628	1.603561
Mo	1.841823	6.379866	1.584189
Mo	4.619993	-1.579596	1.602014
Mo	4.611669	1.603602	1.606452
Mo	4.619408	4.797700	1.600526
Mo	7.411370	-3.137538	1.550956
Mo	7.393137	0.021685	1.514077
Mo	7.394070	3.179677	1.548670
Mo	10.129758	-4.778688	1.572276
Mo	10.189689	-1.582605	1.488632
Mo	10.124214	1.588309	1.486198
Mo	12.869515	-6.388978	1.586230
Mo	12.881116	-3.150649	1.526647
Mo	12.826783	-0.034329	1.486448
S	0.913614	1.595104	0.045848
S	0.951444	4.782919	0.010110
S	0.937775	7.973036	0.007310
S	3.675774	0.010242	0.052653
S	3.682190	3.196692	0.052209
S	3.698822	6.391976	0.039992
S	6.437837	-1.560659	-0.006012
S	6.425717	1.592411	-0.007788
S	6.454466	4.807937	0.024095
S	9.240509	-3.181569	-0.029153
S	9.212947	0.007546	-0.026264
S	9.228838	3.207622	-0.032808
S	11.965844	-4.802705	0.011682
S	11.965253	-1.617848	-0.127309
S	11.954410	1.628708	-0.045023
S	0.892870	1.588194	3.160369
S	0.870526	4.813142	3.139144
S	0.821457	7.943399	3.114584
S	3.674372	0.003802	3.161908
S	3.687661	3.205073	3.164353
S	3.688419	6.390537	3.155881
S	6.528457	-1.543200	3.115084
S	6.515933	1.580163	3.116232
S	6.503883	4.805804	3.118416
S	9.277493	-3.081737	3.095742
S	11.970017	-4.737475	3.123068
S	11.888516	1.494767	3.098801
S	9.224550	3.132510	3.094700
C	11.952307	-1.605959	2.640051
H	11.900911	-1.597145	3.737300

CH_2*

Mo	1.833027	0.007820	1.603467
Mo	1.834583	3.206320	1.608597
Mo	1.812564	6.393774	1.571257
Mo	4.618734	-1.574634	1.598161
Mo	4.617233	1.601963	1.602445
Mo	4.611351	4.800258	1.598360
Mo	7.389457	-3.168356	1.559143
Mo	7.439348	-0.003434	1.541456
Mo	7.381271	3.204734	1.561953
Mo	10.161614	-4.736856	1.529626
Mo	10.155677	-1.536258	1.477661
Mo	10.155547	1.574975	1.480870
Mo	12.889585	-6.370222	1.580587
Mo	12.868387	-3.139073	1.525810
Mo	12.850392	-0.016377	1.503808
S	0.935473	1.609297	0.047151
S	0.914685	4.780560	0.008124
S	0.915243	8.000691	0.000646
S	3.683594	0.015776	0.046734
S	3.683354	3.198862	0.050248
S	3.687765	6.396846	0.038937
S	6.449277	-1.580257	0.015274
S	6.446939	1.602438	0.017261
S	6.438828	4.799756	0.015351
S	9.217687	-3.147353	-0.038996
S	9.218606	-0.002692	-0.099165
S	9.206994	3.225227	-0.022661
S	12.015482	-4.760745	-0.015837
S	11.971819	-1.586396	-0.054963
S	12.024352	1.607602	-0.042198
S	0.905220	1.603107	3.165345
S	0.851170	4.839119	3.127941
S	0.832416	7.947472	3.118271
S	3.687599	0.007325	3.165698
S	3.692481	3.206490	3.164806
S	3.668708	6.398447	3.145228
S	6.509655	-1.566114	3.132493
S	6.507852	1.585645	3.125148
S	6.481803	4.802713	3.134425
S	9.284834	-3.120766	3.076372
S	11.962706	-4.709989	3.108481
S	11.920990	1.522176	3.098815
S	9.257817	3.182516	3.070345
C	9.259276	0.101347	2.782792
H	8.960500	0.438165	3.786804
H	10.026941	-0.676637	3.199807

CH_3*

Mo	1.844115	0.005309	1.588650
Mo	1.856514	3.210562	1.586926
Mo	1.838460	6.392026	1.550657
Mo	4.621987	-1.574043	1.581961
Mo	4.629632	1.603561	1.599029
Mo	4.627632	4.798914	1.578850
Mo	7.398775	-3.162399	1.547885
Mo	7.434301	0.016503	1.577902
Mo	7.399251	3.208169	1.566016
Mo	10.178471	-4.737729	1.544624
Mo	10.141176	-1.521224	1.487402
Mo	10.131776	1.591771	1.570820
Mo	12.908050	-6.358439	1.578536
Mo	12.930738	-3.124562	1.509351
Mo	12.893404	-0.048990	1.518870
S	0.938644	1.606902	0.033976
S	0.945094	4.779712	-0.020013
S	0.921580	8.002214	-0.012886
S	3.694243	0.020413	0.032742
S	3.705604	3.193016	0.031765
S	3.708196	6.396180	0.015023
S	6.468650	-1.557458	0.018949
S	6.470323	1.591727	0.030346
S	6.464428	4.797190	0.005353
S	9.241236	-3.151329	-0.033881
S	9.212569	0.044784	-0.032982
S	9.247215	3.202878	0.006343
S	12.018464	-4.763218	-0.014556
S	11.968646	-1.586636	-0.038910
S	11.982487	1.607919	0.007556
S	0.930925	1.612411	3.147630
S	0.891381	4.847589	3.125568
S	0.871174	7.931200	3.121390
S	3.690705	0.005636	3.152162
S	3.703186	3.212228	3.148956
S	3.682216	6.394142	3.125665
S	6.479787	-1.586481	3.125357
S	6.505207	1.606959	3.140991
S	6.486702	4.812721	3.122742
S	9.284841	-3.122140	3.072583
S	12.005047	-4.682913	3.102299
S	12.002253	1.533283	3.102849
S	9.246622	3.250496	3.107824
C	9.258075	-0.053347	3.036204
H	9.697673	0.920735	3.425896
H	8.590282	-0.265645	3.886434
H	10.157703	-0.747900	3.295615

CH_4*

Mo	1.894328	-0.004260	1.409264
Mo	1.903023	3.193544	1.416706
Mo	1.886043	6.383198	1.367636
Mo	4.695864	-1.576528	1.387086
Mo	4.692475	1.598611	1.395047
Mo	4.692230	4.798948	1.382637
Mo	7.493112	-3.125544	1.322665
Mo	7.505774	0.029992	1.285538
Mo	7.473055	3.197328	1.311389
Mo	10.237235	-4.731237	1.319029
Mo	10.248802	-1.521095	1.220725
Mo	10.185048	1.544336	1.238648
Mo	12.938584	-6.398104	1.394179
Mo	12.947703	-3.147193	1.319186
Mo	12.903168	-0.053130	1.271090
S	0.987359	1.595090	-0.134645
S	0.993423	4.762015	-0.190203
S	0.990780	7.990497	-0.206081
S	3.742553	0.010276	-0.149586
S	3.745835	3.190018	-0.151244
S	3.758497	6.393852	-0.170232
S	6.516448	-1.549446	-0.222539
S	6.501576	1.593205	-0.226411
S	6.521461	4.821926	-0.206486
S	9.326536	-3.127181	-0.274774
S	9.277004	-0.004920	-0.318625
S	9.314686	3.220661	-0.262648
S	12.093870	-4.787055	-0.204051
S	12.054459	-1.622583	-0.297029
S	12.061863	1.605570	-0.254853
S	0.961228	1.585502	2.974820
S	0.923952	4.833655	2.931505
S	0.876669	7.926117	2.906618
S	3.762393	-0.001865	2.959136
S	3.779425	3.203555	2.957829
S	3.752079	6.389369	2.933453
S	6.623890	-1.534332	2.890480
S	6.624418	1.590549	2.888933
S	6.588477	4.815762	2.885595
S	9.391835	-3.020683	2.843981
S	12.025739	-4.715276	2.909254
S	11.905823	1.408959	2.875149
S	9.317590	3.145948	2.836956
C	11.415011	-1.486328	6.092566
H	10.653797	-1.022440	5.452913
H	10.981382	-1.707338	7.076054
H	12.261853	-0.798939	6.210198
H	11.762862	-2.417315	5.628308

2. Adsorption of species on $Cu/MoS_{2-v}(001)$

H_2O*

Mo	1.803835	0.036409	1.599474
Mo	1.816863	3.226983	1.594258
Mo	1.799184	6.414314	1.544264
Mo	4.558066	-1.552740	1.607676
Mo	4.567374	1.641221	1.624592
Mo	4.574199	4.807835	1.596028
Mo	7.287724	-3.129884	1.547346
Mo	7.271910	0.031828	1.606410
Mo	7.350313	3.209703	1.589094
Mo	10.098485	-4.737904	1.512210
Mo	10.126140	1.626267	1.553814
Mo	12.854184	-6.337196	1.575586
Mo	12.944567	-3.133266	1.415394
Mo	12.902550	0.030921	1.446609
Cu	10.369092	-1.898221	1.227913
S	0.888020	1.629946	0.038421
S	0.974518	4.776692	-0.055157
S	0.935467	8.056049	-0.036668
S	3.650535	0.051385	0.053304
S	3.662845	3.211300	0.040642
S	3.673991	6.416108	0.024956
S	6.380017	-1.532098	0.031192
S	6.401190	1.604856	0.042678
S	6.401994	4.797173	0.019889
S	9.075782	-3.282846	-0.140856
S	9.222937	-0.116547	0.217123
S	9.184946	3.178650	0.002753
S	11.944983	-4.782019	-0.041102
S	12.075674	-1.560880	-0.094161
S	11.926149	1.658112	-0.019708
S	0.868949	1.638789	3.153445
S	0.834826	4.866253	3.101477
S	0.824281	7.961140	3.106421
S	3.629006	0.036749	3.174447
S	3.639420	3.239882	3.175625
S	3.617531	6.405119	3.138511
S	6.396497	-1.569974	3.163158
S	6.415130	1.642884	3.178987
S	6.439722	4.833505	3.137638
S	9.300358	-2.931345	2.955237
S	11.951839	-4.629435	3.060284
S	11.948148	1.536078	3.104249
S	9.224893	3.243268	3.109153
O	9.078645	0.128048	3.115447
H	9.471515	-0.799548	3.190851
H	8.868142	0.469744	4.011641

CO*

Mo	1.814183	0.015054	1.607238
Mo	1.822488	3.187700	1.613171
Mo	1.848842	6.386454	1.604262
Mo	4.584082	-1.586520	1.596264
Mo	4.589858	1.607715	1.608989
Mo	4.584288	4.786346	1.593914
Mo	7.316928	-3.165667	1.498015
Mo	7.305383	0.029465	1.493561
Mo	7.357283	3.173867	1.550261
Mo	10.076819	-4.780252	1.526345
Mo	10.088244	1.639708	1.501645
Mo	12.850113	-6.370388	1.590871
Mo	12.906214	-3.153134	1.514196
Mo	12.879508	0.002495	1.531254
Cu	10.312323	-1.855096	1.234951
S	0.889439	1.605132	0.043966
S	0.968587	4.786434	0.029520
S	0.949841	7.977049	0.028853
S	3.651281	0.013488	0.050375
S	3.653767	3.187642	0.046732
S	3.671629	6.387523	0.032987
S	6.379850	-1.590187	-0.024413
S	6.383114	1.591095	-0.016723
S	6.391561	4.761882	-0.006776
S	9.100177	-3.323638	-0.158404

S	9.249696	-0.109905	0.213312
S	9.188359	3.184766	-0.044316
S	11.942069	-4.791228	0.004342
S	12.106287	-1.599789	-0.105836
S	11.949819	1.616699	-0.008961
S	0.871271	1.600266	3.170207
S	0.888695	4.794032	3.151957
S	0.882406	7.987042	3.148817
S	3.665135	0.007974	3.164616
S	3.673888	3.198554	3.173079
S	3.685018	6.384709	3.169505
S	6.489590	-1.544271	3.108422
S	6.483217	1.584165	3.134056
S	6.467193	4.806867	3.102671
S	9.267569	-2.988723	2.932305
S	11.924507	-4.711487	3.102715
S	11.870054	1.541275	3.114645
S	9.184198	3.177038	3.109138
C	12.327807	-1.539334	3.001582
O	11.988885	-1.575534	4.137951

OH*

Mo	1.831061	-0.017612	1.649109
Mo	1.836495	3.169955	1.654922
Mo	1.839977	6.362757	1.633382
Mo	4.614836	-1.585596	1.574937
Mo	4.595176	1.607319	1.589300
Mo	4.597797	4.793581	1.583979
Mo	7.389885	-3.176142	1.461424
Mo	7.345544	0.126337	1.381677
Mo	7.365017	3.209353	1.483755
Mo	10.171905	-4.804534	1.542037
Mo	10.019934	1.629562	1.437862
Mo	12.871045	-6.432478	1.643422
Mo	12.907553	-3.240299	1.644165
Mo	12.872046	-0.092580	1.606163
Cu	9.744005	-1.496436	1.156205
S	0.908865	1.566210	0.096161
S	0.912166	4.749989	0.084208
S	0.902501	7.956379	0.079782
S	3.643242	-0.001682	0.053669
S	3.632469	3.193108	0.052213
S	3.654343	6.383688	0.039767
S	6.402294	-1.580428	-0.066305
S	6.334378	1.656864	-0.087549
S	6.387993	4.798346	-0.045080
S	9.161606	-3.295896	-0.175812
S	9.102198	0.154162	-0.171468
S	9.234528	3.250059	-0.092075
S	12.037037	-4.824850	0.060576
S	11.847748	-1.661625	0.154445
S	11.989094	1.536854	0.034964
S	0.902745	1.561713	3.216145
S	0.930159	4.767616	3.216029
S	0.888568	7.943800	3.191345
S	3.720165	-0.005764	3.166778
S	3.715927	3.193913	3.175893
S	3.720760	6.390520	3.163748
S	6.579520	-1.502135	3.018815
S	6.530824	1.608843	3.069387
S	6.503515	4.823209	3.064905
S	9.327866	-2.952285	2.886348
S	11.934881	-4.814746	3.184892
S	11.786176	1.463587	3.103506
S	9.169149	3.161056	3.067793
O	12.150636	-1.651806	2.881058
H	12.505835	-1.640521	3.792494

H*

Mo	1.822903	-0.026531	1.648272
Mo	1.827186	3.171787	1.660064
Mo	1.838055	6.361875	1.622095
Mo	4.618956	-1.586625	1.590786
Mo	4.594767	1.609515	1.611730
Mo	4.603260	4.795513	1.603637
Mo	7.401207	-3.172151	1.490658
Mo	7.349353	0.127895	1.404594
Mo	7.371034	3.210271	1.512738
Mo	10.182440	-4.806291	1.541014
Mo	10.031335	1.625728	1.442945
Mo	12.869522	-6.436284	1.623445
Mo	12.904547	-3.219646	1.590517
Mo	12.889582	-0.113929	1.545536
Cu	9.820627	-1.512412	1.182540
S	0.912942	1.565963	0.094353
S	0.921570	4.744731	0.069394
S	0.924030	7.952221	0.052795
S	3.652445	0.001336	0.068180
S	3.639702	3.194789	0.072124
S	3.672641	6.382188	0.048335
S	6.416347	-1.585924	-0.040618
S	6.338053	1.661078	-0.058266
S	6.402025	4.801613	-0.016739
S	9.169622	-3.290308	-0.156244
S	9.102435	0.132037	-0.140962
S	9.224428	3.246549	-0.079865
S	12.024065	-4.838283	0.033435
S	11.861599	-1.665671	0.103066
S	11.969091	1.550611	0.002600
S	0.888843	1.554331	3.211128
S	0.897104	4.786866	3.201355
S	0.861870	7.922112	3.180076
S	3.704356	-0.011925	3.177354
S	3.702827	3.198340	3.192036
S	3.708091	6.392076	3.172082
S	6.581808	-1.500912	3.041967
S	6.531461	1.610433	3.098483
S	6.509733	4.826893	3.091069
S	9.359379	-2.949093	2.911479
S	11.958112	-4.784293	3.162503
S	11.808098	1.418907	3.078375
S	9.192527	3.157787	3.079870
H	12.580399	-1.608264	2.634365

O*

Mo	1.824648	0.027883	1.594641
Mo	1.828286	3.200029	1.605143
Mo	1.840788	6.396602	1.566994
Mo	4.579068	-1.577646	1.596481
Mo	4.590992	1.610942	1.614397
Mo	4.584917	4.783988	1.596221
Mo	7.289231	-3.171467	1.525354
Mo	7.301330	0.003176	1.526766
Mo	7.368761	3.163321	1.566468
Mo	10.058970	-4.783721	1.563250
Mo	10.142092	1.630839	1.503236
Mo	12.873637	-6.349383	1.584382
Mo	12.933293	-3.064950	1.513346
Mo	12.894448	0.007605	1.469566
Cu	10.402202	-1.965242	1.326041
S	0.905526	1.624165	0.034495
S	0.965609	4.777384	-0.000828
S	0.961658	8.018009	-0.012753
S	3.665049	0.026888	0.045338
S	3.666353	3.190190	0.044306
S	3.684638	6.390036	0.023542
S	6.378494	-1.586810	-0.014394
S	6.403630	1.576392	0.004450
S	6.396363	4.752190	0.006020
S	9.105099	-3.285550	-0.063728
S	9.294153	-0.183295	0.344125
S	9.209426	3.171495	-0.026022
S	11.964377	-4.738484	0.028262
S	12.131671	-1.577633	-0.213768
S	11.999772	1.639106	-0.031735
S	0.882526	1.612033	3.163446
S	0.891582	4.833265	3.136705
S	0.857113	7.978739	3.110287
S	3.656130	0.012622	3.167049
S	3.668734	3.203753	3.175747
S	3.662086	6.390633	3.153459
S	6.463211	-1.560808	3.131502
S	6.479538	1.578631	3.143930
S	6.456168	4.786885	3.124031
S	9.219389	-3.087319	3.020258
S	11.945035	-4.669894	3.094508
S	11.914460	1.535686	3.099504
S	9.204611	3.141396	3.120678
O	12.095317	-1.566780	2.543603

CO_2*

Mo	1.756294	0.070520	1.575024
Mo	1.762129	3.264390	1.582238
Mo	1.741365	6.452236	1.539832
Mo	4.520132	-1.518712	1.563637
Mo	4.524443	1.674896	1.581456
Mo	4.520413	4.852351	1.564570
Mo	7.267879	-3.108707	1.483654
Mo	7.240690	0.101005	1.456157
Mo	7.304636	3.236039	1.512186
Mo	10.043535	-4.723789	1.480805
Mo	10.072049	1.696201	1.413572
Mo	12.805031	-6.312355	1.541793
Mo	12.868848	-3.110137	1.434553
Mo	12.833417	0.087880	1.412625
Cu	10.231146	-1.835135	1.347251
S	0.849108	1.669858	0.015966
S	0.892950	4.820291	-0.049446
S	0.883057	8.078207	-0.055191
S	3.595788	0.080420	0.020289
S	3.595434	3.255375	0.017611
S	3.603399	6.453185	0.000806
S	6.323173	-1.530944	-0.049917
S	6.316523	1.659922	-0.051414
S	6.332795	4.833649	-0.030243
S	9.049866	-3.230216	-0.150431
S	9.191601	-0.075188	0.208148
S	9.132749	3.254683	-0.100373
S	11.908703	-4.738350	-0.055808
S	11.932464	-1.532708	-0.032014
S	11.928371	1.703024	-0.101133
S	0.814455	1.661941	3.131351
S	0.784817	4.898036	3.100901
S	0.755964	8.011984	3.082482
S	3.600494	0.068169	3.136693
S	3.608130	3.269809	3.146341
S	3.586396	6.453211	3.116070
S	6.429274	-1.481578	3.074987
S	6.424529	1.654018	3.096620
S	6.407610	4.859451	3.076445
S	9.214951	-2.997777	2.979815
S	11.888387	-4.633917	3.049139
S	11.823341	1.554374	3.048614
S	9.161632	3.213619	3.039688
C	9.204390	-0.462006	6.077656
O	9.114663	0.155707	5.079389
O	9.294531	-1.076590	7.075489

HCOO*

Mo	1.794610	0.008354	1.576230
Mo	1.814835	3.204331	1.566536
Mo	1.800360	6.391173	1.514329
Mo	4.564095	-1.563006	1.597218
Mo	4.559516	1.620812	1.612664
Mo	4.577132	4.797002	1.581714
Mo	7.304142	-3.134862	1.562923
Mo	7.298349	0.028089	1.642431
Mo	7.341888	3.209144	1.593253
Mo	10.088940	-4.761822	1.488622
Mo	10.074466	1.582138	1.599509
Mo	12.838235	-6.370927	1.536988
Mo	12.962711	-3.145669	1.382423
Mo	12.920421	-0.026337	1.436964
Cu	10.352656	-1.888737	1.186960
S	0.881062	1.601501	0.010452
S	0.985175	4.750110	-0.090463
S	0.927665	8.027964	-0.064646
S	3.651752	0.031806	0.036621
S	3.671973	3.193896	0.024081
S	3.687254	6.404773	0.007860
S	6.405593	-1.533743	0.042980
S	6.407690	1.591602	0.060012
S	6.417217	4.801352	0.019343
S	9.090923	-3.304160	-0.161308
S	9.207763	-0.123874	0.190541
S	9.167104	3.138340	0.012789
S	11.935367	-4.800670	-0.072591
S	12.092494	-1.597771	-0.141091
S	11.887186	1.595200	-0.017155
S	0.850752	1.613414	3.121241
S	0.837456	4.848221	3.077210
S	0.833967	7.922922	3.093617
S	3.615304	0.017198	3.161223
S	3.630583	3.224923	3.156290
S	3.614010	6.391481	3.118871
S	6.398600	-1.589503	3.171695
S	6.391806	1.645811	3.182346
S	6.432963	4.828631	3.138589
S	9.329840	-2.967593	2.916792
S	11.959131	-4.648851	3.019672
S	11.969029	1.500487	3.074116
S	9.218711	3.251372	3.114202
C	9.089620	0.058741	4.307343
O	9.980301	0.467030	5.015719
O	9.033770	0.228627	2.955384
H	8.220354	-0.526766	4.668520

COOH*

Mo	1.749652	0.060815	1.517523
Mo	1.774381	3.257700	1.501535
Mo	1.756162	6.426637	1.449375
Mo	4.478323	-1.543456	1.553816
Mo	4.498371	1.667302	1.588157
Mo	4.521699	4.831290	1.547448
Mo	7.235551	-3.102414	1.583709
Mo	7.169859	0.033657	1.728063
Mo	7.287320	3.240966	1.638186
Mo	10.034389	-4.698465	1.487081
Mo	10.102972	1.704005	1.698027
Mo	12.830006	-6.281590	1.487534
Mo	12.920175	-3.079734	1.333966
Mo	12.905066	0.013259	1.401672
Cu	10.329464	-1.846716	1.241751
S	0.848203	1.657719	-0.059275
S	0.927965	4.797323	-0.157706
S	0.885767	8.072968	-0.119477
S	3.611920	0.079890	-0.011120
S	3.642764	3.234529	-0.025682
S	3.645636	6.425567	-0.052427
S	6.358920	-1.504406	0.054597
S	6.383351	1.618191	0.089025
S	6.395773	4.821091	0.032517
S	9.035572	-3.231095	-0.140210
S	9.157970	-0.050359	0.417536
S	9.100879	3.180515	0.050791
S	11.868858	-4.731197	-0.106209
S	12.014602	-1.530183	-0.164480
S	11.858294	1.647693	-0.019881
S	0.837582	1.684059	3.066125
S	0.797262	4.896960	3.019706
S	0.820402	7.957814	3.043671
S	3.543993	0.054078	3.116827
S	3.560707	3.273670	3.116799
S	3.533894	6.414369	3.074180
S	6.218082	-1.614309	3.181661
S	6.271688	1.700892	3.209676
S	6.342833	4.866088	3.150050
S	9.261816	-2.935095	2.935763
S	11.932849	-4.570181	2.983544
S	12.072604	1.619788	3.044530
S	9.168742	3.364429	3.160759
C	9.466612	0.553788	3.486517
O	8.448200	-0.181997	3.421854
O	9.974839	0.593998	4.723484
H	10.798769	1.139675	4.704412

CHO*

Mo	1.817465	-0.021852	1.589410
Mo	1.827294	3.161474	1.598656
Mo	1.806464	6.354751	1.623267
Mo	4.588532	-1.588405	1.525681
Mo	4.571828	1.601783	1.525820
Mo	4.567850	4.787760	1.528799
Mo	7.350510	-3.188157	1.418813
Mo	7.314508	0.124220	1.339919
Mo	7.322476	3.203911	1.430838
Mo	10.128015	-4.823237	1.502809
Mo	9.977515	1.658340	1.387318
Mo	12.847214	-6.425407	1.553141
Mo	12.883200	-3.310198	1.693494
Mo	12.861451	0.032295	1.623588

Cu	9.683778	-1.517160	1.199354
S	0.904289	1.566441	0.021289
S	0.864089	4.758235	0.072831
S	0.886954	7.932011	0.046791
S	3.622918	-0.013441	-0.008022
S	3.612315	3.193140	-0.013347
S	3.603679	6.382551	0.006019
S	6.378236	-1.587104	-0.109933
S	6.312889	1.642742	-0.145937
S	6.354884	4.797125	-0.100422
S	9.136715	-3.294039	-0.203002
S	9.092228	0.119528	-0.177494
S	9.182729	3.257051	-0.147078
S	11.993306	-4.795945	0.015903
S	11.822240	-1.649748	0.337853
S	11.922356	1.563491	-0.039983
S	0.881730	1.555463	3.143278
S	0.960268	4.722151	3.197718
S	0.901069	7.968496	3.180107
S	3.698972	-0.003318	3.109421
S	3.703756	3.181352	3.117829
S	3.709588	6.385447	3.122494
S	6.545295	-1.508033	2.975319
S	6.490471	1.605179	3.021411
S	6.459334	4.810704	3.016830
S	9.253905	-3.009672	2.883023
S	11.894850	-4.936692	3.142279
S	11.742129	1.593587	3.052306
S	9.106189	3.160165	3.033108
C	12.187201	-1.044031	3.365141
O	12.058070	-2.288277	3.384713
H	11.979516	-0.559189	4.344149

COH*

Mo	1.812205	0.018912	1.591892
Mo	1.818478	3.192296	1.603665
Mo	1.839539	6.389457	1.576875
Mo	4.573607	-1.579652	1.597889
Mo	4.584714	1.607204	1.612011
Mo	4.573857	4.783187	1.592193
Mo	7.285103	-3.162566	1.501440
Mo	7.300088	0.004783	1.507686
Mo	7.350682	3.168745	1.547939
Mo	10.047865	-4.780430	1.503236
Mo	10.093171	1.618730	1.491482
Mo	12.843457	-6.360572	1.573677
Mo	12.924026	-3.151403	1.475887
Mo	12.901578	0.041988	1.486696
Cu	10.460492	-1.933662	1.285541
S	0.887393	1.612820	0.033675
S	0.997474	4.780908	-0.008993
S	0.970619	7.988467	-0.020492
S	3.654469	0.021752	0.047349
S	3.655210	3.183997	0.044418
S	3.675750	6.390995	0.026759
S	6.365852	-1.581749	-0.023982
S	6.387619	1.575944	-0.008343
S	6.380425	4.759751	-0.008887
S	9.081514	-3.320913	-0.152196
S	9.292823	-0.193254	0.300865
S	9.176000	3.162358	-0.047896
S	11.931391	-4.794284	-0.024894
S	12.156355	-1.613625	-0.186333
S	11.947687	1.632020	-0.037141
S	0.862093	1.604612	3.156515
S	0.866248	4.812615	3.130968
S	0.866262	7.981781	3.121142
S	3.649493	0.013211	3.165262
S	3.661470	3.198246	3.173334
S	3.662842	6.385523	3.159288
S	6.468649	-1.551275	3.121647
S	6.480634	1.578397	3.132491
S	6.449770	4.798282	3.103221
S	9.236028	-2.985485	2.898688
S	11.907056	-4.690574	3.069907
S	11.872005	1.537333	3.101509
S	9.184598	3.169919	3.097045
C	12.158398	-1.540041	2.658812
O	11.869282	-1.579128	3.953250
H	11.754605	-0.660217	4.302439

CH_2O*

Mo	1.869423	0.036746	1.539319
Mo	1.853100	3.219991	1.556929
Mo	1.856163	6.412536	1.536356
Mo	4.607657	-1.567811	1.502471
Mo	4.605408	1.623830	1.516603
Mo	4.592096	4.788044	1.501986
Mo	7.283310	-3.215383	1.442902
Mo	7.314995	0.045341	1.437758
Mo	7.371634	3.151791	1.486191
Mo	10.083202	-4.866259	1.526366
Mo	10.151111	1.641797	1.500849
Mo	12.897916	-6.339819	1.585039
Mo	12.966979	-3.126450	1.590274
Mo	12.961336	0.083566	1.555598
Cu	10.134548	-2.075138	1.551495
S	0.909117	1.637564	-0.000996
S	0.919040	4.810140	-0.008756
S	0.939319	8.019490	-0.030618
S	3.678209	0.030652	-0.046230
S	3.653832	3.204324	-0.045534
S	3.673817	6.405307	-0.049896
S	6.418911	-1.591502	-0.096685
S	6.410615	1.586799	-0.099073
S	6.406997	4.735829	-0.089590
S	9.151152	-3.343987	-0.109074
S	9.314354	-0.174123	0.340946
S	9.234370	3.136794	-0.085699
S	12.000885	-4.722978	0.036767
S	11.924685	-1.568714	0.121698
S	12.020052	1.640604	-0.009677
S	0.946964	1.621713	3.121069
S	0.984403	4.820866	3.136146
S	0.985048	8.029161	3.112684
S	3.716382	0.027033	3.081656
S	3.707278	3.209526	3.091814
S	3.713033	6.403157	3.074655
S	6.490706	-1.559625	3.030793
S	6.472345	1.585323	3.065752
S	6.436728	4.762268	3.039622
S	9.069440	-3.287343	3.059443
S	11.945790	-4.721966	3.106339
S	11.941955	1.595678	3.115129
S	9.169272	3.116165	3.102034
C	11.082325	-1.534323	3.354667
O	12.358783	-1.445677	2.919411
H	10.972683	-2.289618	4.142431
H	10.590167	-0.575564	3.580256

CHOH*

Mo	1.820649	0.023212	1.602950
Mo	1.799587	3.189683	1.611567
Mo	1.841451	6.388294	1.602693
Mo	4.579932	-1.598163	1.545648
Mo	4.582520	1.591555	1.565551
Mo	4.554238	4.765554	1.553998
Mo	7.292697	-3.231514	1.429896
Mo	7.312677	0.028771	1.418028
Mo	7.335993	3.138531	1.499740
Mo	10.039541	-4.818337	1.497490
Mo	10.084442	1.607581	1.510743
Mo	12.830857	-6.344015	1.612299
Mo	12.891267	-3.125608	1.585345
Mo	12.913898	0.052630	1.622302
Cu	9.878492	-1.899404	1.149309
S	0.861478	1.612483	0.052600
S	0.911816	4.801139	0.049794
S	0.927223	7.984930	0.041786
S	3.630605	0.005531	0.013978
S	3.606605	3.172637	0.017185
S	3.635827	6.375283	0.001060
S	6.366921	-1.613497	-0.086926
S	6.358538	1.576944	-0.080399
S	6.337922	4.710207	-0.059289
S	9.019507	-3.468835	-0.258773
S	9.219328	-0.066166	0.078544
S	9.196864	3.117829	-0.068416
S	11.938525	-4.750546	0.025731
S	11.921710	-1.553683	0.139300
S	11.970762	1.617641	0.029991
S	0.866617	1.607062	3.174749
S	0.895899	4.802758	3.167492
S	0.944204	8.005360	3.172442
S	3.691016	-0.001381	3.133518
S	3.670520	3.178935	3.144006
S	3.700863	6.380326	3.137937
S	6.503586	-1.567468	3.028715
S	6.486298	1.550779	3.080048
S	6.434104	4.767062	3.049253
S	9.157243	-3.127488	2.952362
S	11.870920	-4.683026	3.125577
S	11.852506	1.578920	3.157559
S	9.142563	3.145527	3.086093
C	12.238909	-1.461849	3.071424
O	12.517201	-1.490537	4.415000
H	13.457501	-1.258593	4.579374
H	11.144478	-1.550876	3.022916

CH_3O*

Mo	1.828372	0.032608	1.574197
Mo	1.819102	3.204178	1.584102
Mo	1.832945	6.406276	1.561413
Mo	4.581634	-1.583650	1.504661
Mo	4.591113	1.598429	1.528539
Mo	4.562292	4.778579	1.509509
Mo	7.286479	-3.214700	1.388203
Mo	7.329501	0.019702	1.383407
Mo	7.342299	3.143871	1.453930
Mo	10.035024	-4.789394	1.452165
Mo	10.121883	1.596927	1.464550
Mo	12.858048	-6.333190	1.578618
Mo	12.920064	-3.079635	1.568108
Mo	12.897893	0.061248	1.576301
Cu	9.996367	-1.951033	1.151574
S	0.885324	1.628708	0.020465
S	0.916328	4.798120	0.012135
S	0.903759	8.020914	0.010597
S	3.633655	0.018586	-0.023549
S	3.620504	3.180993	-0.020390
S	3.635643	6.392806	-0.040894
S	6.372953	-1.607194	-0.127172
S	6.374117	1.571415	-0.115741
S	6.352055	4.721359	-0.105418
S	9.030770	-3.461446	-0.310242
S	9.259734	-0.124523	0.097326
S	9.217271	3.123143	-0.098935
S	11.982673	-4.711989	0.003618
S	11.980100	-1.560267	0.039011
S	12.004299	1.629557	-0.011814
S	0.889340	1.619536	3.147692
S	0.926596	4.821509	3.139860
S	0.925483	8.013175	3.134958
S	3.700434	0.007275	3.098902
S	3.696034	3.192187	3.106088
S	3.699230	6.393524	3.090744
S	6.500241	-1.569036	2.992376
S	6.499462	1.553131	3.038406
S	6.441174	4.774113	3.003951
S	9.160958	-3.120016	2.917474
S	11.878422	-4.680475	3.061516
S	11.873393	1.607408	3.113532
S	9.159456	3.146001	3.028638
C	12.043873	-1.534386	4.249702
O	12.153790	-1.525875	2.818871
H	13.033456	-1.506778	4.732682
H	11.462453	-0.653606	4.557969
H	11.511005	-2.445886	4.554563

CH_2OH*

Mo	1.841994	-0.018341	1.610344
Mo	1.843015	3.163448	1.620441
Mo	1.820651	6.358369	1.660362
Mo	4.607113	-1.593845	1.534783
Mo	4.589757	1.595858	1.531757
Mo	4.585276	4.780304	1.538915
Mo	7.367152	-3.198792	1.425860
Mo	7.326269	0.115738	1.343322
Mo	7.344155	3.193736	1.435498
Mo	10.146268	-4.839757	1.505969
Mo	10.000462	1.667373	1.403348
Mo	12.875268	-6.407982	1.576004
Mo	12.897461	-3.310142	1.736026
Mo	12.852284	0.060529	1.716320
Cu	9.654221	-1.521425	1.211891
S	0.927953	1.569275	0.040118
S	0.857243	4.772362	0.111291
S	0.871802	7.931068	0.104936
S	3.637074	-0.020025	0.001210
S	3.619537	3.190567	-0.001279
S	3.605647	6.376605	0.025155
S	6.391351	-1.598165	-0.107163
S	6.327885	1.636603	-0.144934
S	6.370637	4.787354	-0.094187
S	9.169406	-3.307659	-0.183962
S	9.115375	0.122749	-0.159994
S	9.206802	3.243159	-0.149977
S	12.027542	-4.770618	0.039151
S	11.806302	-1.612640	0.437488
S	11.964557	1.556599	0.007338
S	0.908804	1.559210	3.165422
S	0.990666	4.721416	3.233659
S	0.931905	7.988054	3.208964
S	3.729060	-0.006613	3.122760
S	3.727155	3.173119	3.127978
S	3.740566	6.380363	3.136590
S	6.563451	-1.518101	2.979575
S	6.508686	1.596555	3.023086
S	6.478103	4.796866	3.021926
S	9.264807	-3.025486	2.894693
S	11.909133	-4.933528	3.161351
S	11.761745	1.660064	3.093682
S	9.118234	3.156667	3.048442
C	11.924472	-0.875166	3.552695
O	12.090102	-2.311457	3.592676
H	12.328646	-0.469423	4.489652
H	10.838683	-0.707800	3.533555
H	12.778216	-2.536457	4.252379

CH*

Mo	1.807454	0.019069	1.598828
Mo	1.819476	3.194736	1.604067
Mo	1.839540	6.390190	1.578545
Mo	4.573594	-1.579517	1.606127
Mo	4.582003	1.609774	1.617805
Mo	4.577165	4.787147	1.594930
Mo	7.294283	-3.155831	1.535421
Mo	7.293635	0.010401	1.533431
Mo	7.354009	3.170298	1.566174
Mo	10.050624	-4.783304	1.527815
Mo	10.101121	1.637742	1.525165
Mo	12.848580	-6.361688	1.583777
Mo	12.933373	-3.145137	1.468253
Mo	12.885103	0.018734	1.508270
Cu	10.479401	-1.944810	1.312875
S	0.887320	1.610974	0.039728
S	1.004244	4.783071	-0.013337
S	0.950188	7.990101	-0.005941
S	3.650600	0.020163	0.055022
S	3.659007	3.186323	0.046373
S	3.678145	6.395180	0.029288
S	6.377177	-1.580111	-0.001121
S	6.391447	1.576879	0.006943
S	6.398309	4.769092	0.009031
S	9.110974	-3.297336	-0.102337
S	9.298886	-0.181002	0.348925
S	9.181333	3.164079	-0.026206
S	11.934513	-4.797636	-0.013257
S	12.173113	-1.615652	-0.212786
S	11.949237	1.623230	-0.011913
S	0.866187	1.608548	3.163711
S	0.863391	4.819381	3.132383
S	0.855380	7.971308	3.129532
S	3.643563	0.013565	3.170981
S	3.658822	3.204029	3.175372
S	3.661379	6.384935	3.163212
S	6.456437	-1.546341	3.145426
S	6.468408	1.585087	3.150126
S	6.443667	4.797202	3.119836
S	9.240617	-2.979349	2.937639
S	11.918159	-4.681820	3.078560

S	11.883952	1.540294	3.121611
S	9.180704	3.180054	3.128698
C	12.058531	-1.564057	2.565979
H	11.734941	-1.598950	3.616118

CH_2*

Mo	1.819876	-0.012927	1.606178
Mo	1.826085	3.188563	1.599432
Mo	1.813727	6.375749	1.556016
Mo	4.599496	-1.572967	1.612742
Mo	4.573955	1.615229	1.622630
Mo	4.583505	4.803796	1.607550
Mo	7.348621	-3.169262	1.562726
Mo	7.326522	0.073072	1.629792
Mo	7.339617	3.221963	1.598792
Mo	10.117791	-4.796643	1.482584
Mo	10.080355	1.603116	1.574054
Mo	12.863355	-6.406438	1.567590
Mo	12.959237	-3.185527	1.425596
Mo	12.930689	-0.046036	1.472665
Cu	10.271791	-1.918105	1.198914
S	0.909582	1.578946	0.041543
S	0.982992	4.735563	-0.048088
S	0.943357	7.999206	-0.027105
S	3.672289	0.015932	0.056914
S	3.673840	3.196125	0.050102
S	3.691854	6.401628	0.035071
S	6.439018	-1.558355	0.045545
S	6.404301	1.631285	0.049749
S	6.403776	4.797704	0.030740
S	9.092467	-3.350213	-0.166843
S	9.224361	-0.092800	0.182442
S	9.149962	3.153628	-0.006188
S	11.977593	-4.839882	-0.051890
S	12.055102	-1.625271	-0.069053
S	11.946766	1.567171	-0.009078
S	0.873319	1.585248	3.153184
S	0.847403	4.824811	3.113049
S	0.848502	7.911057	3.127239
S	3.655954	0.003457	3.179543
S	3.650727	3.215852	3.178504
S	3.641073	6.399151	3.151855
S	6.485427	-1.563778	3.167852
S	6.411998	1.650473	3.186649
S	6.447253	4.832969	3.153919
S	9.338737	-3.060536	2.960691
S	11.970432	-4.700637	3.050737
S	11.937757	1.460853	3.106356
S	9.225168	3.237989	3.111955
C	9.011533	0.329557	3.004189
H	8.796998	0.751378	3.993981
H	9.573485	-0.600857	3.144535

CH_3*

Mo	1.822728	-0.002457	1.592503
Mo	1.844021	3.187775	1.578348
Mo	1.828410	6.375762	1.529444
Mo	4.582209	-1.574746	1.620856
Mo	4.593223	1.607966	1.645366
Mo	4.600241	4.789780	1.603038
Mo	7.325553	-3.141105	1.570212
Mo	7.327544	0.017089	1.673402
Mo	7.358565	3.205808	1.608832
Mo	10.117392	-4.783168	1.463042
Mo	10.081847	1.576237	1.589975
Mo	12.871303	-6.387021	1.524824
Mo	12.993644	-3.165739	1.374566
Mo	12.956258	-0.053045	1.429969
Cu	10.416591	-1.930350	1.161423
S	0.923820	1.585031	0.012303
S	1.026162	4.732273	-0.082628
S	0.973097	8.013906	-0.054347
S	3.684983	0.026711	0.063003
S	3.709084	3.177521	0.049076
S	3.715820	6.395848	0.025939
S	6.424158	-1.539884	0.064714
S	6.435671	1.575575	0.085176
S	6.431519	4.794652	0.035704
S	9.105207	-3.306649	-0.168709
S	9.236031	-0.154173	0.241018
S	9.159267	3.127352	0.003974
S	11.974358	-4.822541	-0.089672
S	12.149276	-1.617111	-0.167368
S	11.928351	1.565510	-0.027500
S	0.867580	1.602076	3.127337
S	0.855711	4.829175	3.083400
S	0.852384	7.906478	3.102529
S	3.636623	0.005769	3.187754
S	3.653684	3.216442	3.178990
S	3.631259	6.378761	3.141743
S	6.403139	-1.608348	3.197381
S	6.432165	1.640496	3.211008
S	6.457517	4.827993	3.155315
S	9.374182	-3.000445	2.898568
S	11.982252	-4.673666	3.003347
S	11.993135	1.495524	3.058590
S	9.245657	3.255714	3.105061
C	9.236583	0.276137	3.233401
H	9.022925	0.815361	4.162414
H	8.496520	-0.583036	3.212039
H	10.130852	-0.355245	3.360517

3. Adsorption of species on Mo edge

H_2O*

Mo	3.216002	9.399402	0.924174
Mo	9.587486	9.162050	0.933636
Mo	-0.061894	9.399116	0.928819
Mo	6.312666	9.165728	0.940811
Mo	11.143921	9.339449	3.683239
Mo	7.945213	9.342063	3.692933
Mo	1.581279	9.343186	3.688240
Mo	4.764608	9.345580	3.699523
Mo	9.548956	9.397687	6.435452
Mo	-0.021024	9.392429	6.441428
Mo	6.345128	9.398879	6.471923
Mo	3.180692	9.399975	6.462698
Mo	4.996525	9.473168	9.265849
Mo	1.327296	9.449793	9.129441
Mo	11.313480	9.446484	9.199341
Mo	7.804459	9.430790	9.223702
S	1.575718	8.122565	-0.282843
S	4.763841	7.700653	0.063346
S	11.141123	7.704068	0.058705
S	1.575664	10.815112	-0.123259
S	7.945720	7.700132	-0.046927
S	7.948049	10.382414	-0.330077
S	4.766854	10.818671	-0.014128
S	11.138479	10.816748	-0.009720
S	3.169465	10.915487	2.775325
S	-0.010208	7.787862	2.736510
S	6.362118	10.856672	2.678786
S	9.538431	7.731747	2.848729
S	6.358735	7.730642	2.856154
S	3.170477	7.793702	2.736267
S	9.538522	10.847715	2.671937
S	-0.012674	10.915964	2.779532
S	1.605286	7.826517	5.556221
S	7.947441	10.939216	5.497582
S	4.744569	7.823760	5.569887
S	1.599529	10.928697	5.501350
S	11.137514	7.814321	5.542056
S	7.947416	7.824127	5.570164
S	4.752562	10.943282	5.506766
S	11.132213	10.938185	5.478959
S	3.179422	7.969931	8.492056
S	-0.058815	11.093080	8.165497
S	6.352554	7.790757	8.282767
S	-0.046354	7.759821	8.235689
S	6.377868	11.074128	8.237559
S	9.556731	7.923509	8.355589
S	9.551779	10.932565	8.306265
S	3.153301	10.944603	8.385752
S	6.407542	9.217113	11.117326
S	0.145984	9.509035	11.062249
S	9.600495	9.496838	10.867089
O	3.642572	9.960541	11.110998
H	3.264643	10.863306	11.084144
H	4.203496	9.893226	11.915983

CO*

Mo	3.111097	9.432081	0.935322
Mo	9.486134	9.232897	0.940765
Mo	0.004355	9.228901	0.939333
Mo	6.378145	9.427461	0.946992
Mo	11.122003	9.339488	3.682053
Mo	7.927191	9.332376	3.699839
Mo	1.560302	9.333833	3.693146
Mo	4.740679	9.322842	3.698762
Mo	9.528630	9.327113	6.443461
Mo	-0.045113	9.332744	6.437247
Mo	6.337346	9.293822	6.466002
Mo	3.151154	9.313746	6.474534
Mo	4.877813	9.307479	9.264718
Mo	1.315694	9.320514	9.144719
Mo	11.292520	9.300176	9.216916
Mo	7.780803	9.256917	9.238365
S	1.551004	7.771290	0.031078
S	4.748446	8.147916	-0.267192
S	11.122316	7.798363	-0.086373
S	1.566435	10.872268	0.007617
S	7.935809	7.774871	0.033076
S	7.925255	10.875622	0.023645
S	4.749393	10.845072	-0.107920
S	11.122504	10.497918	-0.279172
S	3.159292	10.917016	2.811344
S	-0.041880	7.746654	2.815710
S	6.326300	10.918859	2.823421
S	9.529663	7.748541	2.813333
S	6.336689	7.787429	2.725747
S	3.149038	7.792225	2.712022
S	9.521582	10.873855	2.717371
S	-0.036227	10.876282	2.713956
S	1.569458	7.774489	5.527339
S	7.924420	10.880715	5.549361
S	4.727041	7.759844	5.529895
S	1.576894	10.883832	5.536524
S	11.116585	7.777471	5.513149
S	7.948888	7.759300	5.521335
S	4.733882	10.868157	5.556150
S	11.109590	10.898621	5.516805
S	3.114765	7.831772	8.446426
S	-0.092324	10.975561	8.224027
S	6.352450	7.646940	8.234668
S	-0.068712	7.661227	8.200533
S	6.338422	10.916109	8.295382
S	9.547792	7.792333	8.320848
S	9.519728	10.799249	8.370562
S	3.089718	10.841767	8.380649
S	6.381249	8.923128	11.086430
S	0.131724	9.306191	11.077963
S	9.565665	9.264530	10.883107
C	4.068807	10.240386	10.916490
O	3.698771	10.785286	11.870779

OH*

Mo	3.214904	9.319500	0.948295
Mo	9.602517	9.319500	0.970581
Mo	-0.044440	9.319500	0.961080
Mo	6.355237	9.319500	0.961500
Mo	11.161727	9.319500	3.713438
Mo	7.970408	9.319500	3.696810
Mo	1.590466	9.319500	3.669565
Mo	4.788590	9.319500	3.676650
Mo	9.569025	9.319500	6.461441
Mo	0.011063	9.319500	6.448630
Mo	6.365893	9.319500	6.447325
Mo	3.191355	9.319499	6.394400
Mo	4.922754	9.319499	9.222318
Mo	1.458153	9.319499	9.222613
Mo	11.368980	9.319499	9.253235
Mo	7.767801	9.319500	9.251899
S	1.582498	7.953135	-0.154450
S	4.788308	7.796606	0.014319
S	11.154442	7.771987	0.049211
S	1.582498	10.685864	-0.154450
S	7.980834	7.950567	-0.143652
S	7.980834	10.688432	-0.143652
S	4.788308	10.842393	0.014319
S	11.154442	10.867012	0.049211
S	3.189125	10.891075	2.759953
S	-0.009336	7.747248	2.779981
S	6.385197	10.895245	2.774879
S	9.567957	7.749958	2.794153
S	6.385197	7.743754	2.774879
S	3.189125	7.747924	2.759953
S	9.567957	10.889041	2.794153
S	-0.009336	10.891751	2.779981
S	1.596226	7.757685	5.504512
S	7.976481	10.876858	5.544861
S	4.783655	7.753741	5.506225
S	1.596226	10.881315	5.504513
S	11.159009	7.755720	5.552275
S	7.976481	7.762141	5.544861
S	4.783655	10.885259	5.506225
S	11.159009	10.883279	5.552275
S	3.190590	7.807936	8.283460
S	0.030279	10.949723	8.262800
S	6.351569	7.689586	8.261507
S	0.030279	7.689276	8.262799
S	6.351569	10.949413	8.261508
S	9.568214	7.835567	8.382229
S	9.568214	10.803432	8.382228
S	3.190590	10.831063	8.283461
S	6.276694	9.319499	11.115737
S	0.105711	9.319499	11.115898
S	9.568714	9.319499	10.886740
O	3.191549	9.319500	10.533591
H	3.192426	9.319500	11.508394

H*

Mo	3.219819	9.319500	0.949730
Mo	9.602748	9.319500	0.977821
Mo	-0.047401	9.319500	0.963948
Mo	6.351919	9.319500	0.966160
Mo	11.160592	9.319500	3.724077
Mo	7.972585	9.319500	3.714433
Mo	1.593127	9.319500	3.678368
Mo	4.785222	9.319500	3.685398
Mo	9.569749	9.319500	6.478989
Mo	0.013888	9.319500	6.448093
Mo	6.361703	9.319500	6.447883
Mo	3.191336	9.319499	6.417506
Mo	4.862341	9.319499	9.191559
Mo	1.518685	9.319499	9.191454
Mo	11.386961	9.319499	9.272508
Mo	7.750824	9.319500	9.272398
S	1.581941	7.954605	-0.151002
S	4.790316	7.786409	0.028774
S	11.151755	7.768940	0.058586
S	1.581941	10.684394	-0.151002
S	7.980663	7.950892	-0.136488
S	7.980663	10.688107	-0.136488
S	4.790316	10.852590	0.028774
S	11.151755	10.870059	0.058586
S	3.188682	10.889471	2.763980
S	-0.008258	7.749193	2.786456
S	6.386168	10.891568	2.785589

S	9.566443	7.751433	2.806381
S	6.386168	7.747431	2.785589
S	3.188682	7.749528	2.763980
S	9.566443	10.887566	2.806381
S	-0.008258	10.889806	2.786456
S	1.599676	7.757870	5.509085
S	7.977526	10.878239	5.560709
S	4.779529	7.753912	5.512063
S	1.599676	10.881130	5.509086
S	11.157511	7.755979	5.563087
S	7.977526	7.760760	5.560709
S	4.779529	10.885088	5.512063
S	11.157511	10.883020	5.563087
S	3.190634	7.776237	8.294590
S	0.037128	10.941749	8.267707
S	6.343324	7.696590	8.267756
S	0.037128	7.697250	8.267706
S	6.343324	10.942409	8.267757
S	9.568372	7.846504	8.408340
S	9.568372	10.792495	8.408339
S	3.190634	10.862762	8.294591
S	6.162441	9.319499	11.107775
S	0.220713	9.319499	11.106979
S	9.568262	9.319499	10.903307
H	3.192905	9.319500	10.320208

H*

Mo	3.238507	9.208822	0.960277
Mo	9.618697	9.419528	0.960962
Mo	-0.032375	9.210112	0.964743
Mo	6.343285	9.416895	0.967854
Mo	11.171201	9.316922	3.716796
Mo	7.980107	9.317070	3.710805
Mo	1.601179	9.317742	3.718375
Mo	4.784665	9.316374	3.719412
Mo	9.578892	9.320161	6.465170
Mo	-0.000223	9.331951	6.483981
Mo	6.383634	9.321696	6.458072
Mo	3.194181	9.322907	6.492683
Mo	4.996489	9.329208	9.173535
Mo	1.432716	9.343676	9.152459
Mo	11.310980	9.362936	9.256147
Mo	7.788636	9.328601	9.251461
S	1.601819	7.786021	-0.075154
S	4.791752	7.762954	0.048155
S	11.174674	7.761628	0.051045
S	1.602871	10.480623	-0.254748
S	7.980442	8.149555	-0.252252
S	7.978521	10.845793	-0.066826
S	4.791908	10.867021	0.052098
S	11.171262	10.868473	0.050295
S	3.192071	10.850942	2.734496
S	0.012728	7.724846	2.842515
S	6.385666	10.905642	2.840894
S	9.574317	7.779686	2.739602
S	6.385253	7.775785	2.747888
S	3.189130	7.725769	2.837666
S	9.572426	10.905430	2.833821
S	0.012487	10.854821	2.740447
S	1.607563	7.769099	5.574158
S	7.989344	10.878814	5.545913
S	4.767582	7.759545	5.557076
S	1.612759	10.874355	5.553410
S	11.168292	7.760320	5.553994
S	7.990279	7.755864	5.543480
S	4.764665	10.880149	5.549875
S	11.167297	10.886995	5.544054
S	3.205970	7.827682	8.460601
S	-0.020973	11.002626	8.265250
S	6.413102	7.683047	8.241887
S	-0.027578	7.699805	8.315675
S	6.405726	10.973782	8.232930
S	9.568672	7.841188	8.382460
S	9.550476	10.827390	8.363549
S	3.208220	10.836920	8.448676
S	6.217425	9.334762	11.107498
S	0.158060	9.881466	11.171413
S	9.604555	9.281844	10.921020
H	0.228930	8.716823	11.865969

O*

Mo	3.221406	9.319500	0.943636
Mo	9.606142	9.319500	0.963818
Mo	-0.047391	9.319500	0.955365
Mo	6.346889	9.319500	0.953594
Mo	11.161263	9.319500	3.721201
Mo	7.974205	9.319500	3.705270
Mo	1.588600	9.319500	3.681161
Mo	4.787593	9.319500	3.683925
Mo	9.570103	9.319500	6.476561
Mo	0.010839	9.319500	6.467930
Mo	6.370562	9.319500	6.453358
Mo	3.192842	9.319499	6.401533
Mo	4.860239	9.319499	9.221620
Mo	1.590275	9.319499	9.262119
Mo	11.296194	9.319499	9.280942
Mo	7.788145	9.319500	9.268806
S	1.584130	7.956929	-0.161022
S	4.786531	7.774450	0.035483
S	11.155320	7.763463	0.053531
S	1.584130	10.682070	-0.161022
S	7.979172	7.954236	-0.152793
S	7.979172	10.684763	-0.152793
S	4.786531	10.864549	0.035483
S	11.155320	10.875536	0.053531
S	3.185671	10.886278	2.764630
S	-0.009422	7.751156	2.781557
S	6.387093	10.888885	2.775624
S	9.568366	7.753459	2.792893
S	6.387093	7.750114	2.775624
S	3.185671	7.752721	2.764630
S	9.568366	10.885540	2.792893
S	-0.009422	10.887843	2.781557
S	1.590292	7.757058	5.514940
S	7.980671	10.877362	5.551169
S	4.788923	7.753743	5.509910
S	1.590292	10.881942	5.514941
S	11.161062	7.757385	5.564683
S	7.980671	7.761637	5.551169
S	4.788923	10.885257	5.509910
S	11.161062	10.881614	5.564683
S	3.203954	7.762871	8.248862
S	0.041794	10.913822	8.305348
S	6.347524	7.708398	8.276414
S	0.041794	7.725177	8.305347
S	6.347524	10.930601	8.276415
S	9.555733	7.815886	8.383881
S	9.555733	10.823113	8.383880
S	3.203954	10.876128	8.248863
S	6.258862	9.319499	11.100740
S	0.095958	9.319499	11.086728
S	9.555057	9.319499	10.940910
O	3.179829	9.319500	10.410389

H_2*

Mo	3.232826	9.268867	0.849690
Mo	9.611333	9.280687	0.846848
Mo	-0.035435	9.360522	0.855330
Mo	6.334217	9.374759	0.857808
Mo	11.167149	9.320339	3.607775
Mo	7.971831	9.320741	3.602952
Mo	1.601123	9.320602	3.616231
Mo	4.781770	9.320663	3.623643
Mo	9.571631	9.321120	6.354683
Mo	-0.000282	9.319736	6.373045
Mo	6.379941	9.321883	6.375455
Mo	3.193866	9.320660	6.396611
Mo	5.021964	9.324551	9.071171
Mo	1.364150	9.316892	9.069886
Mo	11.333993	9.318902	9.141043
Mo	7.808186	9.324981	9.142242
S	1.574080	7.958341	-0.268380
S	4.749254	7.769448	-0.061938
S	11.137719	7.763128	-0.051708
S	1.619720	10.665440	-0.276324
S	7.948003	7.979852	-0.275724
S	7.991779	10.687188	-0.259150
S	4.816201	10.884227	-0.045697
S	11.199070	10.881206	-0.045229
S	3.195218	10.872956	2.657618
S	0.005566	7.763133	2.666913
S	6.382208	10.895357	2.715637
S	9.562764	7.753191	2.694997
S	6.372007	7.765950	2.661404
S	3.184522	7.751447	2.708124
S	9.572396	10.874599	2.657321
S	0.013652	10.892355	2.706351
S	1.619470	7.769781	5.459982
S	7.981538	10.879089	5.438555
S	4.763047	7.765403	5.462304
S	1.622866	10.871999	5.458770
S	11.158820	7.758382	5.437966
S	7.978381	7.763420	5.439030
S	4.759899	10.876591	5.461370
S	11.158437	10.882263	5.437932
S	3.194987	7.823559	8.394651
S	-0.030704	10.977882	8.140991
S	6.417738	7.664469	8.142719
S	-0.032053	7.660010	8.136166
S	6.418179	10.983522	8.139744
S	9.569160	7.825277	8.262494
S	9.572707	10.819098	8.261175
S	3.190788	10.818605	8.394096
S	6.218612	9.324839	10.997309
S	0.163936	9.294905	10.995579
S	9.571189	9.334416	10.793269
H	2.749055	9.307830	12.964251
H	3.499347	9.341186	12.931390

CO_2*

Mo	3.227492	9.382119	0.906751
Mo	9.606569	9.372799	0.919868
Mo	-0.044711	9.274494	0.920900
Mo	6.334079	9.264973	0.920497
Mo	11.159870	9.320702	3.683819
Mo	7.961116	9.318425	3.678007
Mo	1.590765	9.324401	3.678717
Mo	4.773593	9.322580	3.681739
Mo	9.556520	9.315587	6.428928
Mo	-0.004977	9.319500	6.449038
Mo	6.358250	9.314289	6.449785
Mo	3.180600	9.319322	6.447442
Mo	5.004547	9.308931	9.161189
Mo	1.341764	9.319586	9.161523
Mo	11.311812	9.321149	9.198222
Mo	7.791254	9.312493	9.199637
S	1.614942	7.976371	-0.212479
S	4.819858	7.761623	0.016030
S	11.197410	7.762496	0.024046
S	1.561500	10.685540	-0.206006
S	7.997819	7.958730	-0.195825
S	7.944231	10.666460	-0.210954
S	4.747008	10.876951	0.004275
S	11.120817	10.882792	0.020268
S	3.175318	10.892891	2.767025
S	0.005159	7.751306	2.776772
S	6.369592	10.875173	2.725392
S	9.565563	7.769992	2.729428
S	6.376740	7.747524	2.780034
S	3.184185	7.773796	2.710504
S	9.553210	10.887986	2.779657
S	-0.008919	10.879697	2.730154
S	1.610910	7.768371	5.513749
S	7.960302	10.873490	5.515508
S	4.747245	7.762991	5.514414
S	1.606325	10.873405	5.521639
S	11.151282	7.758089	5.513580
S	7.963946	7.758945	5.511800
S	4.753546	10.875189	5.521688
S	11.149289	10.879340	5.516956
S	3.170266	7.827493	8.429385
S	-0.036534	10.979572	8.209835
S	6.386296	7.650675	8.212966
S	-0.037510	7.660171	8.213527
S	6.384536	10.971239	8.215885
S	9.553665	7.812416	8.323782
S	9.548353	10.817420	8.324396
S	3.176591	10.803266	8.450866
S	6.270432	9.348171	11.066026
S	0.067577	9.374877	11.061690
S	9.548461	9.309501	10.848529
C	3.360279	9.293496	12.692907
O	3.157646	9.063869	11.551208
O	3.558156	9.517674	13.823795

HCOO*

Mo	3.224865	9.492189	1.002748
Mo	9.581630	9.322843	0.993839
Mo	-0.021643	9.478074	1.005455
Mo	6.327079	9.297015	0.998809
Mo	11.163863	9.297919	3.714136
Mo	7.965517	9.293104	3.713506
Mo	1.595764	9.298870	3.731228
Mo	4.770811	9.293439	3.747097
Mo	9.567461	9.190488	6.449600
Mo	0.004337	9.187394	6.466552
Mo	6.366938	9.189860	6.470150
Mo	3.189601	9.214925	6.525350
Mo	5.035074	9.170008	9.297905
Mo	1.346715	9.167307	9.295976
Mo	11.286837	9.008121	9.201532
Mo	7.846663	9.011083	9.202272
S	1.599510	8.235810	-0.242202
S	4.787944	7.891691	0.008446
S	11.160234	7.942772	-0.028584
S	1.594880	10.946796	0.012875
S	7.962576	7.930721	-0.102874
S	7.951122	10.651675	-0.146083
S	4.764552	10.969819	0.126838
S	11.159440	10.939073	0.091388
S	3.183140	10.917659	2.923961
S	0.006785	7.779688	2.714136
S	6.361876	10.874337	2.827899
S	9.562528	7.738642	2.781964
S	6.366620	7.734266	2.810807
S	3.184339	7.785343	2.714441
S	9.560777	10.884356	2.822716
S	0.006112	10.925599	2.911438
S	1.627298	7.675083	5.522335
S	7.972200	10.784682	5.601340
S	4.744548	7.668196	5.535358
S	1.610877	10.789696	5.635092
S	11.165378	7.665753	5.484078
S	7.968010	7.668342	5.492107
S	4.765242	10.795190	5.636008
S	11.154846	10.788568	5.606100
S	3.191034	7.743192	8.532188
S	-0.074053	10.753431	8.334473
S	6.330261	7.480533	8.179889
S	0.048639	7.479597	8.176900
S	6.452982	10.757694	8.337121
S	9.566504	7.541497	8.229484
S	9.568705	10.612733	8.419553
S	3.189290	10.677397	8.449780
S	6.508469	8.481362	11.022516
S	-0.125950	8.477559	11.019469
S	9.569102	8.981775	10.886630
C	3.191488	10.456353	11.533140
O	2.058347	10.094759	11.098267
O	4.327247	10.102979	11.098224
H	3.189091	11.135355	12.405833

COOH*

Mo	3.225985	9.491279	1.007513
Mo	9.529984	9.331067	1.000496
Mo	0.001028	9.427833	1.007745
Mo	6.295973	9.267601	1.007116
Mo	11.147014	9.310831	3.679966
Mo	7.952361	9.307247	3.709474
Mo	1.576559	9.319905	3.722577
Mo	4.754710	9.315445	3.759810
Mo	9.548578	9.245575	6.425845
Mo	-0.017038	9.234110	6.438084
Mo	6.346047	9.244392	6.468302
Mo	3.165604	9.257699	6.522517
Mo	5.034770	9.195020	9.311626
Mo	1.315008	9.208067	9.266172
Mo	11.285845	9.128585	9.174451
Mo	7.816825	9.148637	9.196130
S	1.614860	8.181726	-0.210095
S	4.777956	7.841677	0.047522

S	11.161430	8.009753	-0.103170
S	1.588466	10.916417	-0.000833
S	7.933580	7.885994	-0.062974
S	7.911236	10.622596	-0.159726
S	4.745963	10.955447	0.111644
S	11.127405	10.795462	-0.044566
S	3.169990	10.930333	2.916310
S	0.002119	7.768732	2.736060
S	6.346270	10.877719	2.814976
S	9.544460	7.736316	2.772862
S	6.345968	7.740434	2.846977
S	3.174797	7.797624	2.736489
S	9.536251	10.898253	2.805164
S	-0.013037	10.934099	2.859205
S	1.605468	7.711711	5.526613
S	7.947990	10.829671	5.578308
S	4.726384	7.706207	5.558706
S	1.590048	10.830150	5.613052
S	11.139903	7.701947	5.478504
S	7.945565	7.704089	5.511584
S	4.742422	10.839679	5.632060
S	11.140749	10.827376	5.557935
S	3.176257	7.765478	8.488285
S	-0.054039	10.841763	8.286796
S	6.340425	7.550740	8.219483
S	-0.009624	7.529397	8.180478
S	6.392445	10.839581	8.314257
S	9.543357	7.656478	8.251028
S	9.560919	10.701386	8.363087
S	3.189265	10.708792	8.491980
S	6.524565	8.889824	11.096113
S	-0.107549	8.779012	11.068810
S	9.585282	9.148075	10.855327
C	2.612280	9.654346	11.003400
O	3.848247	9.363915	11.055296
O	2.198682	10.328334	12.074259
H	1.208952	10.356428	12.035586

CHO*

Mo	3.204353	9.224342	0.968103
Mo	9.584494	9.421462	0.930729
Mo	-0.053471	9.220598	0.955463
Mo	6.302899	9.419780	0.952014
Mo	11.145553	9.336081	3.676680
Mo	7.948308	9.333543	3.667744
Mo	1.576200	9.336282	3.729591
Mo	4.753053	9.333619	3.729014
Mo	9.542778	9.349848	6.396069
Mo	-0.033505	9.332168	6.456962
Mo	6.363324	9.321740	6.436101
Mo	3.172632	9.345566	6.524374
Mo	5.045202	9.329470	9.268297
Mo	1.245204	9.329850	9.305379
Mo	11.067786	9.326946	9.174823
Mo	7.998464	9.307433	9.160015
S	1.579576	7.786706	-0.064415
S	4.746501	7.764863	0.052582
S	11.152289	7.771498	0.032307
S	1.578982	10.487587	-0.264350
S	7.937168	8.130767	-0.253770
S	7.936277	10.823625	-0.117255
S	4.753083	10.867443	0.028934
S	11.145612	10.856457	0.005462
S	3.161593	10.870691	2.747506
S	-0.003603	7.740925	2.834794
S	6.343669	10.918610	2.817003
S	9.546471	7.790059	2.706269
S	6.340951	7.789477	2.736211
S	3.159575	7.745321	2.852420
S	9.542324	10.922255	2.787569
S	-0.004550	10.873295	2.724301
S	1.599336	7.782018	5.591332
S	7.939738	10.899008	5.492791
S	4.737925	7.772607	5.573122
S	1.592476	10.896404	5.581459
S	11.139277	7.775376	5.500806
S	7.953629	7.769681	5.487864
S	4.743776	10.897805	5.574113
S	11.152560	10.905663	5.496146
S	3.140640	7.894435	8.525989
S	-0.115860	10.941986	8.291065
S	6.414513	7.680588	8.237350
S	-0.090292	7.698128	8.256732
S	6.433181	10.943948	8.276444
S	9.543371	7.746931	8.235557
S	9.527315	10.948933	8.226296
S	3.140026	10.805043	8.503394
S	6.501749	8.968398	11.027751
S	-0.244430	9.007276	11.054078
S	9.504904	9.689079	10.964085
C	3.761591	9.513340	11.021739
O	2.499559	9.469365	11.042697
H	4.185894	9.653927	12.041632

COH*

Mo	3.206758	9.316486	0.994208
Mo	9.585398	9.334575	0.959688
Mo	-0.056822	9.218401	0.979360
Mo	6.304113	9.227004	0.983071
Mo	11.136348	9.339276	3.721538
Mo	7.950436	9.341038	3.717751
Mo	1.574098	9.326034	3.765022
Mo	4.756155	9.329775	3.769766
Mo	9.543129	9.397366	6.468930
Mo	-0.046163	9.419413	6.488800
Mo	6.370791	9.423240	6.487987
Mo	3.165390	9.390028	6.558025
Mo	5.018763	9.459712	9.239580
Mo	1.300098	9.452664	9.260508
Mo	11.061112	9.474683	9.260389
Mo	8.015849	9.470145	9.262310
S	1.604000	7.886337	-0.107815
S	4.791778	7.689192	0.123142
S	11.183301	7.703820	0.095176
S	1.555705	10.599159	-0.165234
S	7.965757	7.912626	-0.130537
S	7.912112	10.619372	-0.166805
S	4.711948	10.818345	0.064000
S	11.114470	10.815748	0.037488
S	3.156617	10.874421	2.823592
S	-0.011689	7.742447	2.872596
S	6.336114	10.867186	2.758063
S	9.545378	7.766307	2.793841
S	6.356522	7.748012	2.873326
S	3.167883	7.755258	2.845391
S	9.536828	10.894040	2.777792
S	-0.009593	10.862836	2.753921
S	1.571408	7.820113	5.657531
S	7.955281	10.949714	5.506211
S	4.758312	7.819837	5.656820
S	1.592587	10.928428	5.569341
S	11.134785	7.820906	5.581557
S	7.946854	7.827203	5.580649
S	4.732942	10.935027	5.570535
S	11.129686	10.950081	5.506370
S	3.162186	7.874693	8.597276
S	-0.107751	11.094223	8.280450
S	6.463884	7.846244	8.341280
S	-0.139744	7.847936	8.347018
S	6.439599	11.102283	8.285744
S	9.538963	7.838005	8.343951
S	9.539649	11.027914	8.291260
S	3.157504	10.930943	8.417194
S	6.298535	9.605558	11.120318
S	0.003226	9.643757	11.112694
S	9.537176	9.201032	11.076326
C	3.169747	8.981471	10.308457
O	3.142976	8.297343	11.463866
H	4.061982	8.150505	11.787755

CH_2O*

Mo	3.229259	9.362853	0.966261
Mo	9.598132	9.370221	0.925783
Mo	-0.038502	9.268921	0.941596
Mo	6.318395	9.277767	0.956514
Mo	11.146910	9.318067	3.673602
Mo	7.953868	9.316132	3.685665
Mo	1.588353	9.321087	3.730149
Mo	4.768367	9.319737	3.754838
Mo	9.548632	9.318885	6.419275
Mo	-0.032845	9.319101	6.432356
Mo	6.356199	9.318686	6.482035
Mo	3.159987	9.319402	6.519735
Mo	5.052030	9.318923	9.348324
Mo	1.238756	9.319742	9.297404
Mo	11.019107	9.319591	9.177838
Mo	8.099494	9.318874	9.204141
S	1.627211	7.960909	-0.168639
S	4.805240	7.751371	0.069760
S	11.199652	7.762380	0.035631
S	1.580214	10.673410	-0.167464
S	7.972187	7.972050	-0.184309
S	7.928628	10.677087	-0.180894
S	4.737868	10.890281	0.072174
S	11.125983	10.876193	0.034698
S	3.177707	10.886027	2.828812
S	0.012283	7.749678	2.797575
S	6.350738	10.873903	2.772287
S	9.552231	7.761975	2.722927
S	6.356269	7.749580	2.812568
S	3.185388	7.768461	2.786488
S	9.540970	10.890337	2.775432
S	-0.000496	10.872954	2.749029
S	1.592074	7.756403	5.573579
S	7.938555	10.873617	5.513951
S	4.742043	7.752963	5.603906
S	1.589922	10.883051	5.574922
S	11.139651	7.754483	5.490386
S	7.940922	7.762446	5.515568
S	4.744211	10.885419	5.604774
S	11.141866	10.882820	5.490152
S	3.150579	7.894698	8.520229
S	-0.106666	10.937613	8.265103
S	6.430937	7.704496	8.322699
S	-0.106586	7.701668	8.266242
S	6.430195	10.933417	8.322640
S	9.550113	7.687046	8.245034
S	9.548899	10.951114	8.245309
S	3.150945	10.743616	8.520394
S	6.661811	9.320750	11.073382
S	-0.223963	9.322067	11.068510
S	9.592663	9.315130	11.037394
C	2.547354	9.318258	11.098020
O	3.919704	9.318959	10.901250
H	2.279566	10.214053	11.687332
H	2.279846	8.419795	11.684202

CHOH*

Mo	3.249462	9.204375	0.943456
Mo	9.630668	9.406993	0.956863
Mo	-0.018189	9.215428	0.957326
Mo	6.358124	9.410776	0.951237
Mo	11.188139	9.326908	3.717267
Mo	7.995241	9.319359	3.696196
Mo	1.616601	9.321298	3.695461
Mo	4.798417	9.314625	3.694359
Mo	9.591559	9.335704	6.458529
Mo	0.029851	9.331118	6.460373
Mo	6.393504	9.327754	6.436448
Mo	3.197677	9.335317	6.462841
Mo	4.995269	9.355903	9.148018
Mo	1.589341	9.337014	9.283894
Mo	11.363941	9.332190	9.262798
Mo	7.796432	9.348015	9.228567
S	1.608972	7.785568	-0.087506
S	4.799984	7.755903	0.030701
S	11.185608	7.762499	0.038236
S	1.613543	10.480661	-0.268516
S	7.996953	8.124464	-0.248304
S	7.997525	10.820700	-0.096776
S	4.812258	10.849000	0.014917
S	11.182327	10.855031	0.030136
S	3.207912	10.853294	2.710301
S	0.021119	7.730280	2.834591
S	6.400265	10.903884	2.819009
S	9.596188	7.778950	2.744013
S	6.402151	7.773509	2.731262
S	3.201367	7.723434	2.820143
S	9.588846	10.906486	2.821243
S	0.026037	10.862951	2.728649
S	1.620593	7.771162	5.545210
S	8.000105	10.886720	5.528343
S	4.783615	7.766509	5.537167
S	1.621626	10.890683	5.521647
S	11.176412	7.764830	5.557911
S	8.005223	7.768053	5.535735
S	4.781317	10.883203	5.518203
S	11.188701	10.900116	5.550599
S	3.247217	7.814165	8.393957
S	0.082253	10.943417	8.302508
S	6.412927	7.693918	8.237120
S	0.047941	7.722768	8.283769
S	6.421710	10.990044	8.207021
S	9.585195	7.848013	8.373080
S	9.591664	10.832267	8.366423
S	3.257796	10.893849	8.354567
S	6.224344	9.377099	11.083254
S	0.036814	9.053438	11.096971
S	9.561996	9.365982	10.888135
C	2.738567	9.690755	11.022681
O	2.881361	8.931905	12.107098
H	2.379011	8.092928	12.003364
H	3.204725	10.668479	11.226443

CH_2OH*

Mo	3.219403	9.199117	0.965573
Mo	9.524361	9.360430	0.950952
Mo	-0.003411	9.264997	0.962311
Mo	6.286521	9.424086	0.966970
Mo	11.141831	9.312293	3.635302
Mo	7.947256	9.316899	3.658541
Mo	1.573354	9.305304	3.683138
Mo	4.749100	9.311629	3.721195
Mo	9.542921	9.317863	6.377470
Mo	-0.015653	9.316505	6.396480
Mo	6.345857	9.316549	6.423990
Mo	3.157541	9.327610	6.488836
Mo	5.044697	9.355104	9.251763
Mo	1.304575	9.352711	9.271383
Mo	11.279370	9.320403	9.130490
Mo	7.827886	9.316301	9.145688
S	1.583946	7.796592	-0.076446
S	4.737573	7.757288	0.031912
S	11.125009	7.930258	-0.134965
S	1.612055	10.535294	-0.225896
S	7.899840	8.101317	-0.237898
S	7.923478	10.832919	-0.067629
S	4.767351	10.871328	0.041337
S	11.158660	10.711269	-0.116367
S	3.169634	10.851683	2.734224
S	-0.016289	7.711578	2.776645
S	6.339726	10.906775	2.841878
S	9.531655	7.747605	2.714515
S	6.336090	7.768426	2.734627
S	3.166686	7.714866	2.840974
S	9.541805	10.909296	2.762211
S	-0.003991	10.878405	2.731256
S	1.597707	7.753978	5.544286
S	7.945984	10.879104	5.494138
S	4.727385	7.751570	5.565568
S	1.593113	10.877610	5.517912
S	11.137670	7.752826	5.479190
S	7.942213	7.753142	5.491003
S	4.726738	10.884613	5.552505
S	11.140983	10.877256	5.472078
S	3.181208	7.898027	8.509495
S	-0.034173	10.974139	8.199421
S	6.358314	7.675503	8.219206
S	-0.010001	7.677689	8.212559
S	6.386954	10.975757	8.211949
S	9.548863	7.793076	8.256766
S	9.547041	10.850876	8.253818
S	3.167474	10.811950	8.438957
S	6.519213	9.126832	11.064940
S	-0.223221	9.186106	11.059019
S	9.542854	9.382456	10.804039
C	2.429393	9.453847	11.145921
O	3.869298	9.708551	10.982132
H	2.058295	10.245716	11.812957
H	2.332305	8.480629	11.653581
H	4.364838	9.645340	11.826134

CH*			
Mo	3.229776	9.198595	0.963403
Mo	9.614262	9.428107	0.927718
Mo	-0.034851	9.196883	0.952253
Mo	6.324668	9.427370	0.944721
Mo	11.162028	9.333713	3.690150
Mo	7.970946	9.336129	3.670725
Mo	1.597706	9.325114	3.738249
Mo	4.776379	9.328479	3.725517
Mo	9.563917	9.354779	6.423393
Mo	-0.007258	9.349294	6.465902
Mo	6.393302	9.379379	6.442236
Mo	3.178662	9.369172	6.522112
Mo	5.067533	9.460824	9.191640
Mo	1.464935	9.404648	9.229327
Mo	10.990579	9.384306	9.182399
Mo	8.005398	9.423023	9.198098
S	1.601234	7.754758	-0.056920
S	4.775460	7.749027	0.056997
S	11.174021	7.750184	0.043830
S	1.602768	10.449040	-0.281660
S	7.964531	8.162526	-0.281122
S	7.964844	10.849126	-0.100645
S	4.769792	10.870097	0.039096
S	11.175892	10.863801	0.020420
S	3.178137	10.851515	2.736380
S	0.011452	7.732949	2.847217
S	6.364477	10.917233	2.813460
S	9.564947	7.793730	2.709220
S	6.370394	7.791581	2.730274
S	3.182818	7.730351	2.859386
S	9.567344	10.920681	2.790627
S	0.019389	10.853566	2.720390
S	1.607878	7.781226	5.611167
S	7.980536	10.914403	5.477184
S	4.766484	7.799986	5.594626
S	1.595078	10.911933	5.562157
S	11.165148	7.783101	5.526820
S	7.964285	7.792675	5.506686
S	4.747663	10.914665	5.541556
S	11.176169	10.909081	5.506748
S	3.273025	7.931240	8.515558
S	-0.079899	10.958899	8.319623
S	6.472704	7.803865	8.300802
S	-0.130234	7.798766	8.360179
S	6.478247	11.052129	8.196906
S	9.513591	7.768756	8.257472
S	9.541233	10.985672	8.234854
S	3.271070	10.923730	8.432896
S	6.344998	9.706606	11.052172
S	0.362262	9.195620	11.343515
S	9.617218	9.124808	11.025628
C	1.610508	10.281959	10.986743
H	1.978454	11.102729	11.606935

CH_2*			
Mo	3.234888	9.311845	0.913995
Mo	9.613949	9.317389	0.943723
Mo	-0.053893	9.321116	0.933459
Mo	6.333196	9.326234	0.930059
Mo	11.162553	9.319568	3.718786
Mo	7.970150	9.318517	3.715185
Mo	1.597872	9.319070	3.675987
Mo	4.779014	9.318642	3.679065
Mo	9.568375	9.320354	6.466192
Mo	0.012147	9.318894	6.438754
Mo	6.361197	9.319353	6.440001
Mo	3.191031	9.320960	6.443386
Mo	4.690837	9.328376	9.229408
Mo	1.682014	9.327763	9.222755
Mo	11.397887	9.320736	9.273124
Mo	7.735556	9.321022	9.273150
S	1.583753	7.961785	-0.190514
S	4.782472	7.745432	0.042631
S	11.152904	7.743875	0.060355
S	1.585994	10.674155	-0.190125
S	7.976881	7.962237	-0.175828
S	7.979302	10.679157	-0.175949
S	4.795000	10.892401	0.042441
S	11.156414	10.896280	0.062443
S	3.185656	10.882141	2.741461
S	-0.003626	7.758307	2.769077
S	6.386633	10.879765	2.770523
S	9.563311	7.760940	2.786588
S	6.385123	7.758381	2.765102
S	3.184127	7.755023	2.747403
S	9.563272	10.877093	2.785375
S	-0.002992	10.880711	2.770319
S	1.602235	7.762680	5.506077
S	7.973976	10.885512	5.553800
S	4.776138	7.758949	5.507036
S	1.601161	10.875805	5.504609
S	11.157747	7.749332	5.554310
S	7.974884	7.753472	5.555348
S	4.776140	10.879727	5.505044
S	11.158644	10.889478	5.553606
S	3.187682	7.709654	8.317712
S	0.065095	10.916586	8.281769
S	6.307756	7.728476	8.288777
S	0.065390	7.725647	8.285837
S	6.309301	10.915247	8.284599
S	9.566443	7.850199	8.388800
S	9.566594	10.791065	8.388345
S	3.188343	10.940989	8.304017
S	6.215786	9.316088	11.088375
S	0.157571	9.313876	11.086052
S	9.566321	9.319391	10.884030
C	3.183488	9.390020	10.825964
H	3.178252	8.537281	11.518441
H	3.178481	10.337780	11.383362

CH_3*			
Mo	3.243600	9.201242	0.964627
Mo	9.593063	9.387718	0.975016
Mo	-0.003547	9.231521	0.975513
Mo	6.340723	9.422086	0.970811
Mo	11.172220	9.311830	3.689346
Mo	7.979679	9.320453	3.696167
Mo	1.601044	9.306694	3.695765
Mo	4.783912	9.316170	3.713701
Mo	9.570570	9.322963	6.436380
Mo	0.007428	9.324002	6.442037
Mo	6.366371	9.325444	6.440967
Mo	3.200561	9.325627	6.471368
Mo	4.951019	9.355301	9.268291
Mo	1.363661	9.348311	9.212757
Mo	11.325506	9.342877	9.206940
Mo	7.795834	9.345270	9.217604
S	1.605672	7.776353	-0.054413
S	4.785724	7.764886	0.040613
S	11.165602	7.817282	-0.001086
S	1.616828	10.494758	-0.241519
S	7.966768	8.125617	-0.234428
S	7.981925	10.843418	-0.051064
S	4.802159	10.857287	0.036557
S	11.180452	10.798883	-0.004418
S	3.194946	10.851411	2.728379
S	0.010780	7.711572	2.824104
S	6.382763	10.909764	2.842884
S	9.569502	7.759228	2.746030
S	6.380964	7.775331	2.740525
S	3.196257	7.716566	2.839648
S	9.576188	10.908183	2.817053
S	0.016061	10.865241	2.742153
S	1.619355	7.761691	5.554102
S	7.978014	10.883086	5.535528
S	4.775137	7.753585	5.551080
S	1.619153	10.875756	5.526901
S	11.161548	7.756658	5.533125
S	7.975429	7.760273	5.535287
S	4.767847	10.888919	5.538071
S	11.167696	10.881137	5.518456
S	3.164656	7.852733	8.426393
S	-0.015299	10.986014	8.220930
S	6.349491	7.710482	8.272207
S	-0.011694	7.690312	8.245088
S	6.354463	10.971110	8.245304
S	9.561487	7.834254	8.346598
S	9.563683	10.839894	8.326371
S	3.161385	10.835642	8.392486
S	6.409731	9.347857	11.105465
S	0.021843	9.342209	11.093610
S	9.583554	9.353551	10.865161
C	3.517543	9.421139	10.996545
H	3.760050	8.563132	11.639589
H	3.730478	10.366861	11.516845
H	2.390001	9.399680	11.016175

CH_4*			
Mo	3.244193	9.375927	0.849476
Mo	9.621666	9.371461	0.850810
Mo	-0.025712	9.271051	0.859343
Mo	6.350377	9.265590	0.859083
Mo	11.176379	9.321511	3.631350
Mo	7.980640	9.320925	3.627648
Mo	1.611965	9.323275	3.635448
Mo	4.790488	9.322133	3.640464
Mo	9.579711	9.328164	6.393290
Mo	0.012557	9.328371	6.402110
Mo	6.385212	9.327925	6.406915
Mo	3.203347	9.328438	6.426236
Mo	5.027872	9.336982	9.129645
Mo	1.379404	9.339395	9.125003
Mo	11.335878	9.341321	9.177466
Mo	7.825442	9.338954	9.181331
S	1.630404	7.973667	-0.271144
S	4.834079	7.754401	-0.033664
S	11.211928	7.757307	-0.032798
S	1.581570	10.680823	-0.260327
S	8.009239	7.964182	-0.264382
S	7.958931	10.668991	-0.270016
S	4.762449	10.875560	-0.050541
S	11.142305	10.881543	-0.040617
S	3.194815	10.886921	2.716376
S	0.025312	7.754957	2.726336
S	6.384358	10.869290	2.672487
S	9.580628	7.776474	2.671085
S	6.394602	7.753125	2.729349
S	3.203469	7.776240	2.666772
S	9.571369	10.884443	2.716553
S	0.014271	10.871551	2.675831
S	1.634548	7.778967	5.484945
S	7.986555	10.878823	5.465038
S	4.769396	7.775500	5.488214
S	1.629897	10.873189	5.480624
S	11.168572	7.769101	5.469989
S	7.989451	7.771795	5.471937
S	4.770881	10.876374	5.481770
S	11.168536	10.882180	5.462553
S	3.203336	7.841410	8.431540
S	-0.016747	10.987389	8.165795
S	6.423211	7.681169	8.185766
S	-0.018410	7.683561	8.182784
S	6.420844	10.987408	8.172148
S	9.580534	7.835800	8.301230
S	9.578722	10.836139	8.289165
S	3.203865	10.828447	8.429180
S	6.259979	9.365892	11.038209
S	0.141673	9.381224	11.032102
S	9.581626	9.338205	10.832173
C	3.176025	8.951765	12.441195
H	3.190411	9.889274	11.864359
H	2.233988	8.896107	13.002667
H	4.035763	8.943905	13.124664
H	3.244581	8.086365	11.765890

4. Adsorption of species on S edge

H_2O*			
Mo	4.797738	3.172556	0.170518
Mo	7.938454	3.165476	0.127005
Mo	11.128410	3.168130	0.133800
Mo	1.505388	3.173946	0.170102
Mo	6.348305	3.087053	2.739004
Mo	9.530839	3.079933	2.756929
Mo	3.152742	3.102188	2.714703
Mo	-0.041938	3.091482	2.746591
Mo	1.559074	3.004944	5.498710
Mo	4.754704	3.051916	5.483784
Mo	11.114348	3.011972	5.494421
Mo	7.938895	2.962875	5.505517
Mo	6.317602	2.913026	8.099552
Mo	3.199251	3.060976	8.130295
Mo	-0.083690	2.897445	8.099916
Mo	9.584875	2.880787	8.100577
S	6.372982	1.529178	0.830254
S	-0.065300	1.531513	0.842312
S	6.382087	4.761479	0.931645
S	3.150843	4.761347	0.865900
S	9.534124	1.561152	0.845039
S	3.151286	1.551463	0.776211
S	-0.070657	4.764249	0.941383
S	9.530288	4.721094	0.948322
S	1.556757	4.621745	3.700977
S	7.930301	1.484062	3.613902
S	1.570942	1.509967	3.613880
S	7.937498	4.600589	3.731422
S	11.118264	4.625190	3.715316
S	4.753062	4.640424	3.674998
S	4.735158	1.522100	3.614002
S	11.130123	1.500155	3.620041
S	3.209044	1.446590	6.436879
S	6.398788	4.569204	6.490104
S	9.582663	1.340216	6.379280
S	9.495017	4.548313	6.511705
S	-0.025966	4.557133	6.500350
S	3.136337	4.622650	6.420670
S	-0.082446	1.368551	6.366764
S	6.272519	1.370527	6.373603
S	1.575615	1.835262	9.306559
S	4.830744	3.806875	9.588325
S	7.938662	1.906787	9.390075
S	11.121245	3.643925	9.631269
O	1.984211	4.850676	9.310752
H	2.443587	5.711794	9.231773
H	1.984703	4.618652	10.261016

CO*			
Mo	4.815123	3.155441	0.163118
Mo	7.965995	3.141933	0.175610
Mo	11.096328	3.156915	0.192323
Mo	1.631637	3.171751	0.196613
Mo	6.383684	3.094830	2.807429
Mo	9.558549	3.095338	2.794921
Mo	3.195913	3.137834	2.758036
Mo	-0.003800	3.139084	2.734006
Mo	1.593369	3.108219	5.472869
Mo	4.795547	3.087950	5.549707
Mo	11.149560	3.088857	5.539598
Mo	7.972010	2.996492	5.551419
Mo	6.451221	2.961269	8.163056
Mo	3.182069	3.103126	8.198621
Mo	0.004150	3.102255	8.195645
Mo	9.497804	2.959173	8.158286
S	6.379982	1.544263	0.918910
S	-0.009946	1.553134	0.819577
S	6.393104	4.717744	0.979763
S	3.238747	4.769850	0.909277
S	9.536827	1.522233	0.907429

S	3.222693	1.544024	0.873518
S	-0.023914	4.767143	0.853324
S	9.521363	4.740759	0.970058
S	1.590439	4.698270	3.664595
S	7.974753	1.495440	3.679669
S	1.589235	1.565344	3.630741
S	7.974600	4.621582	3.771030
S	11.146820	4.664942	3.713452
S	4.802897	4.665248	3.730245
S	4.759404	1.550908	3.690880
S	11.188184	1.552631	3.674304
S	3.160504	1.547006	6.433724
S	6.459165	4.617768	6.542415
S	9.626945	1.409426	6.461086
S	9.486847	4.616415	6.538028
S	-0.032299	4.674840	6.438223
S	3.218403	4.676167	6.441662
S	0.025411	1.547247	6.430011
S	6.319318	1.409386	6.468660
S	1.592620	1.881910	9.424219
S	4.867438	3.834822	9.585186
S	7.975416	1.989523	9.572042
S	11.076936	3.834915	9.583938
C	1.591896	4.490389	8.654076
O	1.592821	5.555227	9.179310

OH*

Mo	4.819887	3.099663	0.164422
Mo	7.972311	3.097427	0.151096
Mo	11.124279	3.099805	0.164815
Mo	1.594490	3.100956	0.188505
Mo	6.385441	3.101880	2.773973
Mo	9.559238	3.102026	2.773648
Mo	3.190668	3.110023	2.726214
Mo	-0.001986	3.110239	2.725982
Mo	1.594141	3.104968	5.465808
Mo	4.784480	3.139706	5.520933
Mo	11.159499	3.140252	5.520498
Mo	7.972145	3.084538	5.537565
Mo	6.348931	3.110556	8.164116
Mo	3.141699	3.173527	8.154493
Mo	0.045967	3.173874	8.154258
Mo	9.595737	3.111148	8.163850
S	6.397365	1.500942	0.920966
S	-0.026239	1.487554	0.856072
S	6.399606	4.698739	0.914197
S	3.214209	4.718440	0.846200
S	9.546867	1.500503	0.920800
S	3.214612	1.487725	0.856556
S	-0.025575	4.718946	0.845562
S	9.544573	4.699373	0.914115
S	1.594341	4.673609	3.635555
S	7.972454	1.534793	3.705280
S	1.594055	1.543463	3.640198
S	7.972284	4.655190	3.707916
S	11.160674	4.672659	3.665025
S	4.783866	4.672291	3.665571
S	4.773121	1.561952	3.691269
S	11.171364	1.562209	3.691085
S	3.212657	1.558027	6.436931
S	6.420123	4.704867	6.487511
S	9.616479	1.519832	6.482896
S	9.523922	4.705463	6.487173
S	0.019717	4.716591	6.391887
S	3.168500	4.716327	6.392496
S	-0.024753	1.558481	6.436601
S	6.327775	1.519526	6.483021
S	1.593676	1.797697	9.259587
S	4.757202	3.992283	9.579178
S	7.972481	2.176332	9.500215
S	11.186145	3.993380	9.579182
O	1.593740	4.559148	8.820979
H	1.593601	4.492098	9.796406

H*

Mo	4.834276	3.091241	0.157433
Mo	7.971750	3.087858	0.158376
Mo	11.109991	3.091455	0.158937
Mo	1.595381	3.094876	0.181297
Mo	6.385469	3.105467	2.780715
Mo	9.558993	3.105697	2.780629
Mo	3.192788	3.112251	2.723353
Mo	-0.003932	3.111744	2.723183
Mo	1.593984	3.113263	5.455703
Mo	4.784450	3.155886	5.522308
Mo	11.159684	3.156544	5.522088
Mo	7.972267	3.101494	5.531978
Mo	6.396064	3.139360	8.151502
Mo	3.122717	3.163474	8.140054
Mo	0.064693	3.163595	8.139883
Mo	9.548645	3.139445	8.151971
S	6.398912	1.494218	0.937432
S	-0.031946	1.486444	0.852795
S	6.402882	4.693997	0.916141
S	3.222171	4.709481	0.831930
S	9.543819	1.494512	0.937050
S	3.221458	1.486462	0.853262
S	-0.032516	4.709524	0.831163
S	9.540150	4.693701	0.915919
S	1.594184	4.676884	3.624827
S	7.972440	1.539008	3.711683
S	1.594450	1.545467	3.633820
S	7.972221	4.666662	3.701680
S	11.163941	4.680616	3.660313
S	4.780773	4.680753	3.660365
S	4.773253	1.568832	3.700096
S	11.171721	1.568189	3.699535
S	3.206830	1.571331	6.438827
S	6.428898	4.732655	6.471065
S	9.609873	1.539896	6.489296
S	9.515179	4.732235	6.471434
S	0.027577	4.733265	6.393637
S	3.159978	4.733392	6.393836
S	-0.018819	1.570850	6.438473
S	6.334574	1.540094	6.489345
S	1.593285	1.938176	9.379405
S	4.756069	4.032501	9.505368
S	7.972259	2.216846	9.541438
S	11.188287	4.032757	9.505581
H	1.593911	4.222384	8.251658

H*

Mo	4.687208	3.062564	0.190927
Mo	8.035746	3.067634	0.191036
Mo	11.127859	3.078369	0.190135
Mo	1.565850	3.072785	0.171518
Mo	6.357412	3.100491	2.733779
Mo	9.550795	3.126374	2.797779
Mo	3.163496	3.101650	2.775239
Mo	-0.022944	3.127213	2.819255
Mo	1.583548	3.149660	5.578847
Mo	4.767817	3.137122	5.460351
Mo	11.138027	3.224992	5.546934
Mo	7.940853	3.151323	5.556125
Mo	6.081322	3.150509	8.072219
Mo	3.458310	3.149962	8.077372
Mo	-0.124284	3.298728	8.155055
Mo	9.638335	3.298122	8.143864
S	6.365669	1.480733	0.851159
S	-0.028474	1.516336	0.987809
S	6.359997	4.665769	0.804430
S	3.128585	4.697940	0.894949
S	9.583169	1.467129	0.978461
S	3.118194	1.456235	0.940058
S	-0.021797	4.667401	0.926019
S	9.572816	4.711991	0.911169
S	1.593208	4.678314	3.709779
S	7.953175	1.573605	3.729444
S	1.566006	1.570885	3.761541
S	7.927800	4.676798	3.675760
S	11.136305	4.723711	3.675143
S	4.771498	4.682959	3.618261
S	4.770425	1.538842	3.661219
S	11.136711	1.596129	3.771982
S	3.213663	1.532722	6.479800
S	6.304169	4.758163	6.453658
S	9.599983	1.621495	6.539892
S	9.491537	4.824818	6.437055
S	0.026484	4.823866	6.451999
S	3.229701	4.756420	6.460456
S	-0.082193	1.622090	6.552772
S	6.323299	1.532666	6.472751
S	1.577946	2.513875	9.455394
S	4.771711	3.155603	10.138893
S	7.949526	2.496226	9.450555
S	11.128271	4.297511	9.586963
H	4.781787	4.494874	10.393916

O*

Mo	4.816993	3.069345	0.160326
Mo	7.971657	3.062287	0.150113
Mo	11.126761	3.070182	0.161945
Mo	1.595756	3.073824	0.189649
Mo	6.385430	3.102204	2.769096
Mo	9.559057	3.102345	2.768464
Mo	3.184767	3.118664	2.728902
Mo	0.004277	3.118680	2.727908
Mo	1.594174	3.168897	5.456742
Mo	4.801212	3.178232	5.532277
Mo	11.142845	3.178463	5.531441
Mo	7.972232	3.100913	5.518603
Mo	6.468173	3.095345	8.141433
Mo	3.061826	3.284077	8.208972
Mo	0.125406	3.284164	8.208687
Mo	9.476186	3.095270	8.141099
S	6.391739	1.475880	0.935474
S	-0.023779	1.468038	0.878041
S	6.400350	4.674725	0.890966
S	3.216638	4.700199	0.821381
S	9.551843	1.474902	0.934912
S	3.213393	1.468428	0.880466
S	-0.026722	4.700859	0.819583
S	9.542820	4.676219	0.890624
S	1.594162	4.702596	3.609691
S	7.972437	1.539002	3.696487
S	1.593984	1.563502	3.673156
S	7.972409	4.664739	3.685888
S	11.155093	4.683582	3.649501
S	4.789699	4.683465	3.650593
S	4.764874	1.584416	3.714488
S	11.179876	1.584496	3.713461
S	3.196677	1.653193	6.488009
S	6.451923	4.735885	6.492556
S	9.607621	1.528916	6.466713
S	9.492075	4.736226	6.492204
S	-0.001753	4.776792	6.367776
S	3.189971	4.776689	6.368333
S	-0.009184	1.653615	6.487097
S	6.336892	1.529125	6.467148
S	1.592381	1.720605	9.198215
S	4.826363	3.827186	9.591391
S	7.972409	2.084646	9.539579
S	11.117124	3.828485	9.590738
O	1.594021	4.465323	8.719069

HCOO*

Mo	4.696223	3.168559	0.210780
Mo	8.050665	3.160561	0.203670
Mo	11.149470	3.178708	0.190482
Mo	1.598617	3.187123	0.193906
Mo	6.377221	3.101117	2.757497
Mo	9.564646	3.114061	2.799718
Mo	3.181083	3.143701	2.805092
Mo	-0.005731	3.153799	2.831225
Mo	1.601940	3.145563	5.587184
Mo	4.788808	3.062194	5.544687
Mo	11.130724	3.099057	5.565547
Mo	7.964765	2.988771	5.530234
Mo	6.316739	2.813112	8.114072
Mo	3.419844	3.158433	8.210343
Mo	-0.066533	3.179009	8.274292
Mo	9.586143	2.888166	8.163144
S	6.370970	1.557119	0.809024
S	0.000324	1.604919	0.947605
S	6.378013	4.734802	0.889786
S	3.155187	4.792229	0.975143
S	9.610037	1.531184	0.911942
S	3.137317	1.547011	0.929491
S	-0.009386	4.748466	0.984818
S	9.589683	4.774871	0.981238
S	1.599027	4.705461	3.749725
S	7.964875	1.509725	3.635498
S	1.589682	1.595180	3.745367
S	7.953446	4.628647	3.754321
S	11.126547	4.683310	3.759114
S	4.815035	4.656626	3.733109
S	4.763410	1.543476	3.661846
S	11.174238	1.561687	3.709823
S	3.184038	1.527714	6.525579
S	6.420359	4.555551	6.585890
S	9.628553	1.385067	6.407674
S	9.477890	4.586292	6.574756
S	-0.030582	4.684659	6.488391
S	3.246122	4.708000	6.460670
S	-0.020548	1.568751	6.533500
S	6.321141	1.326962	6.373782
S	1.613993	1.968732	9.277916
S	4.931761	2.921393	9.946190
S	7.988353	1.751591	9.330187
S	11.016234	3.410849	9.867672
C	1.728648	5.393189	9.663874
O	0.577537	5.004543	9.312279
O	2.844579	4.858409	9.392066
H	1.771684	6.309078	10.282502

COOH*

Mo	4.785425	3.231468	0.209462
Mo	7.894065	3.214782	0.179085
Mo	11.100686	3.216714	0.181671
Mo	1.451070	3.233353	0.207261
Mo	6.315362	3.115906	2.798872
Mo	9.493799	3.097282	2.821264
Mo	3.122573	3.149207	2.759718
Mo	-0.074758	3.129027	2.798330
Mo	1.524159	3.050395	5.544938
Mo	4.733102	3.048562	5.539317
Mo	11.091287	2.998725	5.561857
Mo	7.901193	2.959019	5.565592
Mo	6.248573	2.857030	8.172420
Mo	3.141409	3.007704	8.230669
Mo	12.493309	2.967408	8.203385
Mo	9.587065	2.813626	8.147498
S	6.337747	1.573657	0.878177
S	-0.095924	1.579846	0.886590
S	6.352911	4.809502	1.009293
S	3.117847	4.805933	0.907725
S	9.498036	1.609880	0.886173
S	3.117419	1.621001	0.803702
S	-0.114100	4.814454	1.005926
S	9.493848	4.748224	1.022671
S	1.526568	4.669576	3.748398
S	7.891538	1.498149	3.660340
S	1.544358	1.557733	3.649864
S	7.906488	4.614616	3.811987
S	11.075413	4.632796	3.791921
S	4.727669	4.661978	3.749806
S	4.694367	1.546579	3.645270
S	11.109591	1.514672	3.661665
S	3.153774	1.458286	6.437268
S	6.363542	4.546008	6.589361
S	9.537493	1.300417	6.423868
S	9.466103	4.523020	6.607072
S	-0.115103	4.588078	6.513667
S	3.131398	4.589228	6.507980
S	-0.043705	1.408007	6.414656
S	6.242300	1.347849	6.411078
S	1.524733	1.699444	9.222645
S	4.778964	3.531818	9.787660
S	7.881095	1.799321	9.377838
S	11.008272	2.978812	9.966613
C	0.827278	4.554252	9.215732
O	2.085783	4.642930	9.258960
O	0.136046	5.577287	9.745500
H	0.781794	6.251709	10.065156

CHO*

Mo	4.849882	3.111579	0.176422
Mo	8.021596	3.102497	0.139098
Mo	11.190268	3.099226	0.146167
Mo	1.587037	3.109869	0.188015
Mo	6.420883	3.112088	2.742528

Mo	9.591435	3.094614	2.769127
Mo	3.222625	3.128351	2.724014
Mo	0.024740	3.109366	2.755916
Mo	1.625740	3.145201	5.493970
Mo	4.841810	3.154158	5.516926
Mo	11.174820	3.087702	5.540792
Mo	8.001676	3.108480	5.483998
Mo	6.672348	3.146291	8.104480
Mo	3.300636	3.211727	8.207645
Mo	-0.004406	3.094916	8.248094
Mo	9.344545	3.094160	8.090496
S	6.439848	1.496589	0.882506
S	0.006287	1.490949	0.901980
S	6.447051	4.721101	0.875486
S	3.220715	4.730321	0.823978
S	9.604088	1.510348	0.905773
S	3.222862	1.502798	0.845171
S	-0.004507	4.720463	0.895239
S	9.605257	4.686916	0.910079
S	1.621882	4.689085	3.645850
S	7.990753	1.533534	3.665811
S	1.637973	1.570699	3.671219
S	8.007569	4.674188	3.659508
S	11.183752	4.646355	3.698542
S	4.826272	4.684991	3.652024
S	4.808374	1.578844	3.682147
S	11.195259	1.540864	3.694820
S	3.230757	1.608936	6.430209
S	6.481128	4.755903	6.467039
S	9.535929	1.467044	6.478044
S	9.584950	4.711964	6.463301
S	-0.015442	4.657493	6.429908
S	3.244796	4.733129	6.403079
S	0.048570	1.547204	6.460875
S	6.406974	1.519632	6.482000
S	1.699285	1.888589	9.298020
S	4.951878	3.973276	9.566424
S	8.024453	3.128704	9.982952
S	11.098537	2.203349	9.488589
C	2.139843	4.803738	9.009422
O	0.884245	4.740926	9.160941
H	2.581260	5.779997	9.301440

COH*

Mo	4.792560	3.036449	0.139068
Mo	7.967517	3.040680	0.134701
Mo	11.107325	3.032328	0.163413
Mo	1.662900	3.029035	0.160140
Mo	6.381105	3.116970	2.771595
Mo	9.563184	3.114108	2.746096
Mo	3.199270	3.101912	2.749777
Mo	0.001380	3.100722	2.709446
Mo	1.591426	3.142113	5.494823
Mo	4.788376	3.200266	5.509430
Mo	11.162872	3.203233	5.485008
Mo	7.976939	3.201826	5.516748
Mo	6.270804	3.311185	8.106871
Mo	3.327720	3.233530	8.109466
Mo	-0.130580	3.236862	8.087428
Mo	9.653270	3.331602	8.102751
S	6.384065	1.481504	0.957778
S	0.005110	1.448603	0.855723
S	6.379441	4.644042	0.863420
S	3.223935	4.666822	0.848250
S	9.528260	1.445340	0.935605
S	3.234403	1.437864	0.938530
S	0.009660	4.648112	0.764296
S	9.537703	4.672334	0.838114
S	1.589481	4.669923	3.618332
S	7.978115	1.585062	3.738318
S	1.590123	1.557614	3.678542
S	7.979595	4.701876	3.631642
S	11.175508	4.699575	3.594801
S	4.776095	4.702897	3.632661
S	4.792116	1.578266	3.727832
S	11.161276	1.580013	3.694040
S	3.210922	1.581779	6.467787
S	6.390807	4.849485	6.402001
S	9.601895	1.646062	6.517451
S	9.558363	4.850186	6.377541
S	0.026713	4.783543	6.388259
S	3.167066	4.786509	6.408404
S	-0.031018	1.571999	6.439518
S	6.354698	1.635980	6.528602
S	1.580984	2.246039	9.467254
S	4.783173	3.631225	9.856732
S	7.983174	2.390756	9.392542
S	11.174508	3.941499	9.755132
C	1.585774	4.076686	9.061756
O	1.637973	5.075569	9.971683
H	0.724688	5.303004	10.255171

CH_2O*

Mo	4.767625	3.126505	0.149734
Mo	7.925148	3.112527	0.176824
Mo	11.220267	3.129448	0.178765
Mo	1.610160	3.138270	0.152443
Mo	6.378669	3.088944	2.750791
Mo	9.567944	3.088279	2.711318
Mo	3.191854	3.129042	2.783974
Mo	0.012404	3.131531	2.763304
Mo	1.607205	3.136669	5.534361
Mo	4.807072	3.106130	5.541255
Mo	11.132357	3.107916	5.498568
Mo	7.980841	2.999909	5.479736
Mo	6.483158	2.971466	8.140899
Mo	3.229344	3.224500	8.323468
Mo	-0.051956	3.206081	8.247021
Mo	9.579553	2.947956	8.126097
S	6.332586	1.495392	0.874378
S	0.045776	1.523237	0.904772
S	6.348518	4.724374	0.910421
S	3.195919	4.719244	0.930037
S	9.580474	1.503563	0.797462
S	3.183765	1.546057	0.923463
S	0.036740	4.747331	0.908666
S	9.564823	4.718460	0.836756
S	1.600551	4.695833	3.697074
S	7.982594	1.495115	3.608874
S	1.598633	1.574812	3.709167
S	7.982881	4.620346	3.685950
S	11.131134	4.667404	3.662652
S	4.815211	4.663622	3.706069
S	4.770958	1.553795	3.693634
S	11.177166	1.553323	3.651382
S	3.196926	1.610439	6.531467
S	6.483774	4.618518	6.483064
S	9.634150	1.413765	6.384134
S	9.488726	4.614124	6.500445
S	-0.032395	4.681672	6.410781
S	3.227387	4.690291	6.465885
S	-0.029050	1.591442	6.475484
S	6.332602	1.427892	6.407291
S	1.518875	1.853550	9.260607
S	5.050691	4.009489	9.568082
S	8.014635	1.870431	9.413838
S	10.992760	3.689608	9.745655
C	2.129804	4.873037	9.181527
O	0.830364	4.886731	9.149586
H	2.602255	5.852115	9.371758
H	2.578747	4.054513	9.931423

CHOH*

Mo	4.771610	3.165539	0.186018
Mo	8.076962	3.164525	0.184277
Mo	11.231208	3.179081	0.177445
Mo	1.601834	3.178895	0.166149
Mo	6.422279	3.097147	2.714441
Mo	9.614226	3.121814	2.779364
Mo	3.217944	3.112151	2.765157
Mo	0.036573	3.131211	2.814216
Mo	1.638277	3.062507	5.584974
Mo	4.820704	3.030898	5.462157
Mo	11.201832	3.087578	5.553499
Mo	8.000798	3.019715	5.516769
Mo	6.165915	2.907584	8.056477
Mo	3.543317	3.034021	8.070561
Mo	-0.179490	3.017163	8.194647
Mo	9.627807	3.025395	8.138352
S	6.424284	1.540437	0.773720
S	0.041742	1.575854	0.930868
S	6.426699	4.752262	0.856804
S	3.189264	4.763679	0.944671
S	9.659862	1.548542	0.889811
S	3.176673	1.547351	0.868654
S	0.043173	4.755541	0.990743
S	9.646335	4.768065	0.952285
S	1.641695	4.652562	3.768570
S	8.014946	1.522651	3.631810
S	1.628772	1.552682	3.709286
S	7.992533	4.635396	3.719877
S	11.193969	4.678957	3.750531
S	4.841397	4.642235	3.673579
S	4.821233	1.512400	3.591855
S	11.201090	1.554527	3.696488
S	3.257365	1.417105	6.445699
S	6.398637	4.594286	6.508875
S	9.650611	1.443387	6.445379
S	9.541604	4.648452	6.509761
S	0.061107	4.639902	6.589697
S	3.292926	4.656525	6.444912
S	-0.002188	1.435420	6.465284
S	6.385251	1.360285	6.371604
S	1.606632	1.930369	9.415862
S	4.871015	2.925363	9.992541
S	7.986178	2.082257	9.393223
S	11.064234	3.704560	9.799178
C	1.237607	3.639754	9.750803
O	2.336495	4.504985	9.365533
H	2.923668	4.645623	10.144347
H	0.884278	3.883793	10.758644

CH_2OH*

Mo	4.781394	3.271406	0.260070
Mo	8.045271	3.260606	0.247032
Mo	11.204746	3.267256	0.228194
Mo	1.590696	3.280434	0.229137
Mo	6.411200	3.129132	2.791208
Mo	9.598260	3.115921	2.840074
Mo	3.208820	3.153200	2.820979
Mo	0.020774	3.137896	2.855373
Mo	1.616657	3.018984	5.607938
Mo	4.837641	3.022508	5.551916
Mo	11.185202	2.978659	5.598482
Mo	7.993921	2.937473	5.573546
Mo	6.338366	2.811311	8.177269
Mo	3.250154	2.953083	8.221245
Mo	-0.193313	2.925444	8.262034
Mo	9.665494	2.762682	8.163739
S	6.412223	1.619762	0.819018
S	0.026721	1.644405	0.921169
S	6.422293	4.841936	0.991298
S	3.180550	4.851763	1.034297
S	9.631314	1.618133	0.892629
S	3.176706	1.635982	0.881080
S	0.014114	4.824791	1.085949
S	9.624374	4.821125	1.072880
S	1.616312	4.658234	3.837220
S	7.987411	1.503984	3.643246
S	1.629700	1.552450	3.700211
S	7.997650	4.617261	3.834806
S	11.173076	4.637632	3.853131
S	4.832590	4.659292	3.788445
S	4.804873	1.542951	3.645141
S	11.199507	1.516563	3.683056
S	3.267911	1.408971	6.443553
S	6.461056	4.515476	6.612618
S	9.631657	1.272248	6.413914
S	9.555722	4.490133	6.642706
S	-0.009837	4.552885	6.614814
S	3.238552	4.557616	6.537345
S	0.035976	1.369155	6.464779
S	6.340378	1.314388	6.404498
S	1.631277	1.665590	9.236083
S	4.871531	3.529347	9.787214
S	7.960846	1.724765	9.368275
S	11.049326	2.977320	10.000270
C	0.771384	4.444577	9.604928
O	2.170626	4.669477	9.250807
H	0.237552	5.398867	9.466797
H	0.725340	4.139071	10.658453
H	2.678809	4.957920	10.035390

CH*

Mo	4.859298	3.080576	0.145697
Mo	7.960840	3.076520	0.118976
Mo	11.178433	3.068340	0.118242
Mo	1.511278	3.066502	0.137092
Mo	6.379287	3.122763	2.736307
Mo	9.567012	3.117770	2.756260
Mo	3.188572	3.107063	2.701790
Mo	-0.004201	3.102554	2.743811
Mo	1.596838	3.116506	5.490397
Mo	4.781134	3.169626	5.477677
Mo	11.160164	3.168356	5.497500
Mo	7.970555	3.183218	5.504321
Mo	6.261409	3.254743	8.075082
Mo	3.344771	3.160779	8.077962
Mo	-0.149827	3.161149	8.083740
Mo	9.678195	3.258326	8.089180
S	6.413111	1.470414	0.906934
S	-0.036407	1.458659	0.915634
S	6.413713	4.714550	0.852293
S	3.177936	4.668662	0.772192
S	9.565703	1.517013	0.914883
S	3.189234	1.494661	0.816034
S	-0.030792	4.695096	0.867591
S	9.573687	4.655527	0.860838
S	1.600960	4.662753	3.631424
S	7.964744	1.583861	3.708075
S	1.605825	1.550287	3.654145
S	7.969158	4.698791	3.633349
S	11.170341	4.690452	3.638481
S	4.766012	4.693075	3.609314
S	4.783012	1.571761	3.662979
S	11.153452	1.564701	3.694989
S	3.212815	1.531579	6.432843
S	6.376007	4.817728	6.390965
S	9.587255	1.599490	6.495800
S	9.560700	4.816358	6.402501
S	0.024638	4.745999	6.419685
S	3.166810	4.747654	6.416093
S	-0.020717	1.530390	6.438593
S	6.349958	1.596825	6.480463
S	1.598118	2.268443	9.535562
S	4.782162	3.478805	9.855630
S	7.969410	2.317419	9.350915
S	11.167785	3.505590	9.856508
C	1.597903	3.957162	9.113036
H	1.599475	4.740529	9.878823

CH_2*

Mo	4.735132	3.088592	0.174718
Mo	8.023534	3.075385	0.164855
Mo	11.177129	3.073312	0.138012
Mo	1.581253	3.083503	0.137259
Mo	6.382881	3.115801	2.708478
Mo	9.576693	3.086094	2.753076
Mo	3.182426	3.126724	2.745942
Mo	-0.003844	3.095437	2.776634
Mo	1.602914	3.132983	5.548937
Mo	4.775993	3.196431	5.475426
Mo	11.165567	3.091458	5.493960
Mo	7.967086	3.105423	5.501646
Mo	6.328642	3.226735	8.098322
Mo	3.366805	3.263668	8.081301
Mo	12.493526	3.073136	8.102811
Mo	9.734796	3.061342	8.072849
S	6.375637	1.483025	0.833759
S	0.007560	1.498816	0.927793
S	6.388056	4.701134	0.791071
S	3.145106	4.712430	0.864676
S	9.603640	1.466191	0.898427
S	3.152553	1.485279	0.912205
S	-0.004990	4.667763	0.904976
S	9.605175	4.684974	0.883370
S	1.579466	4.670652	3.683823
S	7.951766	1.545225	3.666520
S	1.615520	1.568872	3.714594
S	7.982617	4.657979	3.648609
S	11.157212	4.660586	3.672984

S	4.797114	4.707292	3.601230
S	4.785811	1.587307	3.671839
S	11.164640	1.521736	3.673309
S	3.263433	1.580709	6.463104
S	6.438169	4.775038	6.395543
S	9.577605	1.470728	6.436433
S	9.571869	4.697548	6.468153
S	-0.044390	4.712708	6.490699
S	3.174218	4.801824	6.368901
S	0.005392	1.478064	6.442602
S	6.303390	1.575445	6.461578
S	1.644974	2.239505	9.434723
S	4.832515	4.220759	9.553431
S	7.915646	2.334988	9.440942
S	11.107019	3.067507	9.947481
C	1.288952	3.966740	9.388487
H	1.135630	4.438290	10.366029
H	1.996088	4.634588	8.794972

CH_3*			
Mo	4.752066	3.128785	0.180210
Mo	8.024584	3.117365	0.179186
Mo	11.169595	3.125003	0.147758
Mo	1.590282	3.133818	0.148307
Mo	6.385977	3.098104	2.726025
Mo	9.572136	3.096031	2.755798
Mo	3.186330	3.124727	2.744969
Mo	0.008140	3.122255	2.767158
Mo	1.600901	3.118122	5.488285
Mo	4.796302	3.117915	5.520341
Mo	11.160540	3.113736	5.540205
Mo	7.975278	3.027369	5.490181
Mo	6.431438	2.995357	8.126164
Mo	3.142852	3.160095	8.193463
Mo	0.066456	3.158270	8.203081
Mo	9.512508	2.991348	8.134149
S	6.382241	1.506446	0.819908
S	0.006680	1.539363	0.903965
S	6.394848	4.724757	0.850578
S	3.168631	4.747869	0.889044
S	9.608332	1.497286	0.884410
S	3.163780	1.513867	0.878795
S	-0.002489	4.716712	0.914937
S	9.599348	4.728972	0.913375
S	1.602352	4.688997	3.670277
S	7.969760	1.510095	3.630071
S	1.604017	1.554682	3.667659
S	7.972385	4.635586	3.689731
S	11.149083	4.663630	3.697891
S	4.807273	4.665859	3.671610
S	4.776751	1.562141	3.666817
S	11.179286	1.558659	3.691190
S	3.202804	1.569562	6.461730
S	6.459270	4.644788	6.489303
S	9.619105	1.445701	6.424629
S	9.493107	4.641544	6.498503
S	0.006046	4.700313	6.429595
S	3.196690	4.703461	6.419825
S	0.005928	1.569009	6.471961
S	6.329411	1.448152	6.415512
S	1.609549	1.848140	9.343709
S	4.871646	3.856566	9.571979
S	7.967263	1.977835	9.486111
S	11.083714	3.835188	9.580684
C	1.598095	4.739898	8.971044
H	2.451689	4.673489	9.685559
H	1.596849	5.713232	8.474895
H	0.760023	4.678872	9.704302

CH_4*			
Mo	4.733322	3.150597	0.155329
Mo	8.035524	3.145397	0.157481
Mo	11.176371	3.151366	0.130490
Mo	1.581059	3.153734	0.126249
Mo	6.382937	3.110429	2.698801
Mo	9.574359	3.108751	2.740246
Mo	3.188196	3.111008	2.733726
Mo	0.003390	3.112480	2.764023
Mo	1.602725	3.035806	5.501137
Mo	4.791404	3.087968	5.477898
Mo	11.165226	3.082938	5.506069
Mo	7.974459	3.035616	5.480969
Mo	6.383948	3.011220	8.089847
Mo	3.201309	3.004665	8.097952
Mo	0.008414	3.001942	8.108302
Mo	9.564695	3.002620	8.102854
S	6.382176	1.534449	0.774469
S	0.003299	1.557888	0.882074
S	6.386851	4.741965	0.822920
S	3.153575	4.752986	0.901793
S	9.612511	1.523211	0.860012
S	3.152561	1.528217	0.846772
S	0.001400	4.725073	0.931764
S	9.607330	4.749928	0.910132
S	1.604058	4.646544	3.707063
S	7.967505	1.525353	3.609174
S	1.602730	1.526009	3.637141
S	7.968578	4.644293	3.676340
S	11.158731	4.664285	3.698872
S	4.796176	4.663532	3.658409
S	4.794833	1.546887	3.617475
S	11.162374	1.543038	3.653092
S	3.247989	1.442304	6.396927
S	6.428329	4.644428	6.453374
S	9.610762	1.439568	6.404309
S	9.523433	4.637650	6.472459
S	0.051283	4.639092	6.480981
S	3.156333	4.641882	6.466715
S	-0.036689	1.439208	6.411960
S	6.335605	1.446399	6.391642
S	1.611729	2.057862	9.464487
S	4.794107	3.902384	9.492506
S	7.965503	2.062261	9.463910
S	11.161915	3.870869	9.514132
C	1.620158	5.333425	11.913175
H	1.659750	6.300464	12.429945
H	0.715106	4.791725	12.214641
H	2.506022	4.741240	12.172000
H	1.599134	5.500194	10.828802

5. Transition state of elementary reaction on MoS_{2-v}(001)

$H_2O^* + * = OH^* + H^*$			
Mo	1.890518	-0.056073	1.579620
Mo	1.896169	3.149503	1.590902
Mo	1.871533	6.325956	1.553129
Mo	4.658391	-1.655095	1.563438
Mo	4.656448	1.561472	1.568955
Mo	4.665145	4.739319	1.580107
Mo	7.457412	-3.216286	1.583932
Mo	7.340782	-0.041791	1.482536
Mo	7.442759	3.130990	1.581194
Mo	10.227823	-4.818552	1.608403
Mo	10.286608	-1.642738	1.557399
Mo	10.227573	1.487332	1.621609
Mo	12.967444	-6.419256	1.602967
Mo	12.942822	-3.202167	1.545583
Mo	12.933953	-0.093579	1.515668
S	0.981343	1.550642	0.035162
S	0.959472	4.715137	-0.003527
S	0.964198	7.936368	-0.016689
S	3.734630	-0.046082	0.018770
S	3.730000	3.154578	0.019292
S	3.734930	6.318594	0.009003
S	6.483989	-1.688959	-0.025125
S	6.477108	1.603095	-0.027585
S	6.531363	4.743280	0.034021
S	9.320178	-3.211515	0.030102
S	9.269861	-0.081770	0.069591
S	9.324157	3.105373	0.066654
S	12.053259	-4.825463	0.023753
S	12.030863	-1.661852	-0.031859
S	12.031981	1.550661	0.021599
S	1.001278	1.544083	3.156668
S	0.934470	4.776860	3.127792
S	0.919934	7.879478	3.113540
S	3.744263	-0.055088	3.128202
S	3.748318	3.150146	3.146976
S	3.723713	6.332486	3.126540
S	6.538571	-1.610053	3.114989
S	6.532189	1.520918	3.118772
S	6.528620	4.743752	3.132695
S	9.341428	-3.181893	3.132192
S	12.053362	-4.763163	3.149536
S	12.076717	1.482828	3.129918
S	9.286329	3.105481	3.151095
O	9.832790	-0.143507	3.186026
H	10.269121	-0.112041	4.076405
H	8.661205	-0.097690	2.987023

$OH^* + * = O^* + H^*$			
Mo	1.829576	0.008708	1.611177
Mo	1.824586	3.199053	1.621729
Mo	1.828431	6.389568	1.590295
Mo	4.614002	-1.576447	1.599166
Mo	4.611139	1.606968	1.606423
Mo	4.605224	4.798060	1.605536
Mo	7.390707	-3.153958	1.563729
Mo	7.390706	0.047141	1.502110
Mo	7.383127	3.181271	1.552531
Mo	10.137084	-4.774573	1.546986
Mo	10.222545	-1.577560	1.410925
Mo	10.098761	1.528124	1.524095
Mo	12.870814	-6.382873	1.600714
Mo	12.860488	-3.133947	1.542486
Mo	12.857164	-0.026188	1.509437
S	0.914186	1.604516	0.056119
S	0.918824	4.776425	0.036826
S	0.934381	7.996539	0.017009
S	3.677460	0.015860	0.053735
S	3.668468	3.200534	0.058300
S	3.685371	6.392291	0.042982
S	6.435294	-1.574020	-0.001729
S	6.417913	1.603049	-0.013417
S	6.436720	4.802227	0.026666
S	9.186825	-3.206367	-0.046764
S	9.201579	-0.014657	-0.060591
S	9.231605	3.168077	-0.013947
S	11.991725	-4.784676	0.021307
S	12.022834	-1.601040	-0.142961
S	11.960009	1.611162	-0.009356
S	0.893768	1.593849	3.176542
S	0.860514	4.821501	3.150042
S	0.853169	7.964319	3.131132
S	3.686939	0.008448	3.167610
S	3.688007	3.203381	3.173162
S	3.680760	6.396822	3.160141
S	6.527997	-1.531599	3.110252
S	6.521951	1.587228	3.127980
S	6.487585	4.799011	3.124420
S	9.275906	-3.084904	3.063037
S	11.954123	-4.732451	3.128411
S	11.898333	1.497692	3.107055
S	9.220862	3.131616	3.097691
O	11.938191	-1.517152	2.672356
H	10.782967	-1.017301	3.075597

$2OH^* = H_2O^* + O^*$			
Mo	1.827986	0.051033	1.546574
Mo	1.833948	3.248221	1.559532
Mo	1.820219	6.433717	1.540369
Mo	4.602172	-1.547898	1.517493
Mo	4.600970	1.645011	1.521959
Mo	4.599771	4.833155	1.529351
Mo	7.367588	-3.131747	1.510257
Mo	7.356996	0.056362	1.409983
Mo	7.367975	3.214836	1.516154
Mo	10.150000	-4.752322	1.568397
Mo	10.144446	-1.518188	1.500474
Mo	10.087316	1.554858	1.584007
Mo	12.904940	-6.300374	1.558894
Mo	12.851506	-3.096282	1.553150
Mo	12.861176	0.031847	1.511222
S	0.921762	1.657161	-0.009760
S	0.881695	4.829658	0.001545
S	0.898958	8.035305	-0.024725
S	3.665105	0.048280	-0.024595
S	3.661566	3.243686	-0.022263
S	3.662250	6.423409	-0.029219
S	6.423121	-1.568937	-0.078646
S	6.416001	1.657298	-0.081682
S	6.447264	4.824430	-0.036313
S	9.234042	-3.152980	-0.024290
S	9.212143	0.029088	-0.054130
S	9.257338	3.181858	0.015162
S	11.978965	-4.712549	0.006850
S	11.940705	-1.548550	-0.089219
S	11.940499	1.659056	0.010686
S	0.934038	1.648844	3.123584
S	0.888209	4.859404	3.111443
S	0.878626	8.013320	3.095868
S	3.690245	0.045028	3.087298
S	3.698480	3.239509	3.101472
S	3.684203	6.432758	3.090839
S	6.503339	-1.500874	3.053473
S	6.499761	1.595124	3.059248
S	6.457739	4.830223	3.071003
S	9.211168	-3.112469	3.070585
S	11.973322	-4.699582	3.131476
S	11.988519	1.645710	3.083465
S	9.178973	3.168245	3.117722
O	11.917652	-1.469333	2.702023
O	10.052315	-0.250302	3.297942
H	11.173152	-0.940754	3.426057
H	9.247525	-0.380597	3.841819

$CO^* + O^* = CO_2^* + *$			
Mo	1.861790	0.009131	1.563025
Mo	1.875979	3.211068	1.547720
Mo	1.848642	6.400102	1.524198
Mo	4.654686	-1.567039	1.575514
Mo	4.641425	1.610514	1.573740
Mo	4.644099	4.803389	1.553862
Mo	7.422771	-3.155473	1.532364
Mo	7.452942	0.025161	1.564311
Mo	7.417126	3.200948	1.522404
Mo	10.186982	-4.775518	1.470072
Mo	10.293189	-1.618988	1.487498
Mo	10.160220	1.584349	1.506290
Mo	12.932792	-6.350312	1.516062
Mo	12.932350	-3.133147	1.454285
Mo	12.897744	-0.031901	1.484820
S	0.977285	1.606355	-0.011996
S	0.971927	4.785240	-0.058722
S	0.937248	8.010543	-0.036436
S	3.718541	0.016213	0.016725
S	3.729358	3.199891	0.000698
S	3.731528	6.412170	0.000996
S	6.494333	-1.538698	0.005260
S	6.482891	1.577752	0.001664
S	6.480356	4.809791	-0.018574
S	9.239311	-3.197709	-0.099602
S	9.279135	-0.061421	-0.027229
S	9.251644	3.169481	-0.057338
S	12.045665	-4.760624	-0.086936
S	12.035724	-1.577288	-0.106238
S	12.013584	1.604211	-0.049586
S	0.940323	1.619516	3.108074
S	0.890432	4.839702	3.075401
S	0.873596	7.941039	3.093622
S	3.707824	0.013940	3.134371

S	3.713936	3.219023	3.121959
S	3.697525	6.397302	3.104747
S	6.536729	-1.569005	3.118187
S	6.510686	1.620043	3.112093
S	6.508606	4.804555	3.091379
S	9.309877	-3.207840	3.026316
S	12.007415	-4.694852	3.036251
S	12.001430	1.587569	3.050971
S	9.276214	3.205969	3.054458
C	10.264991	-0.708354	3.397415
O	10.484021	-0.654050	4.562219
O	9.149567	0.293167	2.854713

CO* + OH* = COOH* + *

Mo	1.843131	-0.039636	1.597874
Mo	1.862075	3.149373	1.623040
Mo	1.835838	6.345498	1.622065
Mo	4.620192	-1.627607	1.584160
Mo	4.619344	1.561511	1.581438
Mo	4.616984	4.749995	1.590484
Mo	7.386310	-3.211620	1.555849
Mo	7.361744	-0.008276	1.482270
Mo	7.388838	3.131090	1.545906
Mo	10.148376	-4.830414	1.592220
Mo	10.135995	-1.629952	1.551244
Mo	10.138924	1.545323	1.535537
Mo	12.910693	-6.391890	1.595953
Mo	12.889672	-3.201992	1.711698
Mo	12.845083	0.014668	1.542795
S	0.944877	1.570270	0.039548
S	0.881940	4.745474	0.101141
S	0.929807	7.929161	0.030872
S	3.683622	-0.037734	0.033594
S	3.679361	3.161876	0.036144
S	3.670152	6.342218	0.043705
S	6.436306	-1.632640	-0.021393
S	6.424109	1.565595	-0.038288
S	6.449740	4.750175	0.011984
S	9.235305	-3.235829	-0.005714
S	9.226220	-0.029897	0.014580
S	9.255625	3.148328	0.000069
S	12.013413	-4.758035	0.074609
S	11.977878	-1.667945	0.043668
S	11.961498	1.619922	-0.009987
S	0.938182	1.547286	3.172694
S	0.974439	4.737302	3.194375
S	0.862373	7.940129	3.145155
S	3.699494	-0.038015	3.146313
S	3.726477	3.149274	3.161470
S	3.709583	6.350877	3.159119
S	6.520743	-1.588184	3.102549
S	6.512237	1.531646	3.111163
S	6.485053	4.742604	3.117217
S	9.224227	-3.228394	3.110748
S	11.963299	-4.859152	3.181164
S	11.964333	1.584301	3.124630
S	9.210540	3.083810	3.118289
C	11.728486	-1.313634	2.926515
O	12.246289	-2.065830	3.774249
O	10.233928	-0.496072	3.489183
H	9.870356	-1.091108	4.185489

CO* + H* = CHO* + *

Mo	1.798215	-0.019119	1.581902
Mo	1.825100	3.165070	1.604822
Mo	1.802450	6.364789	1.606864
Mo	4.585301	-1.593892	1.561468
Mo	4.589006	1.581727	1.558558
Mo	4.583464	4.781364	1.564832
Mo	7.351069	-3.162889	1.515322
Mo	7.364251	0.025513	1.456279
Mo	7.350198	3.176597	1.500446
Mo	10.108722	-4.765918	1.559784
Mo	10.068579	-1.530918	1.504359
Mo	10.081623	1.588794	1.440842
Mo	12.851026	-6.379848	1.582538
Mo	12.865377	-3.181678	1.689526
Mo	12.763700	0.035330	1.502940
S	0.895362	1.588303	0.028704
S	0.859558	4.769124	0.080474
S	0.883168	7.948262	0.016827
S	3.639212	-0.011464	0.014338
S	3.644338	3.182749	0.017701
S	3.632456	6.373595	0.023175
S	6.399274	-1.580632	-0.049156
S	6.392129	1.587561	-0.065025
S	6.404590	4.795600	-0.026827
S	9.206489	-3.154271	-0.036666
S	9.180052	0.018297	-0.089122
S	9.204842	3.232097	-0.062926
S	11.980631	-4.734134	0.060029
S	11.927832	-1.642835	0.021516
S	11.933440	1.652331	-0.057633
S	0.884983	1.562272	3.156146
S	0.951464	4.748329	3.175665
S	0.795318	7.956276	3.112068
S	3.661200	-0.012132	3.128248
S	3.698630	3.171317	3.136325
S	3.679515	6.379975	3.138968
S	6.496377	-1.544740	3.067047
S	6.498669	1.567573	3.072371
S	6.458041	4.783260	3.079054
S	9.182726	-3.119845	3.077378
S	11.910213	-4.832375	3.158709
S	11.844621	1.570556	3.094202
S	9.169225	3.122523	3.058041
C	11.618547	-1.221613	2.942676
O	12.261981	-2.119733	3.597151
H	10.686578	-0.767537	3.458166

CO* + H* = COH* + *

Mo	1.855636	-0.008993	1.575683
Mo	1.852098	3.180525	1.597631
Mo	1.867650	6.369683	1.578427
Mo	4.632224	-1.599094	1.589277
Mo	4.629617	1.584524	1.600086
Mo	4.626478	4.770744	1.593075
Mo	7.384643	-3.188661	1.568686
Mo	7.387154	0.012506	1.535722
Mo	7.400114	3.144309	1.571663
Mo	10.145837	-4.813482	1.584694
Mo	10.228698	-1.580761	1.573666
Mo	10.145739	1.518223	1.560752
Mo	12.889092	-6.382707	1.590201
Mo	12.883454	-3.166464	1.589625
Mo	12.903674	-0.008697	1.459891
S	0.925697	1.595530	0.032215
S	0.940052	4.772495	0.032377
S	0.997769	7.959261	-0.024967
S	3.709882	-0.002176	0.032739
S	3.696040	3.176394	0.040595
S	3.716703	6.367671	0.027414
S	6.461551	-1.594649	0.001437
S	6.448364	1.568729	-0.001670
S	6.467625	4.762748	0.027241
S	9.239693	-3.185839	0.017546
S	9.236419	-0.052571	0.029228
S	9.246322	3.143947	0.012691
S	11.978614	-4.785483	0.035224
S	11.988232	-1.634272	-0.075266
S	11.949799	1.630828	-0.024859
S	0.927388	1.576029	3.149541
S	0.917886	4.794817	3.150372
S	0.886176	7.953793	3.101149
S	3.693053	-0.014324	3.150039
S	3.702492	3.181297	3.159839
S	3.706662	6.372603	3.148896
S	6.514390	-1.570725	3.123606
S	6.514344	1.561862	3.144466
S	6.485538	4.760733	3.130454
S	9.218866	-3.188216	3.092904
S	11.969331	-4.763504	3.162640
S	11.975534	1.512881	3.109783
S	9.232820	3.096954	3.128105
C	12.072693	-1.517417	2.688167
O	11.182353	-1.271168	3.633340
H	10.392073	-0.319795	3.103852

CHO* + O* = HCOO* + *

Mo	1.916080	0.004887	1.578641
Mo	1.889809	3.192121	1.612996
Mo	1.892996	6.377478	1.588366
Mo	4.652654	-1.617143	1.529115
Mo	4.658902	1.578118	1.542704
Mo	4.643478	4.750959	1.545487
Mo	7.373759	-3.245707	1.499327
Mo	7.390787	-0.022348	1.441924
Mo	7.422319	3.121917	1.545075
Mo	10.177368	-4.837140	1.602287
Mo	10.039649	-1.673300	1.509755
Mo	10.262745	1.462861	1.622761
Mo	12.958189	-6.357549	1.641631
Mo	12.941955	-3.130074	1.688368
Mo	13.015258	0.027320	1.614488
S	0.958625	1.613059	0.047499
S	0.908924	4.781556	0.076566
S	0.980286	7.980169	0.012467
S	3.724903	-0.007972	-0.015140
S	3.690116	3.171406	0.002735
S	3.705197	6.349654	-0.008576
S	6.460578	-1.632123	-0.075644
S	6.471705	1.583371	-0.058891
S	6.472959	4.705737	-0.033516
S	9.230977	-3.328023	-0.050239
S	9.258931	-0.009327	-0.031945
S	9.331526	3.085078	0.058514
S	12.056234	-4.735674	0.102948
S	11.987516	-1.595371	0.127847
S	12.071083	1.603594	0.062030
S	1.008173	1.589694	3.174873
S	0.999872	4.799963	3.192974
S	1.046758	8.000514	3.156332
S	3.774206	-0.016905	3.110695
S	3.763910	3.166771	3.130817
S	3.761972	6.363502	3.116453
S	6.530661	-1.597675	3.056146
S	6.540368	1.518425	3.086825
S	6.488969	4.735894	3.087146
S	9.137159	-3.265216	3.083289
S	11.998084	-4.757245	3.201451
S	12.075928	1.593072	3.184303
S	9.258071	3.068188	3.133209
C	11.085410	-1.442678	3.284291
O	9.804636	-0.200006	2.934095
O	12.401854	-1.324171	3.186477
H	10.731975	-1.657028	4.301934

COH* + O* = COOH* + *

Mo	1.899551	-0.066782	1.617617
Mo	1.914045	3.126867	1.600380
Mo	1.878983	6.313610	1.600700
Mo	4.671574	-1.664913	1.598330
Mo	4.674113	1.526742	1.599376
Mo	4.665714	4.711935	1.595086
Mo	7.432628	-3.259001	1.556966
Mo	7.411762	-0.049154	1.492879
Mo	7.441529	3.090433	1.557291
Mo	10.206397	-4.871198	1.524730
Mo	10.205530	-1.672970	1.472583
Mo	10.232779	1.473577	1.540703
Mo	12.966490	-6.415670	1.558423
Mo	12.963041	-3.270025	1.502576
Mo	12.925280	-0.038275	1.592640
S	1.015949	1.527458	0.032531
S	1.009808	4.703248	0.003626
S	0.971643	7.927755	0.047605
S	3.739164	-0.072081	0.052692
S	3.748757	3.117849	0.038192
S	3.731575	6.313378	0.045746
S	6.479390	-1.676839	-0.010880
S	6.473525	1.528940	-0.022463
S	6.496325	4.701232	0.018305
S	9.232796	-3.294190	-0.052335
S	9.260768	-0.091613	-0.024169
S	9.282093	3.073791	-0.013166
S	12.053085	-4.857131	-0.043814
S	12.084622	-1.643378	0.001899
S	12.069796	1.527608	-0.000218
S	0.977226	1.543391	3.157501
S	0.923639	4.731907	3.131666
S	0.940752	7.891314	3.165811
S	3.756230	-0.070116	3.165529
S	3.757081	3.123625	3.165345
S	3.740592	6.308194	3.157363
S	6.578846	-1.632997	3.115306
S	6.572759	1.499597	3.129784
S	6.535287	4.703279	3.122178
S	9.302746	-3.262739	3.055858
S	12.025614	-4.791995	3.097438
S	12.043122	1.601434	3.123932
S	9.295211	3.052945	3.096458
C	10.397485	-0.567241	3.182688
O	11.641070	-1.139072	3.053530
O	9.952906	-0.472556	4.434456
H	8.984132	-0.305290	4.410234

HCOO* + * = CO_2* + H*

Mo	1.863129	-0.047544	1.604998
Mo	1.888157	3.134193	1.627868
Mo	1.846659	6.334667	1.631617
Mo	4.641794	-1.627191	1.573477
Mo	4.648913	1.544957	1.565835
Mo	4.638854	4.746425	1.577321
Mo	7.413337	-3.205734	1.528888
Mo	7.439399	-0.039539	1.477850
Mo	7.412584	3.134953	1.520692
Mo	10.163917	-4.796141	1.598713
Mo	10.041060	-1.537551	1.519734
Mo	10.160766	1.536814	1.461531
Mo	12.914536	-6.418465	1.611936
Mo	12.921031	-3.237524	1.762915
Mo	12.839182	0.029077	1.544263
S	0.954162	1.560601	0.053619
S	0.886554	4.736158	0.118916
S	0.918393	7.929855	0.044489
S	3.693482	-0.044400	0.024955
S	3.699081	3.150264	0.029030
S	3.673434	6.339795	0.040799
S	6.458517	-1.612548	-0.036723
S	6.464509	1.545617	-0.043511
S	6.463967	4.752014	-0.011367
S	9.270450	-3.204516	-0.018411
S	9.234965	-0.009431	-0.096377
S	9.273373	3.193985	-0.028134
S	12.041102	-4.754908	0.106235
S	11.974815	-1.668482	0.142322
S	12.011347	1.611851	-0.032925
S	0.956487	1.531343	3.180196
S	1.033634	4.707517	3.213625
S	0.862921	7.932036	3.144403
S	3.731415	-0.042579	3.142911
S	3.767376	3.135515	3.149607
S	3.736976	6.348205	3.150462
S	6.555524	-1.594544	3.086731
S	6.559707	1.516526	3.078713
S	6.512419	4.744946	3.092904
S	9.214711	-3.139971	3.120835
S	11.963367	-4.906129	3.198485
S	11.910704	1.548821	3.137624
S	9.232990	3.069078	3.082062
C	11.477315	-1.462226	4.102133
O	10.868413	-0.864315	4.928094
O	12.352589	-2.285824	3.838006
H	11.296642	-0.773056	2.675706

COOH* + * = CO_2* + H*

Mo	1.885074	-0.074851	1.652317
Mo	1.882445	3.109076	1.658586
Mo	1.874948	6.302673	1.648789
Mo	4.648356	-1.678580	1.597934
Mo	4.651594	1.498540	1.605247
Mo	4.633448	4.684293	1.594243
Mo	7.380407	-3.302050	1.511390
Mo	7.448187	-0.118780	1.528672
Mo	7.415073	3.066354	1.555534
Mo	10.157964	-4.866861	1.594948
Mo	9.924448	-1.681377	1.464813
Mo	10.170913	1.495857	1.536362
Mo	12.932881	-6.432495	1.661163
Mo	12.929370	-3.228135	1.707869
Mo	12.933575	-0.061169	1.681170

S	0.955396	1.524899	0.095469
S	0.917549	4.706491	0.116518
S	0.931550	7.902292	0.101134
S	3.699538	-0.083849	0.059339
S	3.690465	3.089664	0.057334
S	3.691593	6.293048	0.055131
S	6.450684	-1.665570	-0.016993
S	6.468335	1.477134	0.003583
S	6.443545	4.646470	-0.008318
S	9.230923	-3.359303	-0.074256
S	9.222940	-0.018898	-0.075130
S	9.280496	3.097645	0.007901
S	12.053535	-4.813714	0.109700
S	11.964393	-1.658345	0.159202
S	12.066402	1.516941	0.080216
S	0.967877	1.517402	3.225252
S	0.987803	4.703841	3.229828
S	0.979652	7.908915	3.216643
S	3.755471	-0.089097	3.182257
S	3.756573	3.096382	3.182532
S	3.751554	6.292319	3.174227
S	6.552572	-1.690186	3.110857
S	6.559182	1.453008	3.120266
S	6.499177	4.676863	3.108550
S	9.155422	-3.276841	3.105905
S	11.967672	-4.834749	3.209886
S	11.967208	1.538202	3.179298
S	9.238060	3.035664	3.127338
C	11.110729	-1.339640	3.138624
O	12.375784	-1.690597	3.252254
O	10.483598	-0.708293	4.057339
H	9.496657	-0.294124	3.114434

$2H^* = H_2 + 2^*$

Mo	1.825184	-0.004604	1.607223
Mo	1.831349	3.194332	1.618353
Mo	1.812661	6.382109	1.574321
Mo	4.616695	-1.578401	1.602234
Mo	4.616894	1.597030	1.609656
Mo	4.612839	4.793036	1.597351
Mo	7.397168	-3.149204	1.561825
Mo	7.419275	0.032152	1.536674
Mo	7.394392	3.181720	1.542898
Mo	10.153366	-4.762266	1.553007
Mo	10.169027	-1.527002	1.571894
Mo	10.118934	1.560822	1.461572
Mo	12.877045	-6.383928	1.594164
Mo	12.881516	-3.145507	1.552367
Mo	12.847426	-0.029764	1.482006
S	0.920689	1.598136	0.058387
S	0.908339	4.765211	0.018414
S	0.920776	7.986895	-0.007039
S	3.678655	0.009549	0.055615
S	3.677815	3.189162	0.055268
S	3.687780	6.391176	0.041156
S	6.449088	-1.555020	0.011675
S	6.435076	1.579994	0.000156
S	6.449800	4.808134	0.018698
S	9.260981	-3.106752	0.012012
S	9.217423	-0.039330	-0.023577
S	9.229656	3.212397	-0.041968
S	12.006021	-4.771198	0.014594
S	11.935461	-1.613375	-0.011898
S	11.987697	1.616208	-0.045692
S	0.897423	1.585693	3.172353
S	0.864821	4.831346	3.147446
S	0.816890	7.930950	3.114463
S	3.679964	-0.000632	3.168993
S	3.695382	3.200838	3.169152
S	3.671373	6.388150	3.145935
S	6.526245	-1.545762	3.122705
S	6.530816	1.591285	3.127556
S	6.492625	4.792288	3.116386
S	9.256117	-3.136433	3.093025
S	11.961007	-4.724632	3.127165
S	11.874886	1.466548	3.073854
S	9.235119	3.122317	3.074956
H	10.868484	-1.019932	4.018598
H	10.208916	-0.635610	4.009266

CHO* + * = CH* + O*

Mo	1.803094	0.005714	1.629787
Mo	1.820283	3.204999	1.619612
Mo	1.784299	6.389493	1.614987
Mo	4.586472	-1.583011	1.615925
Mo	4.589309	1.588398	1.622964
Mo	4.577829	4.786302	1.607981
Mo	7.338522	-3.189313	1.521240
Mo	7.401501	-0.007862	1.523049
Mo	7.354924	3.173066	1.555614
Mo	10.110613	-4.771136	1.499017
Mo	10.042773	-1.590384	1.358154
Mo	10.166696	1.574997	1.505541
Mo	12.874925	-6.328153	1.559768
Mo	12.862061	-3.156280	1.508539
Mo	12.773888	0.060707	1.571063
S	0.935049	1.608909	0.045218
S	0.919326	4.786762	0.022991
S	0.868836	7.999342	0.064459
S	3.647832	0.004653	0.069086
S	3.660620	3.182383	0.061589
S	3.641332	6.394256	0.064084
S	6.389588	-1.567387	-0.001331
S	6.401351	1.572462	0.017902
S	6.383029	4.760454	0.005791
S	9.119158	-3.250353	-0.120620
S	9.151611	0.029439	-0.119150
S	9.167750	3.182132	-0.039743
S	11.977509	-4.758237	-0.041826
S	11.976309	-1.566285	-0.040879
S	11.998838	1.638400	-0.037129
S	0.876595	1.617010	3.168106
S	0.823054	4.816366	3.147433
S	0.794551	7.967471	3.159742
S	3.659942	-0.001802	3.187298
S	3.671049	3.197704	3.180224
S	3.651245	6.385588	3.169519
S	6.506445	-1.581352	3.109676
S	6.508474	1.558576	3.121838
S	6.458203	4.788922	3.118643
S	9.205287	-3.137549	3.013497
S	11.919162	-4.693992	3.084576
S	11.939470	1.680219	3.118064
S	9.226354	3.157955	3.072588
C	9.870398	-0.140374	2.827555
O	11.305166	-1.022572	2.853210
H	9.500514	-0.210806	3.856763

$CHO^* + H^* = CH_2O^* + *$

Mo	1.872377	0.002936	1.560649
Mo	1.841124	3.179766	1.595228
Mo	1.848787	6.371622	1.567791
Mo	4.609612	-1.625819	1.510532
Mo	4.617470	1.566642	1.521894
Mo	4.591646	4.738103	1.522275
Mo	7.322802	-3.257131	1.474394
Mo	7.347502	-0.046803	1.428965
Mo	7.374843	3.109240	1.515579
Mo	10.115962	-4.833205	1.585606
Mo	9.977488	-1.692689	1.527075
Mo	10.184088	1.497449	1.550103
Mo	12.898049	-6.369226	1.631878
Mo	12.887671	-3.144160	1.680035
Mo	12.967031	0.035920	1.594966
S	0.899660	1.607461	0.033596
S	0.854440	4.773181	0.062702
S	0.937489	7.979122	-0.001971
S	3.681205	-0.015489	-0.033661
S	3.640454	3.157485	-0.018391
S	3.659296	6.341918	-0.029758
S	6.415166	-1.643344	-0.099411
S	6.431376	1.561378	-0.085769
S	6.419285	4.692181	-0.059256
S	9.173274	-3.319842	-0.073990
S	9.227891	-0.027291	-0.037803
S	9.270405	3.108568	0.010547
S	11.998174	-4.741693	0.094941
S	11.938671	-1.582998	0.132842
S	12.028147	1.599542	0.036180
S	0.955575	1.578973	3.160574
S	0.961012	4.785008	3.170044
S	1.008443	8.000369	3.133836
S	3.732839	-0.023787	3.091849
S	3.717690	3.153398	3.110221
S	3.717184	6.353493	3.094355
S	6.490141	-1.615472	3.037909
S	6.499935	1.503485	3.060964
S	6.435649	4.718466	3.057955
S	9.060815	-3.264306	3.088532
S	11.943351	-4.773754	3.190746
S	11.972464	1.570004	3.168075
S	9.197587	3.056291	3.105791
C	11.163377	-1.633159	3.225984
O	12.447587	-1.364792	3.162242
H	10.869151	-1.956620	4.241754
H	10.171626	-0.373151	2.857095

CHO* + H* = CHOH* + *

Mo	1.804644	-0.022658	1.599067
Mo	1.812500	3.180585	1.593683
Mo	1.776316	6.370687	1.570746
Mo	4.593112	-1.595821	1.605510
Mo	4.580575	1.587481	1.602213
Mo	4.572895	4.783920	1.591964
Mo	7.358715	-3.186205	1.570294
Mo	7.386229	0.019583	1.604358
Mo	7.337732	3.194326	1.555570
Mo	10.131224	-4.785995	1.479615
Mo	10.165648	-1.635660	1.518117
Mo	10.108018	1.594149	1.498673
Mo	12.874298	-6.398848	1.566252
Mo	12.864148	-3.190107	1.508444
Mo	12.798212	-0.038783	1.547585
S	0.921000	1.574176	0.031654
S	0.901233	4.756090	-0.010417
S	0.864543	7.971401	0.013691
S	3.660790	-0.012296	0.048142
S	3.661005	3.178383	0.037899
S	3.654855	6.386147	0.039970
S	6.433338	-1.575425	0.040977
S	6.417802	1.583339	0.027417
S	6.402233	4.796489	0.014549
S	9.177125	-3.182932	-0.058173
S	9.197819	-0.047654	0.015375
S	9.147080	3.188708	-0.055973
S	12.009157	-4.803569	-0.049361
S	11.945254	-1.612501	-0.036466
S	11.982758	1.573179	-0.022374
S	0.886063	1.579466	3.152636
S	0.831825	4.801531	3.116683
S	0.805507	7.922617	3.131071
S	3.655177	-0.014292	3.164373
S	3.655533	3.190655	3.157877
S	3.632636	6.375938	3.145387
S	6.481926	-1.585393	3.156318
S	6.440940	1.608069	3.149861
S	6.436618	4.786543	3.133301
S	9.245269	-3.246898	3.052105
S	11.937790	-4.747341	3.073452
S	11.893693	1.548799	3.114497
S	9.221747	3.205677	3.055057
C	9.123808	0.322126	3.044039
O	9.902297	-0.747489	3.449369
H	8.839429	0.880655	3.951914
H	11.189862	-0.759219	2.927854

COH* + H* = CHOH* + *

Mo	1.844002	0.018840	1.579023
Mo	1.838844	3.214874	1.591796
Mo	1.855528	6.400877	1.570611
Mo	4.638914	-1.573389	1.587171
Mo	4.627389	1.603204	1.593712
Mo	4.632182	4.797999	1.587145
Mo	7.422170	-3.147672	1.533170
Mo	7.424237	0.000811	1.512876
Mo	7.414047	3.163408	1.541198
Mo	10.137968	-4.778408	1.531942
Mo	10.190323	-1.565310	1.427034
Mo	10.165100	1.547460	1.490303
Mo	12.882990	-6.355170	1.563270
Mo	12.853732	-3.113028	1.512834
Mo	12.852569	0.021141	1.462826
S	0.932051	1.623552	0.024393
S	0.945327	4.808139	0.009109
S	0.963315	7.992664	-0.010964
S	3.699525	0.017581	0.033025
S	3.692981	3.201669	0.040071
S	3.714054	6.395931	0.026072
S	6.460686	-1.556056	-0.020165
S	6.448690	1.575933	-0.011194
S	6.467824	4.787987	0.013966
S	9.219730	-3.216629	-0.081374
S	9.225791	0.018024	-0.073981
S	9.246151	3.168710	-0.035123
S	11.976202	-4.767139	-0.009945
S	11.990742	-1.574631	-0.137902
S	11.970247	1.656506	-0.059517
S	0.907392	1.611256	3.139922
S	0.865839	4.840572	3.122094
S	0.853811	7.980372	3.092503
S	3.690706	0.010249	3.147214
S	3.700035	3.209690	3.149633
S	3.704789	6.398125	3.139009
S	6.542951	-1.560124	3.104539
S	6.533781	1.566773	3.101174
S	6.517311	4.797513	3.102419
S	9.282135	-3.096065	3.054983
S	11.960496	-4.716447	3.104761
S	11.949512	1.543894	3.097570
S	9.257263	3.123760	3.076875
C	11.923223	-1.521558	2.763189
O	11.983797	-1.559385	4.132134
H	12.833566	-1.970058	4.402880
H	10.609021	-0.666259	2.882266

$CH_2O^* + * = CH_2^* + O^*$

Mo	1.841034	0.007440	1.575341
Mo	1.848899	3.195453	1.578230
Mo	1.833524	6.390651	1.571875
Mo	4.616067	-1.590535	1.568372
Mo	4.623225	1.591531	1.572191
Mo	4.603605	4.780952	1.562524
Mo	7.360245	-3.200012	1.524681
Mo	7.414360	0.042280	1.512559
Mo	7.384328	3.158201	1.511667
Mo	10.144189	-4.832698	1.502098
Mo	10.217766	-1.616478	1.546964
Mo	10.076676	1.581620	1.488840
Mo	12.920367	-6.339148	1.528607
Mo	12.864746	-3.137032	1.554985
Mo	12.867307	-0.014005	1.528100
S	0.958785	1.607976	-0.006499
S	0.911456	4.788952	0.021238
S	0.917774	7.991447	0.005741
S	3.688556	-0.000354	0.019649
S	3.685286	3.184006	0.011832
S	3.679068	6.387838	0.010710
S	6.449838	-1.578707	-0.013178
S	6.436487	1.558097	-0.035547
S	6.428200	4.773472	-0.024981
S	9.200151	-3.207921	-0.033965
S	9.239936	-0.065741	0.001570
S	9.229736	3.149143	-0.075595
S	12.010283	-4.747176	-0.028613
S	11.986160	-1.581998	-0.080034
S	11.987968	1.610038	-0.028112
S	0.921745	1.605607	3.131696
S	0.888968	4.805460	3.125393
S	0.875679	7.974624	3.122921
S	3.695617	-0.001322	3.134033
S	3.702019	3.189904	3.135091
S	3.691009	6.381399	3.130708
S	6.519748	-1.560844	3.088912
S	6.527793	1.584105	3.116268
S	6.467280	4.761097	3.086797
S	9.202631	-3.283481	3.026912
S	11.960187	-4.753931	3.091651
S	11.955034	1.639449	3.036250
S	9.198873	3.114305	3.088293
C	10.381858	-0.893957	3.505115
O	11.965486	-1.534154	2.716377

H	10.861984	0.022634	3.851581
H	10.058481	-1.504642	4.361380

CHOH* + * = CH* + OH*

Mo	1.833575	0.003576	1.580580
Mo	1.836053	3.202050	1.583570
Mo	1.813245	6.391256	1.550552
Mo	4.607661	-1.585749	1.579495
Mo	4.612273	1.587342	1.583619
Mo	4.599963	4.776745	1.575222
Mo	7.334111	-3.192642	1.569291
Mo	7.419164	-0.035511	1.578273
Mo	7.381364	3.180719	1.567109
Mo	10.148954	-4.760961	1.558742
Mo	10.225457	-1.517043	1.670005
Mo	10.169983	1.585750	1.524118
Mo	12.891023	-6.349828	1.566908
Mo	12.891841	-3.129410	1.525739
Mo	12.882323	0.002031	1.496944
S	0.928609	1.609632	0.025156
S	0.912427	4.780796	-0.012639
S	0.917212	7.999923	-0.023769
S	3.682185	0.005967	0.022726
S	3.681669	3.180139	0.022340
S	3.685414	6.384656	0.015446
S	6.450272	-1.604557	0.007728
S	6.467096	1.566732	0.020044
S	6.439818	4.768494	0.009724
S	9.235676	-3.112895	0.059708
S	9.272491	-0.065136	0.005870
S	9.211511	3.211745	-0.009671
S	11.994099	-4.738445	-0.011837
S	11.933401	-1.569981	0.002677
S	12.019492	1.618706	-0.039667
S	0.911016	1.604052	3.141833
S	0.869968	4.840925	3.119909
S	0.851622	7.942451	3.114509
S	3.676481	-0.001913	3.144842
S	3.682512	3.189675	3.144421
S	3.661279	6.382398	3.121108
S	6.460736	-1.590939	3.149172
S	6.481736	1.568874	3.131037
S	6.441554	4.763523	3.132295
S	9.183621	-3.209637	3.086765
S	11.976102	-4.697843	3.112650
S	11.966958	1.558750	3.101019
S	9.248360	3.174771	3.103789
C	9.171379	0.230212	2.810034
O	10.561013	-0.903722	3.666137
H	8.980998	0.514951	3.847999
H	10.070133	-1.500310	4.274282

$CH_2O^* + H^* = CH_3O^* + *$

Mo	1.881798	0.004969	1.563890
Mo	1.869183	3.186718	1.579527
Mo	1.870296	6.374391	1.562059
Mo	4.626469	-1.617241	1.522333
Mo	4.635641	1.572841	1.526918
Mo	4.621177	4.749664	1.525145
Mo	7.349692	-3.228426	1.496393
Mo	7.366966	-0.070080	1.462669
Mo	7.406205	3.122190	1.534502
Mo	10.150947	-4.795213	1.613512
Mo	9.959001	-1.559448	1.618740
Mo	10.216034	1.494113	1.565193
Mo	12.916791	-6.359814	1.627770
Mo	12.921682	-3.146050	1.651631
Mo	12.966405	0.013368	1.607179
S	0.919194	1.606813	0.027939
S	0.892179	4.780620	0.037036
S	0.939412	7.978793	0.006747
S	3.696458	-0.009373	-0.025622
S	3.678562	3.164954	-0.022105
S	3.687822	6.353129	-0.027461
S	6.436143	-1.620988	-0.085327
S	6.467207	1.565217	-0.058911
S	6.464376	4.709879	-0.040903
S	9.235825	-3.227982	-0.011540
S	9.232032	-0.005328	-0.013273
S	9.299293	3.142272	0.032028
S	12.012585	-4.738550	0.087991
S	11.890002	-1.582201	0.153219
S	12.037708	1.597459	0.041868
S	0.975100	1.594075	3.150951
S	0.990951	4.784758	3.157879
S	1.014035	7.989395	3.137249
S	3.738914	-0.014239	3.098454
S	3.735821	3.165013	3.107273
S	3.731488	6.358036	3.096262
S	6.495278	-1.618061	3.071428
S	6.515840	1.507593	3.067557
S	6.460795	4.732699	3.071515
S	9.076913	-3.221617	3.113333
S	11.978850	-4.746271	3.191189
S	12.013298	1.577972	3.175899
S	9.235783	3.072447	3.115446
C	11.203432	-1.336848	3.622354
O	12.453941	-1.511818	3.029459
H	10.904843	-2.243771	4.165128
H	11.258526	-0.517314	4.361565
H	10.335119	-0.304261	2.907520

$CH_2O^* + H^* = CH_2OH^* + *$

Mo	1.839251	-0.016205	1.534283
Mo	1.854625	3.191333	1.535900
Mo	1.817552	6.358861	1.525075
Mo	4.587978	-1.623412	1.551671
Mo	4.598773	1.589194	1.561222
Mo	4.622851	4.773444	1.558517
Mo	7.415913	-3.187005	1.587633
Mo	7.310151	-0.029369	1.671076
Mo	7.401152	3.159869	1.589237
Mo	10.177396	-4.788777	1.528815
Mo	10.274501	-1.646622	1.498467
Mo	10.246247	1.585399	1.539592
Mo	12.932541	-6.366938	1.525990
Mo	12.883027	-3.211668	1.453935
Mo	12.835660	0.017148	1.477168
S	0.960311	1.591763	-0.028917
S	0.939835	4.763752	-0.059962
S	0.921080	7.963295	-0.044549
S	3.694157	-0.012022	-0.011997
S	3.709519	3.185660	-0.010879
S	3.687691	6.351807	-0.014897
S	6.467799	-1.604084	0.036180
S	6.470921	1.568795	0.037651
S	6.496252	4.771950	0.029080
S	9.246710	-3.185548	-0.030803
S	9.183909	-0.037557	0.112321
S	9.243676	3.151023	0.002193
S	12.000996	-4.805912	-0.071495
S	12.010785	-1.605622	-0.083573
S	12.007450	1.619630	-0.067775
S	0.952155	1.595019	3.097908
S	0.856379	4.797624	3.070742
S	0.840943	7.935185	3.064151
S	3.661110	-0.023885	3.109678
S	3.678995	3.193763	3.114522
S	3.649820	6.353601	3.102500
S	6.373934	-1.661744	3.143205
S	6.393068	1.612996	3.152841
S	6.479071	4.773813	3.130291
S	9.335213	-3.174385	3.095220
S	12.001731	-4.732759	3.083696
S	12.056662	1.626153	3.112489
S	9.279678	3.158775	3.100386
C	8.670516	-0.111026	3.504440
O	10.013127	-0.090561	2.942567
H	8.589677	0.769205	4.158322
H	8.565938	-1.019444	4.110544
H	11.166559	-0.493243	3.047655

$CHOH^* + H^* = CH_2OH^* + *$

Mo	1.865608	-0.052343	1.594084
Mo	1.888840	3.134080	1.606858
Mo	1.849147	6.331575	1.628006
Mo	4.638964	-1.631898	1.581869
Mo	4.645609	1.553659	1.571767
Mo	4.637430	4.747655	1.588718
Mo	7.407926	-3.201188	1.558611
Mo	7.381301	-0.015626	1.469558
Mo	7.399964	3.137089	1.538309
Mo	10.167907	-4.810163	1.574216
Mo	10.174832	-1.532517	1.554201
Mo	10.173338	1.525685	1.495781
Mo	12.926769	-6.405047	1.552550
Mo	12.922934	-3.263462	1.674639
Mo	12.841430	0.031898	1.570373
S	0.982920	1.552330	0.017510
S	0.924297	4.735085	0.075489
S	0.936902	7.914158	0.045646
S	3.705433	-0.047965	0.027307
S	3.711334	3.156091	0.027503
S	3.680929	6.337522	0.047076
S	6.453010	-1.641237	-0.025318
S	6.448282	1.569291	-0.047871
S	6.469958	4.761103	0.010968
S	9.249645	-3.197769	-0.002871
S	9.240524	-0.027578	-0.035524
S	9.254943	3.168463	-0.017621
S	12.016629	-4.774355	0.032750
S	12.014079	-1.656543	0.091373
S	11.987466	1.600348	-0.041645
S	0.950438	1.535671	3.146391
S	0.993583	4.706840	3.186276
S	0.873876	7.934817	3.153731
S	3.724603	-0.039708	3.141686
S	3.750748	3.137012	3.150787
S	3.729542	6.345179	3.158782
S	6.537893	-1.581858	3.101539
S	6.538995	1.527435	3.100660
S	6.508711	4.747585	3.115361
S	9.262075	-3.153513	3.100061
S	11.978168	-4.910268	3.144569
S	11.962290	1.631498	3.108855
S	9.234208	3.082627	3.083777
C	11.601090	-0.987510	3.167524
O	12.136850	-2.269129	3.555293
H	11.574832	-0.411953	4.107739
H	10.254446	-0.521802	3.034132
H	12.868334	-2.158957	4.210576

$CH_3O^* + * = CH_3^* + O^*$

Mo	1.827383	0.017533	1.562046
Mo	1.831372	3.205243	1.572675
Mo	1.829590	6.397968	1.545883
Mo	4.618136	-1.562157	1.538194
Mo	4.619870	1.612444	1.546407
Mo	4.613079	4.812133	1.538915
Mo	7.397739	-3.126244	1.480072
Mo	7.427679	0.039323	1.448001
Mo	7.393345	3.199900	1.477097
Mo	10.141474	-4.751685	1.492791
Mo	10.201279	-1.548801	1.393143
Mo	10.094838	1.571242	1.431630
Mo	12.876254	-6.374007	1.548776
Mo	12.853297	-3.117805	1.505194
Mo	12.820148	-0.039285	1.464811
S	0.918124	1.612922	0.007610
S	0.917814	4.787966	-0.004560
S	0.913437	7.999251	-0.018876
S	3.671593	0.026039	-0.002249
S	3.671641	3.206760	0.001821
S	3.678974	6.406672	-0.013828
S	6.439813	-1.544393	-0.067642
S	6.434517	1.599643	-0.068602
S	6.441197	4.820403	-0.048827
S	9.235742	-3.151504	-0.101445
S	9.216114	-0.002080	-0.127109
S	9.236856	3.211947	-0.095953
S	12.002905	-4.767017	-0.025212
S	11.989490	-1.602333	-0.182917
S	11.974595	1.619856	-0.068191
S	0.895856	1.602071	3.129664
S	0.867907	4.827611	3.104202
S	0.836249	7.969607	3.078382
S	3.693608	0.018809	3.111167
S	3.706441	3.214851	3.112593
S	3.693278	6.408265	3.101031
S	6.538311	-1.524860	3.048456
S	6.543392	1.595637	3.054680
S	6.500912	4.819697	3.045836
S	9.261851	-3.053330	3.008228
S	11.950988	-4.729685	3.079367
S	11.863801	1.507827	3.045827
S	9.217471	3.152195	3.028038
C	11.788516	-1.473265	4.748493
O	11.899447	-1.544456	2.622714
H	12.829327	-1.238514	4.959509
H	11.058686	-0.666765	4.772482
H	11.438325	-2.490115	4.908662

$CH_2OH^* + * = CH_3^* + OH^*$

Mo	1.887357	-0.001771	1.602914
Mo	1.885849	3.189265	1.614571
Mo	1.887196	6.380653	1.604509
Mo	4.669531	-1.587979	1.580763
Mo	4.666023	1.591351	1.579625
Mo	4.653491	4.781325	1.576542
Mo	7.417591	-3.182272	1.555813
Mo	7.452324	0.038579	1.508410
Mo	7.427686	3.167262	1.520805
Mo	10.189238	-4.815130	1.561991
Mo	10.172145	-1.494567	1.667609
Mo	10.145598	1.578531	1.472480
Mo	12.944717	-6.382536	1.586122
Mo	12.942437	-3.163088	1.627062
Mo	12.910948	-0.027677	1.599600
S	0.978319	1.597656	0.039887
S	0.942597	4.782487	0.058803
S	0.954877	7.967842	0.041533
S	3.725723	-0.002340	0.032717
S	3.714136	3.185799	0.031878
S	3.723046	6.384708	0.030516
S	6.499839	-1.576316	-0.009094
S	6.478416	1.575065	-0.035234
S	6.484742	4.793406	-0.005971
S	9.297292	-3.130185	0.051379
S	9.280571	-0.047109	-0.005737
S	9.275274	3.195532	-0.057238
S	12.044112	-4.766572	0.040186
S	11.957438	-1.604503	0.077349
S	12.037711	1.589242	-0.003523
S	0.964625	1.585423	3.167108
S	0.969422	4.803152	3.182235
S	0.956851	7.968676	3.160927
S	3.751022	-0.000355	3.146633
S	3.754701	3.185754	3.148835
S	3.755949	6.381329	3.145661
S	6.570865	-1.548466	3.103738
S	6.571004	1.581761	3.110371
S	6.515108	4.764210	3.103315
S	9.235663	-3.245323	3.097829
S	12.005237	-4.813442	3.153309
S	11.948059	1.574187	3.108083
S	9.239235	3.100292	3.089660
C	11.983361	-1.406271	3.104351
O	10.296410	-0.926212	3.763781
H	11.894042	-2.501288	3.365060
H	12.449031	-1.034315	4.022281
H	10.389237	0.051259	3.847449

$CH^* + H^* = CH_2^* + *$

Mo	1.833938	-0.004679	1.612890
Mo	1.841181	3.191235	1.617610
Mo	1.803908	6.383664	1.583736
Mo	4.617719	-1.583839	1.598398
Mo	4.625193	1.587368	1.606768
Mo	4.605995	4.789653	1.603040
Mo	7.380762	-3.186084	1.545086
Mo	7.456428	-0.003002	1.522035
Mo	7.372635	3.195861	1.559284
Mo	10.154466	-4.743570	1.517275
Mo	10.133562	-1.526278	1.423050
Mo	10.152490	1.566260	1.461801
Mo	12.892073	-6.375458	1.585453
Mo	12.872926	-3.166821	1.527373
Mo	12.824992	-0.011222	1.524582
S	0.942089	1.596184	0.052295
S	0.919984	4.763507	0.014850
S	0.901183	7.992917	0.020173

S	3.682532	0.004783	0.051977
S	3.685699	3.184369	0.056700
S	3.676049	6.387725	0.047449
S	6.441647	-1.594135	0.008316
S	6.443322	1.596888	0.011443
S	6.422118	4.782450	0.010043
S	9.185005	-3.200610	-0.076364
S	9.210565	0.012874	-0.150811
S	9.195691	3.218547	-0.028141
S	12.017938	-4.774890	-0.020401
S	11.996865	-1.589101	-0.056616
S	12.027631	1.605876	-0.040978
S	0.908514	1.590629	3.171097
S	0.854336	4.814476	3.128598
S	0.821798	7.946122	3.126823
S	3.695885	-0.005112	3.170420
S	3.702850	3.189656	3.170095
S	3.667614	6.390755	3.152100
S	6.522354	-1.568286	3.118802
S	6.533977	1.562745	3.124980
S	6.479409	4.795416	3.131979
S	9.275298	-3.094456	3.046647
S	11.950019	-4.724036	3.101267
S	11.903454	1.550007	3.106287
S	9.254100	3.166034	3.061943
C	9.304905	0.010902	2.683550
H	9.241264	0.111747	3.773734
H	10.778397	-0.756472	2.893002

CH_2* + H* = CH_3* + *

Mo	1.840227	0.010287	1.599081
Mo	1.858239	3.213781	1.589675
Mo	1.831800	6.395407	1.559282
Mo	4.624383	-1.568101	1.584269
Mo	4.628755	1.608595	1.600564
Mo	4.621761	4.805668	1.582764
Mo	7.395791	-3.156464	1.534660
Mo	7.435574	0.030636	1.541232
Mo	7.387338	3.218500	1.553154
Mo	10.172315	-4.731081	1.528630
Mo	10.132574	-1.480869	1.445439
Mo	10.125480	1.601949	1.537987
Mo	12.904166	-6.353646	1.571580
Mo	12.937633	-3.147947	1.482100
Mo	12.855531	-0.030045	1.534432
S	0.945748	1.608337	0.035414
S	0.963735	4.782171	-0.028296
S	0.906651	8.007714	0.008045
S	3.688052	0.023728	0.040847
S	3.704492	3.197262	0.036208
S	3.699551	6.404085	0.022525
S	6.456393	-1.562574	0.003601
S	6.451388	1.613416	0.014127
S	6.447160	4.806273	-0.002165
S	9.222894	-3.174944	-0.063474
S	9.205123	0.068416	-0.095567
S	9.230885	3.220957	-0.013865
S	12.012730	-4.772531	-0.035648
S	11.991055	-1.573958	-0.050570
S	11.996725	1.610980	-0.005696
S	0.924371	1.619954	3.149617
S	0.882792	4.840827	3.120456
S	0.855870	7.942689	3.122258
S	3.695979	0.010075	3.158079
S	3.705086	3.214744	3.154651
S	3.682426	6.402933	3.131941
S	6.504216	-1.562942	3.113212
S	6.520946	1.601963	3.130216
S	6.487098	4.822625	3.117064
S	9.288098	-3.087468	3.041971
S	11.995930	-4.680694	3.086630
S	11.978392	1.569068	3.100232
S	9.237933	3.253783	3.088717
C	9.250302	-0.083395	2.870213
H	9.689626	0.910707	3.275155
H	8.918893	-0.404022	3.871160
H	10.624505	-0.745559	2.990760

CH_3* + H* = CH_4* + *

Mo	1.833236	0.003333	1.572332
Mo	1.837964	3.200933	1.575594
Mo	1.810969	6.391669	1.541944
Mo	4.614187	-1.584219	1.568293
Mo	4.618117	1.589532	1.579202
Mo	4.605931	4.779616	1.556639
Mo	7.371410	-3.196205	1.516047
Mo	7.423997	0.030903	1.524097
Mo	7.391575	3.151828	1.504844
Mo	10.146463	-4.811076	1.505844
Mo	10.173583	-1.568046	1.612629
Mo	10.127143	1.558497	1.456745
Mo	12.902644	-6.346120	1.536416
Mo	12.881350	-3.130102	1.524485
Mo	12.862273	0.001021	1.471455
S	0.943885	1.607629	0.006677
S	0.906263	4.782265	-0.016969
S	0.914545	7.999043	-0.034302
S	3.683239	0.005452	0.020073
S	3.680527	3.179098	0.014597
S	3.683689	6.390534	0.005627
S	6.454176	-1.562307	-0.014091
S	6.437414	1.548834	-0.031488
S	6.436470	4.770590	-0.029225
S	9.237312	-3.165759	-0.017547
S	9.249413	-0.076905	-0.022091
S	9.232390	3.164075	-0.080891
S	12.012345	-4.742861	-0.037322
S	11.919521	-1.578958	-0.011245
S	12.001431	1.625743	-0.062514
S	0.909320	1.604438	3.130773
S	0.866506	4.837665	3.110832
S	0.830994	7.943774	3.094680
S	3.681558	-0.005587	3.138387
S	3.691397	3.198340	3.133314
S	3.669830	6.381577	3.107687
S	6.515169	-1.571674	3.082134
S	6.520595	1.584122	3.105670
S	6.473374	4.759632	3.078635
S	9.188807	-3.275903	3.041701
S	11.959078	-4.717114	3.082450
S	11.940127	1.575616	3.037401
S	9.227705	3.104418	3.056207
C	10.399476	-1.051318	3.957202
H	9.682342	-0.183184	2.733845
H	9.445700	-1.147678	4.492917
H	10.886853	-0.115917	4.251903
H	11.062196	-1.881396	4.234475

6. Transition state of elementary reaction on Cu/MoS_{2-v}(001)

H_2O* + * = OH* + H*

Mo	1.807130	0.008993	1.632995
Mo	1.820415	3.207366	1.621538
Mo	1.812335	6.396595	1.583169
Mo	4.587760	-1.555831	1.644067
Mo	4.571119	1.636004	1.651396
Mo	4.588277	4.815764	1.627397
Mo	7.344282	-3.117583	1.576597
Mo	7.315495	0.073049	1.612748
Mo	7.345412	3.235146	1.591928
Mo	10.125755	-4.778725	1.486554
Mo	10.060545	1.614173	1.545130
Mo	12.851955	-6.385992	1.580141
Mo	12.930437	-3.172096	1.429045
Mo	12.901937	-0.038006	1.469941
Cu	10.315911	-1.850479	1.141735
S	0.903060	1.599023	0.061195
S	0.985581	4.758317	-0.019622
S	0.941785	8.023487	0.000849
S	3.659747	0.034500	0.088556
S	3.670369	3.212157	0.074439
S	3.688266	6.418676	0.062103
S	6.411539	-1.519007	0.064731
S	6.383798	1.629449	0.059029
S	6.413690	4.837836	0.043992
S	9.103384	-3.309638	-0.175503
S	9.168344	-0.041791	0.091611
S	9.159027	3.184251	-0.018124
S	11.975796	-4.824497	-0.048447
S	12.117964	-1.601893	-0.130016
S	11.914446	1.599315	-0.002534
S	0.858273	1.609160	3.172992
S	0.828366	4.838836	3.122830
S	0.823451	7.934850	3.142049
S	3.642760	0.026031	3.206449
S	3.647298	3.234950	3.202427
S	3.638626	6.404280	3.176503
S	6.463358	-1.544496	3.184593
S	6.430077	1.660102	3.191723
S	6.467507	4.852144	3.156871
S	9.385962	-2.938044	2.946746
S	11.955338	-4.687411	3.063613
S	11.911998	1.484423	3.092028
S	9.222379	3.251759	3.106020
O	9.079603	0.215558	2.836051
H	8.913984	0.556983	3.738066
H	10.830794	-1.909482	2.674427

OH* + * = O* + H*

Mo	1.820378	0.045826	1.654236
Mo	1.806669	3.220586	1.667536
Mo	1.832517	6.425605	1.635662
Mo	4.588259	-1.587632	1.585551
Mo	4.590461	1.599496	1.617655
Mo	4.563123	4.776884	1.602343
Mo	7.309209	-3.241598	1.452571
Mo	7.341427	0.027919	1.448979
Mo	7.355376	3.122427	1.542646
Mo	10.046923	-4.813691	1.528509
Mo	10.141667	1.541905	1.595108
Mo	12.867463	-6.302425	1.665284
Mo	12.863484	-2.993263	1.635170
Mo	12.890744	0.054380	1.626110
Cu	9.915065	-1.940408	1.088950
S	0.886080	1.647630	0.102704
S	0.896496	4.822156	0.100887
S	0.913206	8.036673	0.072038
S	3.635250	0.021033	0.064775
S	3.615090	3.186026	0.072845
S	3.643255	6.389220	0.042922
S	6.378771	-1.618203	-0.050729
S	6.364700	1.573893	-0.033679
S	6.346468	4.693520	-0.015304
S	9.009321	-3.547739	-0.273798
S	9.214790	-0.080694	0.077797
S	9.233088	3.064769	0.004351
S	11.974730	-4.693435	0.086440
S	11.972964	-1.536632	-0.001225
S	11.987549	1.664385	0.075956
S	0.889458	1.637700	3.235971
S	0.885960	4.860907	3.209703
S	0.903335	8.011326	3.213383
S	3.694812	0.001709	3.182016
S	3.682556	3.197734	3.196750
S	3.696214	6.399587	3.175303
S	6.525198	-1.574639	3.053500
S	6.505827	1.541439	3.125308
S	6.458476	4.768037	3.083852
S	9.194404	-3.091618	2.937295
S	11.872701	-4.632459	3.147566
S	11.922323	1.626695	3.223195
S	9.175336	3.118683	3.122540
O	12.132024	-1.511738	2.795229
H	11.203862	-0.549412	2.138200

2OH* = H_2O* + O*

Mo	1.801925	0.073050	1.628394
Mo	1.768963	3.263143	1.644163
Mo	1.787157	6.455113	1.624069
Mo	4.557660	-1.577673	1.581900
Mo	4.558078	1.608342	1.619010
Mo	4.527072	4.790382	1.598043
Mo	7.276835	-3.253712	1.420651
Mo	7.318394	-0.004795	1.480604
Mo	7.323978	3.119570	1.555880
Mo	10.010024	-4.813760	1.471665
Mo	10.185082	1.588696	1.632144
Mo	12.856084	-6.245471	1.622493
Mo	12.772803	-2.941043	1.615876
Mo	12.868855	0.108713	1.596906
Cu	9.925268	-2.033428	0.926523
S	0.878898	1.685538	0.069573
S	0.826879	4.871186	0.092947
S	0.892448	8.065850	0.048683
S	3.621580	0.038423	0.051700
S	3.589014	3.202825	0.064537
S	3.606762	6.402981	0.039710
S	6.352830	-1.596064	-0.059522
S	6.353165	1.558726	-0.008321
S	6.301857	4.669582	-0.017934
S	8.932116	-3.579608	-0.336378
S	9.234710	-0.064010	0.107401
S	9.189476	3.032268	0.000206
S	11.956318	-4.638482	0.040465
S	11.912051	-1.457458	-0.029915
S	11.978422	1.706146	0.063051
S	0.869685	1.678707	3.198667
S	0.805874	4.899345	3.185179
S	0.874249	8.049091	3.192798
S	3.656734	0.014943	3.174824
S	3.635708	3.220338	3.185100
S	3.649265	6.414217	3.167396
S	6.482138	-1.608456	3.048470
S	6.463745	1.535983	3.128793
S	6.424165	4.778375	3.078749
S	9.158880	-3.129564	2.888515
S	11.825918	-4.597656	3.106877
S	11.993169	1.715774	3.193213
S	9.172989	3.173454	3.119471
O	11.988162	-1.355462	2.746398
O	9.831314	-0.148648	3.017129
H	10.797145	-0.819156	2.954424
H	9.728027	0.135159	3.947630

CO* + O* = CO_2* + *

Mo	1.841129	0.011942	1.584189
Mo	1.848674	3.203155	1.564931
Mo	1.828646	6.402312	1.539837
Mo	4.614943	-1.552768	1.615543
Mo	4.594011	1.613173	1.607483
Mo	4.587936	4.800288	1.579738
Mo	7.318877	-3.200094	1.594023
Mo	7.430634	0.097504	1.634639
Mo	7.350229	3.213289	1.564397
Mo	10.118024	-4.794640	1.459972
Mo	10.084925	1.607874	1.530400
Mo	12.876754	-6.360585	1.522665
Mo	12.984966	-3.181918	1.398555
Mo	12.925086	0.022198	1.458672
Cu	10.263997	-1.827162	1.473225
S	0.933758	1.598610	0.004533
S	1.009456	4.764536	-0.076927
S	0.945665	8.030144	-0.037554
S	3.696282	0.018939	0.040457
S	3.697864	3.191213	0.020985
S	3.710261	6.429135	0.023720
S	6.480638	-1.530928	0.083802

S	6.433533	1.587886	0.041029
S	6.416895	4.804256	0.003637
S	9.120826	-3.286482	-0.102883
S	9.229304	-0.104543	0.074696
S	9.171310	3.157851	-0.045263
S	11.981386	-4.799541	-0.095003
S	11.996743	-1.590081	0.031760
S	11.934425	1.618908	-0.043643
S	0.885605	1.615553	3.115620
S	0.873604	4.830503	3.084117
S	0.861148	7.953104	3.104368
S	3.665194	0.022561	3.171876
S	3.660867	3.216812	3.153844
S	3.652934	6.402068	3.134151
S	6.490947	-1.551695	3.174729
S	6.442258	1.658428	3.174923
S	6.409294	4.779053	3.144298
S	9.152791	-3.270516	3.056598
S	11.971989	-4.675619	3.021511
S	11.958390	1.565006	3.067920
S	9.231589	3.225894	3.084490
C	10.474688	-1.010548	3.371807
O	10.659447	-0.964108	4.514929
O	9.062276	0.342573	2.795058

CO* + OH* = COOH* + *

Mo	1.843131	-0.039636	1.597874
Mo	1.843111	0.014908	1.562559
Mo	1.842140	3.217089	1.545640
Mo	1.805812	6.407029	1.561307
Mo	4.600250	-1.608939	1.520841
Mo	4.596671	1.583369	1.548569
Mo	4.568243	4.763646	1.532641
Mo	7.327869	-3.271002	1.407118
Mo	7.322664	-0.004243	1.412822
Mo	7.357712	3.112397	1.517361
Mo	10.070429	-4.839160	1.422663
Mo	10.235507	1.607921	1.615903
Mo	12.907418	-6.274667	1.526962
Mo	12.917757	-3.153909	1.419458
Mo	12.870760	0.172262	1.653031
Cu	9.879661	-2.013163	1.091461
S	0.943317	1.616373	-0.017470
S	0.947831	4.803391	-0.056370
S	0.880559	8.006255	0.010803
S	3.664683	-0.004230	-0.013182
S	3.662926	3.171245	-0.022592
S	3.640555	6.378244	-0.017313
S	6.401798	-1.633751	-0.109054
S	6.388578	1.564422	-0.075570
S	6.364297	4.670329	-0.059688
S	9.003959	-3.547429	-0.332427
S	9.267090	-0.064830	0.125583
S	9.217933	3.024811	-0.034320
S	11.955983	-4.752189	-0.108548
S	11.873755	-1.493261	0.179086
S	11.993556	1.661112	0.019698
S	0.935860	1.648918	3.104846
S	0.851411	4.826527	3.082696
S	0.926555	8.011580	3.159309
S	3.699260	-0.016131	3.105548
S	3.677567	3.188144	3.112311
S	3.675945	6.381337	3.097254
S	6.518329	-1.612222	3.007667
S	6.487923	1.522048	3.077820
S	6.441283	4.758756	3.041403
S	9.186581	-3.190102	2.918548
S	11.917886	-4.624896	3.011287
S	12.047393	1.848370	3.185586
S	9.203524	3.180597	3.089764
C	11.591813	-0.692824	3.238744
O	11.725104	-1.349562	4.223809
O	10.086533	-0.109888	3.065256
H	9.695609	-0.022627	3.962844

CO* + H* = CHO* + *

Mo	1.856035	-0.000423	1.592431
Mo	1.849692	3.194424	1.608964
Mo	1.819720	6.386771	1.609326
Mo	4.613051	-1.611347	1.553282
Mo	4.610896	1.576839	1.574472
Mo	4.585061	4.757763	1.567333
Mo	7.345864	-3.260013	1.435052
Mo	7.344610	0.010500	1.441210
Mo	7.371289	3.125119	1.526531
Mo	10.098317	-4.832231	1.475707
Mo	10.173715	1.609867	1.557355
Mo	12.902587	-6.320895	1.585382
Mo	12.921546	-3.180853	1.548743
Mo	12.901734	0.154115	1.610462
Cu	9.866522	-1.941450	1.144243
S	0.939862	1.608329	0.034710
S	0.925886	4.779013	0.029489
S	0.929330	7.978761	0.020642
S	3.676409	-0.012516	0.015146
S	3.658137	3.167119	0.020087
S	3.648138	6.365475	0.021999
S	6.410688	-1.628242	-0.077223
S	6.397442	1.564763	-0.058791
S	6.373096	4.687062	-0.040061
S	9.047087	-3.505564	-0.280491
S	9.261437	-0.048390	0.119302
S	9.231679	3.084733	-0.037834
S	11.996206	-4.756410	-0.020257
S	11.905302	-1.551798	0.200978
S	11.998904	1.663628	0.012556
S	0.936382	1.604155	3.157590
S	0.896820	4.802962	3.161034
S	0.916506	7.999450	3.173495
S	3.713188	-0.022525	3.137007
S	3.705927	3.172779	3.152541
S	3.700415	6.374145	3.136080
S	6.539789	-1.601714	3.034872
S	6.507770	1.534178	3.095014
S	6.465827	4.760655	3.065420
S	9.204425	-3.151656	2.957099
S	11.928070	-4.707639	3.093463
S	11.957821	1.731328	3.188018
S	9.197614	3.162687	3.098291
C	11.670043	-0.824949	3.094380
O	11.872990	-1.709295	3.907681
H	10.586971	-0.369870	3.049478

CO* + H* = COH* + *

Mo	1.792296	-0.018008	1.595518
Mo	1.813943	3.155687	1.598021
Mo	1.854800	6.352614	1.578617
Mo	4.575058	-1.614974	1.586468
Mo	4.578984	1.573257	1.600889
Mo	4.575442	4.756332	1.576200
Mo	7.300575	-3.187556	1.498696
Mo	7.311116	-0.005264	1.499830
Mo	7.335798	3.154946	1.535889
Mo	10.062427	-4.809021	1.481717
Mo	10.019187	1.596400	1.478145
Mo	12.811807	-6.364855	1.585563
Mo	12.881590	-3.192534	1.469691
Mo	12.896530	-0.072335	1.515670
Cu	10.338051	-1.866548	1.181583
S	0.852506	1.577180	0.038900
S	0.971872	4.751494	0.005822
S	0.959826	7.939064	0.003026
S	3.636485	-0.015736	0.044324
S	3.646450	3.150318	0.032443
S	3.676041	6.359363	0.011935
S	6.375287	-1.603971	-0.028237
S	6.377268	1.553120	-0.017507
S	6.382607	4.745419	-0.023114
S	9.090608	-3.347265	-0.180473
S	9.235572	-0.132448	0.153242
S	9.156760	3.137910	-0.067404
S	11.923418	-4.828459	-0.037420
S	12.155035	-1.634518	-0.183565
S	11.931880	1.568914	0.020999
S	0.852485	1.580878	3.152355
S	0.865787	4.764971	3.115923
S	0.895904	7.929672	3.129457
S	3.645453	-0.021952	3.154028
S	3.663780	3.168823	3.158572
S	3.680340	6.348853	3.154627
S	6.476066	-1.570554	3.107478
S	6.473535	1.561089	3.124797
S	6.444279	4.779992	3.092058
S	9.252818	-2.992276	2.879281
S	11.891082	-4.704174	3.079802
S	11.897486	1.429955	3.124602
S	9.161385	3.164371	3.089424
C	12.266086	-1.598441	2.922822
O	11.905673	-1.612948	4.062298
H	10.829159	1.078697	3.923483

CHO* + O* = HCOO* + *

Mo	1.852435	0.015522	1.655783
Mo	1.844446	3.221538	1.668824
Mo	1.833189	6.411440	1.635213
Mo	4.644618	-1.548881	1.617782
Mo	4.614205	1.630738	1.643126
Mo	4.626000	4.822803	1.645197
Mo	7.414434	-3.154385	1.549062
Mo	7.482593	0.052571	1.453844
Mo	7.396184	3.248537	1.567209
Mo	10.213973	-4.772096	1.592628
Mo	10.103204	1.582326	1.447809
Mo	12.905177	-6.374835	1.631324
Mo	12.839697	-3.174158	1.577570
Mo	12.881869	-0.023711	1.526300
Cu	9.983719	-1.302492	0.208407
S	0.951861	1.619640	0.097478
S	0.919006	4.788932	0.086047
S	0.956425	8.014551	0.055264
S	3.690388	0.039905	0.083771
S	3.677459	3.229615	0.100157
S	3.692454	6.411034	0.084066
S	6.462180	-1.549117	-0.002732
S	6.398645	1.670489	0.030498
S	6.423330	4.827163	0.027028
S	9.200210	-3.285272	-0.057261
S	8.993586	0.458570	-0.465322
S	9.235983	3.292614	-0.010780
S	12.022518	-4.781286	0.048408
S	12.110636	-1.591314	-0.155478
S	12.009704	1.624399	0.002324
S	0.921028	1.604758	3.216501
S	0.849219	4.840956	3.183734
S	0.846790	7.973497	3.174350
S	3.718152	0.017264	3.203092
S	3.709480	3.228870	3.218154
S	3.704137	6.431931	3.188472
S	6.581686	-1.507581	3.085429
S	6.564423	1.576264	3.094784
S	6.522834	4.846557	3.156049
S	9.373508	-3.015768	3.129522
S	12.001942	-4.763629	3.195860
S	11.892384	1.519653	3.085833
S	9.264259	3.148771	3.088032
C	10.399400	-1.496003	3.140392
O	9.336010	-0.072356	2.418235
O	11.599100	-1.556252	2.617125
H	10.301737	-0.976955	4.103912

COH* + O* = COOH* + *

Mo	1.772815	0.012040	1.668939
Mo	1.808570	3.211562	1.626405
Mo	1.752550	6.401734	1.627435
Mo	4.568558	-1.561838	1.638409
Mo	4.540817	1.619289	1.645140
Mo	4.528167	4.811539	1.618762
Mo	7.309908	-3.209744	1.510512
Mo	7.353094	0.087432	1.553962
Mo	7.293780	3.226737	1.563378
Mo	10.090939	-4.816067	1.435807
Mo	10.055358	1.685891	1.605062
Mo	12.852016	-6.309214	1.603338
Mo	12.884380	-3.200733	1.412928
Mo	12.722844	0.077250	1.694282
Cu	9.669027	-1.749485	1.117641
S	0.905153	1.593825	0.077568
S	0.951299	4.779807	-0.006914
S	0.787445	8.015936	0.120670
S	3.608795	0.014988	0.099468
S	3.631614	3.199322	0.066568
S	3.607455	6.431134	0.078342
S	6.377516	-1.553854	0.027079
S	6.329802	1.645651	0.032579
S	6.319176	4.781989	0.001322
S	9.009072	-3.419559	-0.264906
S	9.061292	0.123091	-0.048931
S	9.110841	3.150564	-0.049782
S	11.956715	-4.820778	-0.073158
S	11.869272	-1.589052	0.155577
S	11.983509	1.620142	0.051423
S	0.864875	1.645504	3.197220
S	0.782366	4.817503	3.131480
S	0.771903	7.962241	3.204984
S	3.639731	0.013092	3.215877
S	3.631795	3.226820	3.204350
S	3.612886	6.412646	3.185214
S	6.513496	-1.566939	3.120743
S	6.424999	1.633405	3.164455
S	6.400683	4.827994	3.128646
S	9.235697	-3.088746	2.886763
S	11.884505	-4.620075	3.073640
S	11.898017	1.777307	3.227539
S	9.154366	3.293206	3.110337
C	9.097882	0.368626	2.905610
O	10.676929	-0.352174	2.208914
O	9.167487	0.239782	4.212950
H	8.536083	-0.452980	4.520595

HCOO* + * = CO_2* + H*

Mo	1.801012	0.054737	1.557019
Mo	1.817913	3.223981	1.580354
Mo	1.776413	6.439278	1.587887
Mo	4.548820	-1.545889	1.540974
Mo	4.566170	1.633639	1.548998
Mo	4.536860	4.817212	1.545197
Mo	7.256597	-3.166616	1.446487
Mo	7.295030	0.052413	1.446349
Mo	7.313958	3.188738	1.502508
Mo	10.008617	-4.755675	1.483370
Mo	10.119568	1.681331	1.486970
Mo	12.846335	-6.276347	1.542061
Mo	12.900812	-3.109844	1.672262
Mo	12.828887	0.235947	1.552659
Cu	10.104089	-1.977772	1.270455
S	0.892930	1.662421	-0.008890
S	0.855238	4.827813	0.053663
S	0.875407	8.034332	-0.012168
S	3.626460	0.045357	-0.011960
S	3.623927	3.224454	-0.010422
S	3.597284	6.427593	0.000612
S	6.353525	-1.565219	-0.072736
S	6.367998	1.605460	-0.069735
S	6.332958	4.772770	-0.055297
S	8.999161	-3.384097	-0.246222
S	9.276787	-0.121265	0.249185
S	9.166800	3.182754	-0.070526
S	11.952592	-4.633708	0.015404
S	11.989365	-1.545872	0.166431
S	11.943175	1.733849	-0.062743
S	0.876726	1.641472	3.124164
S	0.963370	4.807724	3.158024
S	0.838051	8.058715	3.131158
S	3.646534	0.046475	3.113067
S	3.672130	3.219321	3.126269
S	3.646766	6.432045	3.120199
S	6.452443	-1.525259	3.051500
S	6.452925	1.597638	3.082358
S	6.406665	4.817193	3.056554
S	9.150673	-3.085024	2.967680
S	11.856765	-4.746558	3.076937
S	11.881817	1.764134	3.117597
S	9.136423	3.191081	3.072148
C	11.574904	-1.232952	4.132425
O	10.882175	-0.530744	4.784747
O	12.260423	-2.208447	3.913842
H	11.663822	-0.565314	2.623353

COOH* + * = CO_2* + H*

Mo	1.748859	0.144535	1.616974
Mo	1.731827	3.352730	1.609909

Mo	1.736280	6.527719	1.587875
Mo	4.501552	-1.487216	1.609361
Mo	4.492540	1.700565	1.644300
Mo	4.482506	4.886563	1.610755
Mo	7.248030	-3.162779	1.513376
Mo	7.262804	0.116783	1.713847
Mo	7.266889	3.225202	1.623897
Mo	9.981382	-4.725375	1.459054
Mo	10.221929	1.709449	1.624759
Mo	12.828608	-6.160030	1.564369
Mo	12.803000	-2.920153	1.513741
Mo	12.836619	0.205002	1.573368
Cu	9.825349	-1.935888	1.098259
S	0.861884	1.758951	0.034641
S	0.823772	4.940163	0.015038
S	0.832956	8.145017	0.024457
S	3.588333	0.125295	0.059294
S	3.576551	3.291804	0.059894
S	3.592283	6.499012	0.036620
S	6.364206	-1.447325	0.059570
S	6.340189	1.634593	0.097429
S	6.287955	4.780775	0.036427
S	8.881959	-3.452958	-0.292730
S	9.126870	0.036093	0.239468
S	9.091366	3.142029	0.007309
S	11.878828	-4.584876	-0.028305
S	11.782817	-1.375477	0.106421
S	11.950755	1.794281	0.002492
S	0.824174	1.772370	3.163715
S	0.757629	4.989325	3.149985
S	0.810445	8.094131	3.172166
S	3.571712	0.099885	3.190345
S	3.557022	3.322335	3.185534
S	3.565731	6.497587	3.165223
S	6.344447	-1.566500	3.148954
S	6.314606	1.707417	3.227391
S	6.346377	4.871656	3.138607
S	9.106635	-3.105599	2.968422
S	11.831557	-4.498513	3.053977
S	12.021865	1.829517	3.174748
S	9.174001	3.270326	3.124903
C	9.919663	0.082367	3.016619
O	8.674983	-0.072168	3.347089
O	10.757701	-0.749212	3.540641
H	11.908599	-1.088626	2.834241

$2H^* = H_2 + 2^*$

Mo	1.853206	-0.021016	1.667830
Mo	1.861540	3.176483	1.663594
Mo	1.836092	6.360407	1.629673
Mo	4.607654	-1.627054	1.629508
Mo	4.608209	1.577349	1.653396
Mo	4.608074	4.743308	1.636004
Mo	7.336880	-3.226275	1.535832
Mo	7.295001	-0.048129	1.508552
Mo	7.400447	3.119423	1.623008
Mo	10.129865	-4.831402	1.596868
Mo	10.181131	1.580688	1.679831
Mo	12.918813	-6.373034	1.661386
Mo	12.971683	-3.187752	1.534075
Mo	12.944370	-0.001475	1.571501
Cu	10.359662	-1.992735	1.406011
S	0.938196	1.578324	0.107876
S	0.983335	4.733721	0.036856
S	0.951966	7.993112	0.055905
S	3.676471	-0.018879	0.095199
S	3.682426	3.154524	0.086117
S	3.683976	6.346693	0.073405
S	6.392538	-1.653204	-0.005521
S	6.409162	1.557760	0.030215
S	6.425073	4.689400	0.047121
S	9.132228	-3.379986	-0.073929
S	9.303168	-0.179294	0.360517
S	9.259371	3.077112	0.071498
S	11.993783	-4.825745	0.051626
S	12.053861	-1.599284	0.073140
S	11.990152	1.603365	0.090855
S	0.942896	1.589081	3.230106
S	0.889808	4.808142	3.192584
S	0.893347	7.918418	3.204043
S	3.703894	-0.033536	3.211655
S	3.704756	3.173210	3.226286
S	3.686638	6.350556	3.191438
S	6.511301	-1.605742	3.147384
S	6.500864	1.513885	3.166188
S	6.488285	4.760793	3.154083
S	9.286350	-3.081421	3.041414
S	11.983571	-4.693799	3.158413
S	12.038215	1.557870	3.210516
S	9.228668	3.167797	3.208637
H	10.040092	-0.135035	3.341063
H	9.505471	0.382805	3.549401

$CHO^* + * = CH^* + O^*$

Mo	1.852248	0.009079	1.642188
Mo	1.856173	3.194995	1.647785
Mo	1.862470	6.382056	1.625621
Mo	4.612226	-1.610371	1.575965
Mo	4.621329	1.575901	1.602328
Mo	4.613525	4.748665	1.588828
Mo	7.303017	-3.254377	1.467911
Mo	7.352522	-0.033523	1.426987
Mo	7.397649	3.104139	1.541689
Mo	10.119022	-4.859045	1.505056
Mo	10.268551	1.499304	1.593660
Mo	12.931670	-6.327310	1.644065
Mo	12.917990	-3.052834	1.596482
Mo	12.900160	0.014094	1.633566
Cu	9.882810	-1.814381	1.199483
S	0.945650	1.615158	0.080442
S	0.945664	4.786830	0.070753
S	0.925993	7.992715	0.080058
S	3.662970	-0.005500	0.048382
S	3.664156	3.164399	0.053690
S	3.674238	6.358774	0.035663
S	6.390638	-1.648889	-0.065316
S	6.402274	1.558380	-0.039128
S	6.408199	4.675822	-0.029932
S	9.106425	-3.444399	-0.195337
S	9.209896	-0.051297	-0.023608
S	9.258617	3.044053	-0.019508
S	12.023557	-4.732159	0.058157
S	11.999777	-1.575266	0.004895
S	12.064240	1.630405	0.055923
S	0.947256	1.612506	3.216901
S	0.920416	4.820102	3.201258
S	0.929865	7.969942	3.202159
S	3.722408	-0.020760	3.168501
S	3.725242	3.174339	3.181379
S	3.727581	6.366029	3.159008
S	6.527179	-1.601380	3.057854
S	6.537961	1.506103	3.097794
S	6.495879	4.738067	3.093538
S	9.232544	-3.102965	2.917226
S	11.925390	-4.677422	3.128648
S	12.040316	1.637125	3.249994
S	9.250421	3.086731	3.096690
C	10.611103	-0.510742	2.457691
O	12.142742	-1.528584	2.783174
H	10.424373	-0.636395	3.531534

$CHO^* + H^* = CH_2O^* + *$

Mo	1.868193	-0.009019	1.616775
Mo	1.870152	3.185948	1.630095
Mo	1.857960	6.373298	1.613483
Mo	4.621463	-1.615242	1.566544
Mo	4.619160	1.566141	1.583302
Mo	4.612141	4.740920	1.579066
Mo	7.293455	-3.263160	1.461795
Mo	7.368481	-0.059231	1.439865
Mo	7.390062	3.104218	1.556717
Mo	10.106224	-4.901328	1.558696
Mo	10.239187	1.557724	1.601658
Mo	12.933272	-6.349769	1.638918
Mo	12.954955	-3.136185	1.625761
Mo	12.943716	0.045724	1.631453
Cu	10.050009	-2.017531	1.348388
S	0.946249	1.604406	0.063810
S	0.938020	4.774940	0.059966
S	0.927080	7.974853	0.052276
S	3.676565	-0.018956	0.025847
S	3.673056	3.158276	0.031121
S	3.677698	6.354274	0.027543
S	6.406480	-1.642044	-0.068732
S	6.423401	1.535165	-0.029078
S	6.405083	4.665859	-0.032805
S	9.120342	-3.434077	-0.133662
S	9.280241	-0.083677	0.116685
S	9.242014	3.060542	-0.001247
S	12.018488	-4.755310	0.073116
S	11.941550	-1.613691	0.112256
S	12.058247	1.606861	0.060058
S	0.966087	1.594619	3.191589
S	0.958659	4.793409	3.199091
S	0.965557	7.976776	3.192449
S	3.726767	-0.025999	3.151243
S	3.730450	3.161965	3.166436
S	3.726609	6.361151	3.146134
S	6.528208	-1.612466	3.076082
S	6.518359	1.488659	3.090730
S	6.478093	4.735436	3.101141
S	9.182526	-3.241986	3.009238
S	11.948528	-4.726376	3.144376
S	12.037812	1.634850	3.211818
S	9.211972	3.081978	3.149487
C	10.866142	-1.164783	2.916846
O	12.170540	-1.458906	2.977999
H	10.420281	-1.110942	3.925033
H	9.916975	0.227113	2.759438

$CHO^* + H^* = CHOH^* + *$

Mo	1.834195	0.016827	1.635586
Mo	1.822888	3.218514	1.640287
Mo	1.806083	6.414436	1.626653
Mo	4.617538	-1.570878	1.624878
Mo	4.597057	1.598465	1.641104
Mo	4.565760	4.794861	1.623343
Mo	7.339522	-3.234500	1.534913
Mo	7.436450	0.058522	1.580571
Mo	7.336374	3.188965	1.575175
Mo	10.088740	-4.808565	1.480192
Mo	10.131121	1.644398	1.521774
Mo	12.876534	-6.321687	1.589595
Mo	12.903462	-3.127214	1.528530
Mo	12.877573	0.112480	1.587237
Cu	9.841220	-1.933775	1.156082
S	0.933010	1.622149	0.069629
S	0.925491	4.800367	0.038283
S	0.919705	8.009691	0.042199
S	3.677230	0.014959	0.076796
S	3.655822	3.187820	0.076973
S	3.662726	6.412126	0.072765
S	6.447752	-1.557127	0.040600
S	6.409589	1.593941	0.042777
S	6.350682	4.752615	0.017153
S	9.019549	-3.444847	-0.225114
S	9.213755	0.016136	0.026146
S	9.152048	3.156068	-0.040670
S	11.986931	-4.745218	-0.020159
S	11.872315	-1.529123	0.172078
S	12.002437	1.659758	-0.006523
S	0.889710	1.623184	3.183150
S	0.851440	4.847249	3.171678
S	0.856512	7.988194	3.189752
S	3.683002	0.002285	3.200878
S	3.666848	3.204751	3.199542
S	3.667803	6.409789	3.183571
S	6.539734	-1.573224	3.131040
S	6.484265	1.598485	3.172412
S	6.428138	4.787037	3.143947
S	9.169573	-3.270107	3.050669
S	11.922703	-4.665858	3.087511
S	11.933011	1.651187	3.158270
S	9.208102	3.205490	3.091399
C	9.256053	0.231993	2.969220
O	10.165503	-0.761009	2.852280
H	9.043855	0.523899	4.009610
H	11.530648	-0.645756	2.810096

$COH^* + H^* = CHOH^* + *$

Mo	1.818458	0.023458	1.608960
Mo	1.815774	3.207772	1.613622
Mo	1.833406	6.395562	1.597312
Mo	4.578843	-1.589396	1.601193
Mo	4.573588	1.602338	1.615850
Mo	4.570733	4.771443	1.598198
Mo	7.289861	-3.236068	1.518893
Mo	7.293446	0.036831	1.510570
Mo	7.345125	3.125806	1.571828
Mo	10.066598	-4.863610	1.535087
Mo	10.138198	1.575605	1.574676
Mo	12.873285	-6.342922	1.609841
Mo	12.903255	-3.132827	1.537168
Mo	12.888546	0.071167	1.542763
Cu	10.342659	-2.117154	1.310057
S	0.896742	1.621315	0.049052
S	0.958045	4.802809	0.013966
S	0.943341	8.000764	0.013848
S	3.652619	0.009677	0.051598
S	3.643045	3.184929	0.046522
S	3.667233	6.387559	0.036889
S	6.389622	-1.621286	-0.000216
S	6.368505	1.569337	-0.010862
S	6.381837	4.713417	0.003948
S	9.073672	-3.433557	-0.138401
S	9.245261	-0.212700	0.337644
S	9.192482	3.075560	-0.004376
S	11.945769	-4.784995	0.017759
S	12.090246	-1.572048	-0.118672
S	11.944676	1.659934	0.007174
S	0.895403	1.620148	3.179372
S	0.873316	4.821568	3.159141
S	0.881495	7.989042	3.153068
S	3.659440	0.002892	3.172115
S	3.656380	3.197630	3.178483
S	3.672029	6.382853	3.165818
S	6.488195	-1.577700	3.107964
S	6.448923	1.562569	3.157000
S	6.436442	4.755406	3.121034
S	9.174282	-3.126757	3.000628
S	11.911577	-4.703389	3.111231
S	11.934410	1.611021	3.196170
S	9.174892	3.113013	3.143506
C	12.072243	-1.579098	2.713774
O	11.815740	-1.571083	4.018002
H	11.791079	-0.647840	4.368058
H	11.219505	-0.415066	2.046404

$CH_2O^* + * = CH_2^* + O^*$

Mo	1.838072	0.040667	1.635121
Mo	1.820436	3.235270	1.630659
Mo	1.828537	6.414217	1.629689
Mo	4.593079	-1.616763	1.563170
Mo	4.582708	1.578882	1.599308
Mo	4.564087	4.757123	1.583627
Mo	7.313335	-3.303453	1.410347
Mo	7.301992	-0.024137	1.449551
Mo	7.360199	3.070819	1.563672
Mo	10.059645	-4.884980	1.486150
Mo	10.300493	1.520022	1.721369
Mo	12.930226	-6.253086	1.632583
Mo	12.835384	-2.983262	1.635151
Mo	12.881937	0.076269	1.681626
Cu	9.913136	-2.112962	0.938501
S	0.932003	1.649676	0.061259
S	0.861177	4.841854	0.086438
S	0.882691	8.027362	0.095774
S	3.642042	-0.002015	0.039969
S	3.625925	3.176344	0.041847
S	3.632801	6.368295	0.026637
S	6.381027	-1.648367	-0.087168
S	6.368792	1.549468	-0.035256
S	6.346196	4.619294	-0.021061
S	8.976563	-3.658514	-0.335991
S	9.257608	-0.085659	0.193193
S	9.236913	2.953322	0.031798
S	11.990812	-4.670304	0.056671
S	11.915420	-1.479334	0.053869
S	12.042248	1.669804	0.103195
S	0.945457	1.664296	3.204025
S	0.873223	4.854893	3.194155

S	0.935956	8.013623	3.218093
S	3.702900	-0.021570	3.161423
S	3.680284	3.190261	3.173066
S	3.698900	6.381365	3.159654
S	6.529348	-1.641517	3.033132
S	6.475555	1.499213	3.121510
S	6.452715	4.739346	3.071632
S	9.160769	-3.235927	2.912842
S	11.880591	-4.631402	3.126602
S	12.126054	1.791805	3.272818
S	9.217285	3.100424	3.148825
C	10.624237	-0.277048	2.968480
O	12.126055	-1.432924	2.861170
H	10.856304	-0.163829	4.034879
H	9.931467	-1.114831	2.832179

CHOH* + * = CH* + OH*

Mo	1.799666	-0.000593	1.623673
Mo	1.837942	3.189967	1.600148
Mo	1.788696	6.395986	1.592386
Mo	4.591858	-1.582238	1.612327
Mo	4.592028	1.573784	1.620003
Mo	4.552427	4.776513	1.599820
Mo	7.289793	-3.238377	1.549777
Mo	7.430939	0.014263	1.584728
Mo	7.323578	3.171781	1.557703
Mo	10.052809	-4.807181	1.459100
Mo	10.137585	1.693104	1.487527
Mo	12.872406	-6.316179	1.548075
Mo	12.950036	-3.171338	1.404901
Mo	12.789177	0.069822	1.596150
Cu	9.659819	-1.810187	1.364926
S	0.931041	1.598777	0.035427
S	0.990013	4.764561	-0.035274
S	0.838692	8.007243	0.054027
S	3.646412	-0.004397	0.063083
S	3.674403	3.159999	0.046766
S	3.649318	6.404355	0.049621
S	6.423547	-1.585462	0.030115
S	6.413665	1.559221	0.024870
S	6.349633	4.748770	0.003945
S	9.041655	-3.376638	-0.167780
S	9.264035	-0.004679	0.037246
S	9.104535	3.182340	-0.082886
S	11.942308	-4.776940	-0.078933
S	11.899415	-1.595122	0.106397
S	11.998992	1.642670	-0.026512
S	0.873702	1.623588	3.153984
S	0.841665	4.813040	3.111001
S	0.805655	7.956854	3.164384
S	3.653838	-0.008895	3.183413
S	3.663971	3.180847	3.176647
S	3.638430	6.390814	3.158711
S	6.487697	-1.593298	3.142369
S	6.483542	1.566381	3.161107
S	6.395633	4.756038	3.134380
S	9.141177	-3.254924	3.046581
S	11.910062	-4.624753	3.030907
S	11.930552	1.706756	3.122811
S	9.193109	3.200530	3.090731
C	9.227892	0.243498	2.771845
O	10.937591	-0.869528	2.729495
H	9.261668	0.225918	3.868343
H	11.045978	-1.193878	3.651086

$CH_2O^* + H^* = CH_3O^* + *$

Mo	1.873499	0.003029	1.608333
Mo	1.854041	3.199597	1.614464
Mo	1.842965	6.389182	1.601792
Mo	4.621702	-1.626111	1.531769
Mo	4.612421	1.569358	1.566322
Mo	4.588358	4.743648	1.553700
Mo	7.336003	-3.293425	1.396918
Mo	7.340056	-0.021618	1.417424
Mo	7.378818	3.087530	1.530462
Mo	10.095849	-4.879137	1.469323
Mo	10.252031	1.550875	1.659942
Mo	12.930033	-6.319408	1.619568
Mo	12.899706	-3.137162	1.608944
Mo	12.956970	0.086575	1.636790
Cu	9.858176	-1.999899	1.060645
S	0.943010	1.612682	0.049841
S	0.897386	4.790924	0.054617
S	0.925298	7.996594	0.041616
S	3.673663	-0.014929	0.007643
S	3.650080	3.160051	0.013061
S	3.655440	6.353005	0.001160
S	6.412369	-1.649895	-0.111559
S	6.397469	1.551567	-0.066453
S	6.376979	4.637958	-0.052581
S	9.039497	-3.589509	-0.316039
S	9.267026	-0.068082	0.127158
S	9.246045	2.998106	-0.009634
S	12.014135	-4.742134	0.021638
S	11.895534	-1.541695	0.167572
S	12.035904	1.629428	0.075842
S	0.966813	1.614086	3.177700
S	0.921162	4.808036	3.173495
S	0.981454	7.995305	3.192715
S	3.741900	-0.033739	3.130057
S	3.717458	3.169099	3.147484
S	3.721496	6.367176	3.124441
S	6.546255	-1.637432	3.008030
S	6.506867	1.499158	3.086093
S	6.469985	4.740991	3.047370
S	9.175740	-3.200453	2.916985
S	11.904763	-4.709567	3.112207
S	12.063966	1.694861	3.201546
S	9.214695	3.134911	3.119932
C	11.265160	-1.072179	3.891832
O	12.122709	-1.430424	3.010454
H	10.557202	-1.822043	4.265950
H	11.455919	-0.161412	4.473245
H	10.116627	0.104663	2.857943

$CH_2O^* + H^* = CH_2OH^* + *$

Mo	1.833563	0.030008	1.585730
Mo	1.804306	3.236875	1.596327
Mo	1.792707	6.421130	1.575197
Mo	4.574884	-1.591817	1.577528
Mo	4.567787	1.602138	1.607588
Mo	4.553380	4.781113	1.590045
Mo	7.313075	-3.270249	1.508189
Mo	7.336157	0.008994	1.620503
Mo	7.339383	3.146633	1.579259
Mo	10.083535	-4.828753	1.454473
Mo	10.257985	1.572633	1.521098
Mo	12.895336	-6.289686	1.548216
Mo	12.877341	-3.078419	1.499997
Mo	12.899022	0.142626	1.542454
Cu	9.828709	-1.905148	1.202516
S	0.935232	1.640579	0.016348
S	0.889381	4.818142	-0.002222
S	0.925272	8.025156	-0.013371
S	3.670511	0.019866	0.025590
S	3.640983	3.192904	0.036015
S	3.649326	6.387923	0.021576
S	6.420158	-1.592506	0.018682
S	6.400635	1.572567	0.046052
S	6.357486	4.701144	0.002137
S	8.996322	-3.477339	-0.241429
S	9.124556	-0.007943	0.044822
S	9.182732	3.075749	-0.031537
S	11.963798	-4.709998	-0.053369
S	11.820866	-1.469503	0.180027
S	12.012502	1.693155	-0.049357
S	0.899828	1.642288	3.139313
S	0.831727	4.870755	3.129916
S	0.868505	8.004040	3.144677
S	3.658541	-0.001770	3.159294
S	3.636207	3.210299	3.164108
S	3.636269	6.394545	3.141370
S	6.427227	-1.649715	3.108402
S	6.415731	1.593876	3.167166
S	6.412180	4.757682	3.124821
S	9.186370	-3.236717	2.973056
S	11.922687	-4.645038	3.047434
S	12.020824	1.709087	3.143409
S	9.249837	3.141897	3.060777
C	8.886874	-0.102858	3.396989
O	10.108195	-0.248541	2.686782
H	8.878528	0.786715	4.041544
H	8.669572	-0.997172	3.997692
H	11.514559	-0.570266	2.859426

CHOH* + H* = CH_2OH^* + *

Mo	1.915549	0.003995	1.599985
Mo	1.897752	3.200094	1.608590
Mo	1.864200	6.389061	1.631644
Mo	4.659993	-1.623334	1.549348
Mo	4.656113	1.564833	1.571683
Mo	4.624834	4.746621	1.569097
Mo	7.372403	-3.286656	1.425223
Mo	7.394588	-0.028394	1.427749
Mo	7.409102	3.097097	1.538019
Mo	10.128880	-4.877943	1.463148
Mo	10.289098	1.557176	1.613086
Mo	12.972477	-6.297678	1.570337
Mo	12.932614	-3.172440	1.626055
Mo	12.952799	0.193250	1.690680
Cu	9.834148	-1.952171	1.065629
S	1.008362	1.613420	0.024732
S	0.933546	4.801052	0.065164
S	0.960475	7.981898	0.057650
S	3.722979	-0.021132	0.011813
S	3.701337	3.162637	0.017463
S	3.676673	6.356007	0.028846
S	6.447918	-1.649439	-0.091046
S	6.442836	1.547282	-0.056292
S	6.409158	4.654833	-0.038824
S	9.072979	-3.564588	-0.296601
S	9.293216	-0.042095	0.075500
S	9.259483	3.014716	-0.014418
S	12.036509	-4.720255	-0.006788
S	11.941379	-1.516423	0.263294
S	12.059741	1.659853	0.034380
S	1.001350	1.616125	3.154050
S	0.961017	4.791986	3.184958
S	0.998891	8.016818	3.207559
S	3.773629	-0.029967	3.137131
S	3.753684	3.162917	3.150895
S	3.755657	6.369260	3.141384
S	6.584178	-1.628170	3.031397
S	6.550706	1.498402	3.089012
S	6.501355	4.741893	3.066709
S	9.224013	-3.190202	2.938097
S	11.948433	-4.767130	3.097182
S	12.068834	1.840566	3.210032
S	9.246245	3.124140	3.108351
C	11.737779	-0.633546	3.196877
O	11.825985	-1.995387	3.257356
H	11.443973	-0.251168	4.185323
H	10.187459	0.095448	2.779974
H	11.165999	-2.450460	3.845560

$CH_3O^* + * = CH_3^* + O^*$

Mo	1.811025	0.047239	1.513043
Mo	1.800259	3.212197	1.521807
Mo	1.828915	6.414357	1.503178
Mo	4.575009	-1.567836	1.453303
Mo	4.577069	1.620792	1.473572
Mo	4.557106	4.801908	1.462650
Mo	7.303853	-3.183211	1.340857
Mo	7.307741	0.061344	1.325918
Mo	7.341958	3.176384	1.407621
Mo	10.051357	-4.766856	1.427950
Mo	10.084199	1.625156	1.400891
Mo	12.849893	-6.333770	1.523170
Mo	12.880369	-3.032508	1.508720
Mo	12.869899	-0.004448	1.485840
Cu	10.008451	-1.847138	1.078450
S	0.869403	1.634920	-0.040597
S	0.894465	4.809223	-0.042997
S	0.901890	8.022974	-0.051649
S	3.624202	0.033420	-0.076181
S	3.610317	3.205673	-0.072373
S	3.632739	6.405613	-0.094013
S	6.364508	-1.577920	-0.180098
S	6.356945	1.614866	-0.171174
S	6.349086	4.753470	-0.147946
S	9.043360	-3.398839	-0.322705
S	9.219623	-0.053175	-0.000637
S	9.213476	3.172485	-0.152160
S	11.970353	-4.708450	-0.038247
S	11.978676	-1.555909	-0.138186
S	11.987168	1.625968	-0.068447
S	0.871999	1.626156	3.091703
S	0.900933	4.839620	3.082283
S	0.892031	8.006959	3.065677
S	3.680066	0.022630	3.042882
S	3.672867	3.212738	3.051830
S	3.687378	6.411445	3.041847
S	6.502188	-1.535260	2.938594
S	6.483860	1.588454	2.985189
S	6.444248	4.808267	2.956638
S	9.183152	-3.073639	2.867226
S	11.892504	-4.664663	3.034032
S	11.851198	1.565490	3.039354
S	9.155084	3.166573	2.986105
C	11.310796	-1.255988	4.947212
O	12.193359	-1.525880	2.629512
H	10.507379	-0.561083	4.714437
H	11.092806	-2.316818	5.032872
H	12.287446	-0.875059	5.233675

$CH_2OH^* + * = CH_2^* + OH^*$

Mo	1.848890	0.015994	1.623725
Mo	1.860395	3.212723	1.602419
Mo	1.824299	6.410740	1.614727
Mo	4.615606	-1.599162	1.576117
Mo	4.620692	1.574871	1.604565
Mo	4.583610	4.759539	1.576478
Mo	7.322101	-3.272559	1.422297
Mo	7.401906	-0.014551	1.505688
Mo	7.368390	3.115562	1.543156
Mo	10.079596	-4.822611	1.420171
Mo	10.252052	1.605475	1.619996
Mo	12.911881	-6.264872	1.567090
Mo	12.949057	-3.132118	1.464219
Mo	12.867282	0.166460	1.707231
Cu	9.873687	-2.018248	0.991826
S	0.958326	1.618639	0.039190
S	0.982101	4.806492	-0.002531
S	0.892480	8.011315	0.068930
S	3.670942	-0.000656	0.043394
S	3.678614	3.157367	0.031000
S	3.656300	6.386632	0.034870
S	6.422199	-1.595744	-0.046666
S	6.426382	1.527674	-0.007312
S	6.358295	4.661985	-0.037605
S	8.990571	-3.568497	-0.348106
S	9.289474	-0.056253	0.094132
S	9.224514	3.026866	-0.016573
S	11.988217	-4.733979	-0.077779
S	11.925752	-1.488855	0.189673
S	12.013073	1.670987	0.044019
S	0.932226	1.650701	3.157280
S	0.873427	4.830433	3.138256
S	0.917681	8.006743	3.221736
S	3.710927	-0.015026	3.164959
S	3.701265	3.185363	3.163955
S	3.697592	6.380754	3.146255
S	6.530135	-1.631086	3.052931
S	6.518618	1.529860	3.128854
S	6.461320	4.760191	3.072023
S	9.184780	-3.177335	2.903054
S	11.908677	-4.602813	3.038011
S	12.040998	1.840803	3.212778
S	9.228180	3.199696	3.089135
C	11.536692	-0.772534	3.147873
O	9.730618	-0.008766	3.016315
H	11.130485	-1.782926	3.024155
H	11.656800	-0.564550	4.222736
H	9.539380	0.344692	3.912317

CH* + H* = CH_2^* + *

Mo	1.833004	-0.037888	1.608093
Mo	1.827833	3.175051	1.617683
Mo	1.798902	6.362510	1.593569
Mo	4.618645	-1.619901	1.570190
Mo	4.590397	1.568766	1.593951

Mo	4.588855	4.761172	1.596740
Mo	7.398149	-3.245196	1.474429
Mo	7.374281	0.021493	1.473869
Mo	7.352591	3.172191	1.543292
Mo	10.148816	-4.838095	1.473980
Mo	10.123954	1.564730	1.545309
Mo	12.886740	-6.394410	1.594508
Mo	12.871945	-3.224179	1.503988
Mo	12.887328	0.008642	1.571571
Cu	9.913673	-1.313314	1.502152
S	0.929198	1.567603	0.055050
S	0.903798	4.742723	0.018833
S	0.906129	7.953340	0.009254
S	3.666721	-0.026844	0.035327
S	3.654518	3.166385	0.045930
S	3.657108	6.351530	0.036578
S	6.432158	-1.638378	-0.045433
S	6.384755	1.621065	-0.023613
S	6.388084	4.732955	-0.012316
S	9.112142	-3.411207	-0.161940
S	9.139292	0.093874	-0.146509
S	9.185083	3.120619	-0.040171
S	11.996230	-4.837465	-0.032378
S	11.831390	-1.627496	0.125483
S	12.000829	1.587360	0.004422
S	0.914118	1.568808	3.167176
S	0.841596	4.796986	3.142310
S	0.864359	7.923020	3.169814
S	3.695451	-0.044129	3.154757
S	3.681307	3.167719	3.169058
S	3.672978	6.369266	3.143345
S	6.542664	-1.604540	3.062093
S	6.478660	1.555504	3.110830
S	6.480598	4.788768	3.107410
S	9.360702	-3.057769	2.910955
S	11.952740	-4.736250	3.109997
S	11.959048	1.579927	3.175736
S	9.220215	3.174038	3.091439
C	9.084466	0.154249	2.690161
H	11.132330	-0.297864	2.247726
H	9.200420	-0.104238	3.751989

$CH_2^* + H^* = CH_3^* + *$

Mo	1.832394	0.002295	1.625799
Mo	1.834287	3.211668	1.607514
Mo	1.810087	6.398671	1.585887
Mo	4.625351	-1.588003	1.594177
Mo	4.592110	1.592249	1.619331
Mo	4.579693	4.786363	1.599061
Mo	7.375817	-3.251413	1.478687
Mo	7.410443	0.064800	1.578023
Mo	7.350304	3.176018	1.565584
Mo	10.118958	-4.840611	1.420775
Mo	10.181461	1.583003	1.614785
Mo	12.895882	-6.341277	1.581600
Mo	12.930319	-3.146125	1.445674
Mo	12.873393	0.044161	1.590485
Cu	9.934396	-1.987626	1.062649
S	0.938514	1.598495	0.051024
S	0.960548	4.781282	-0.019365
S	0.881962	8.011024	0.040228
S	3.671487	0.001391	0.056798
S	3.669474	3.180488	0.049445
S	3.675749	6.397957	0.038607
S	6.462556	-1.574901	0.007298
S	6.407105	1.598378	0.032485
S	6.367199	4.726144	-0.003908
S	9.004908	-3.545807	-0.317267
S	9.217097	-0.045595	0.080527
S	9.186852	3.057816	-0.029729
S	11.998406	-4.803132	-0.067181
S	11.904071	-1.566887	0.090064
S	12.003715	1.610504	0.026562
S	0.910503	1.625190	3.167357
S	0.842139	4.842283	3.129826
S	0.863213	7.944711	3.175292
S	3.690807	-0.016205	3.177765
S	3.668975	3.204010	3.176033
S	3.668765	6.400260	3.150744
S	6.549067	-1.601947	3.095461
S	6.459052	1.610350	3.162137
S	6.458518	4.800508	3.110353
S	9.285255	-3.156396	2.908066
S	11.945048	-4.652949	3.041906
S	12.015791	1.645852	3.201268
S	9.238404	3.228624	3.089752
C	9.087541	0.230760	3.026605
H	8.948253	0.783477	3.965702
H	9.362232	-0.794761	3.301750
H	10.613511	-0.016942	2.247539

$CH_3^* + H^* = CH_4 + 2^*$

Mo	1.940180	-0.108835	1.581992
Mo	1.936826	3.098757	1.587039
Mo	1.908222	6.283720	1.555353
Mo	4.716009	-1.678113	1.545246
Mo	4.695389	1.504977	1.573972
Mo	4.691157	4.695826	1.560940
Mo	7.486780	-3.311577	1.475816
Mo	7.478764	0.012892	1.452511
Mo	7.456312	3.097735	1.515671
Mo	10.266798	-4.933869	1.466615
Mo	10.213196	1.487836	1.496164
Mo	12.985746	-6.487466	1.560294
Mo	13.015075	-3.319928	1.479520
Mo	12.989833	-0.076959	1.483310
Cu	9.849785	-1.733682	1.227939
S	1.029031	1.491155	0.026428
S	1.027854	4.659970	-0.024389
S	1.011115	7.898652	-0.022951
S	3.772132	-0.089677	0.009402
S	3.761411	3.095053	0.015852
S	3.767437	6.293218	0.000870
S	6.545658	-1.682621	-0.050247
S	6.481094	1.539290	-0.049683
S	6.499436	4.676782	-0.036576
S	9.211918	-3.500775	-0.220637
S	9.250086	-0.030614	-0.083384
S	9.309756	3.052528	-0.067008
S	12.105692	-4.926662	-0.055196
S	11.900609	-1.711714	0.224488
S	12.063662	1.513939	-0.042259
S	1.011665	1.488718	3.134780
S	0.966526	4.717599	3.119825
S	0.952130	7.844087	3.114708
S	3.794266	-0.109096	3.132766
S	3.783347	3.106033	3.140566
S	3.773797	6.303004	3.109416
S	6.641836	-1.643691	3.029127
S	6.578634	1.515295	3.101153
S	6.568058	4.712628	3.080176
S	9.411132	-3.174533	2.914248
S	12.066511	-4.833245	3.085980
S	12.029506	1.427869	3.089902
S	9.319602	3.088914	3.058636
C	9.583354	-0.106289	4.512686
H	8.956213	0.372319	2.665900
H	8.640598	-0.609396	4.722228
H	9.749104	0.886692	4.925865
H	10.448098	-0.724090	4.277014

7. Transition state of elementary reaction on Mo edge

$H_2O^* + \# = OH^* + H^\#$

Mo	3.225508	9.404950	0.931775
Mo	9.604272	9.189913	0.954996
Mo	-0.054775	9.397530	0.949344
Mo	6.329132	9.189322	0.944922
Mo	11.157055	9.340594	3.720471
Mo	7.962929	9.347492	3.709969
Mo	1.588388	9.338897	3.696557
Mo	4.782206	9.345306	3.695211
Mo	9.561878	9.395518	6.473325
Mo	0.008902	9.386897	6.474335
Mo	6.368516	9.401668	6.470519
Mo	3.196381	9.391342	6.436827
Mo	4.951649	9.475697	9.197255
Mo	1.428272	9.443534	9.236023
Mo	11.367109	9.446069	9.263317
Mo	7.797203	9.448299	9.256847
S	1.580625	8.113694	-0.257445
S	4.783265	7.724295	0.057403
S	11.149436	7.716327	0.077564
S	1.578504	10.807511	-0.118529
S	7.968697	7.745502	-0.056749
S	7.970343	10.434488	-0.294004
S	4.773216	10.840829	0.004313
S	11.152682	10.838972	0.022428
S	3.177020	10.914134	2.785796
S	-0.007476	7.785321	2.759981
S	6.378930	10.865506	2.693277
S	9.554474	7.742707	2.862602
S	6.379944	7.739812	2.849154
S	3.182024	7.793262	2.737871
S	9.559750	10.859201	2.711692
S	-0.006013	10.913483	2.801754
S	1.606037	7.811921	5.556256
S	7.974308	10.943001	5.517349
S	4.779809	7.817113	5.556001
S	1.601610	10.928672	5.505853
S	11.155127	7.813025	5.588281
S	7.967996	7.822706	5.583388
S	4.779574	10.941490	5.497193
S	11.155053	10.934740	5.530425
S	3.202108	7.936725	8.391953
S	0.017142	11.059292	8.235694
S	6.367822	7.802434	8.303126
S	0.017145	7.787966	8.303500
S	6.388048	11.080475	8.239385
S	9.567724	7.941826	8.410619
S	9.573804	10.917292	8.355686
S	3.179797	10.943255	8.307104
S	6.132854	9.451768	11.269091
S	0.097836	9.541405	11.130305
S	9.511583	9.470359	10.902850
O	3.313568	9.527487	10.791919
H	3.203647	10.417692	11.188647
H	4.628738	9.270549	11.348661

$OH^* + \# = O^* + H^\#$

Mo	3.215622	9.319500	0.937554
Mo	9.596269	9.319500	0.957992
Mo	-0.059281	9.319500	0.952070
Mo	6.333283	9.319500	0.943946
Mo	11.150630	9.319500	3.720434
Mo	7.962665	9.319500	3.704198
Mo	1.582748	9.319500	3.676389
Mo	4.785364	9.319500	3.679281
Mo	9.553709	9.319500	6.473805
Mo	0.001522	9.319500	6.458940
Mo	6.363731	9.319500	6.461339
Mo	3.191962	9.319499	6.392166
Mo	4.865776	9.319499	9.198742
Mo	1.567624	9.319499	9.234484
Mo	11.360374	9.319499	9.275206
Mo	7.798101	9.319500	9.257087
S	1.574346	7.957474	-0.164183
S	4.776052	7.768351	0.033364
S	11.144590	7.759699	0.054071
S	1.574346	10.681525	-0.164183
S	7.968753	7.954426	-0.158398
S	7.968753	10.684573	-0.158398
S	4.776052	10.870648	0.033364
S	11.144590	10.879300	0.054071
S	3.180928	10.885330	2.760123
S	-0.017988	7.752400	2.779382
S	6.380475	10.888512	2.768787
S	9.556937	7.755227	2.790729
S	6.380475	7.750487	2.768787
S	3.180928	7.753669	2.760123
S	9.556937	10.883772	2.790729
S	-0.017988	10.886599	2.779382
S	1.586176	7.757897	5.507441
S	7.964679	10.880811	5.550952
S	4.790221	7.753349	5.506523
S	1.586176	10.881103	5.507442
S	11.144633	7.757323	5.562353
S	7.964679	7.758188	5.550952
S	4.790221	10.885651	5.506523
S	11.144633	10.881676	5.562353
S	3.204217	7.776415	8.243933
S	0.044412	10.923040	8.284438
S	6.355550	7.697462	8.289307
S	0.044412	7.715959	8.284437
S	6.355550	10.941537	8.289308
S	9.565818	7.831430	8.387912
S	9.565818	10.807569	8.387911
S	3.204217	10.862584	8.243934
S	6.063450	9.319499	11.329994
S	0.088604	9.319499	11.105530
S	9.480517	9.319499	10.917237
O	3.195589	9.319500	10.427337
H	4.715529	9.319500	11.622250

$CO^* + O^* = CO_2^* + *$

Mo	3.254828	9.218770	0.970642
Mo	9.640043	9.430913	0.960847
Mo	-0.017300	9.218111	0.973678
Mo	6.358018	9.435088	0.954971
Mo	11.185930	9.339407	3.732796
Mo	7.998794	9.339414	3.709366
Mo	1.615842	9.347651	3.740862
Mo	4.813201	9.345827	3.722794
Mo	9.585032	9.352606	6.483695
Mo	0.020409	9.386495	6.502436
Mo	6.411154	9.363280	6.473793
Mo	3.229775	9.373277	6.469650
Mo	4.985479	9.401920	9.277253
Mo	1.606371	9.428485	9.309218
Mo	11.013310	9.442132	9.279586
Mo	8.025711	9.397259	9.269533
S	1.618210	7.782243	-0.048527
S	4.798384	7.763961	0.064535
S	11.194877	7.758322	0.072919
S	1.616208	10.479969	-0.254547
S	7.998687	8.158899	-0.253510
S	8.002274	10.851590	-0.084600
S	4.805580	10.880132	0.046746
S	11.188605	10.878588	0.050841
S	3.207519	10.872684	2.741931
S	0.032365	7.749227	2.865469
S	6.410330	10.926795	2.822307
S	9.592935	7.797906	2.750709
S	6.404280	7.801892	2.741908
S	3.205248	7.753804	2.863671
S	9.591970	10.922752	2.829695
S	0.026636	10.871316	2.746345
S	1.615487	7.806092	5.605183
S	8.001205	10.908336	5.534583
S	4.816967	7.794910	5.564539
S	1.620108	10.933948	5.559187
S	11.193855	7.797306	5.589483
S	7.996843	7.789650	5.550177
S	4.820059	10.926100	5.539267
S	11.178007	10.917597	5.550631
S	3.283641	7.828955	8.318112
S	-0.023363	10.961945	8.332615
S	6.447375	7.789071	8.339718

S	-0.016218	7.872205	8.401282
S	6.437708	10.988016	8.296377
S	9.559140	7.770441	8.355292
S	9.547123	10.995995	8.292431
S	3.260962	10.929508	8.307744
S	6.362763	9.449296	11.108824
S	-0.102823	9.867109	11.000517
S	9.518816	9.354235	11.113164
C	2.152643	8.217234	10.895904
O	2.295680	7.495254	11.799667
O	3.329272	9.497522	10.559898

CO* + OH* = COOH* + *

Mo	3.227309	9.242710	0.960617
Mo	9.565567	9.400752	0.968480
Mo	-0.015093	9.287641	0.971796
Mo	6.318467	9.438797	0.968114
Mo	11.155509	9.327218	3.681014
Mo	7.965452	9.330179	3.681811
Mo	1.585470	9.326268	3.689057
Mo	4.770003	9.329567	3.710801
Mo	9.561207	9.306886	6.429922
Mo	0.004558	9.309118	6.424471
Mo	6.363354	9.312948	6.439430
Mo	3.165747	9.309550	6.462568
Mo	5.021074	9.296310	9.186778
Mo	1.403585	9.271334	9.272506
Mo	11.328089	9.291971	9.206131
Mo	7.808443	9.281868	9.201626
S	1.586559	7.853316	-0.093590
S	4.756294	7.792247	0.031346
S	11.146625	7.883377	-0.041597
S	1.605331	10.584034	-0.205516
S	7.941276	8.114493	-0.215719
S	7.957573	10.840691	-0.077806
S	4.792091	10.891614	0.041296
S	11.160868	10.819620	-0.021796
S	3.183668	10.878307	2.740740
S	-0.004833	7.738831	2.794773
S	6.366982	10.923920	2.843956
S	9.555860	7.771399	2.732933
S	6.360238	7.786467	2.732292
S	3.179117	7.743382	2.821613
S	9.559168	10.924980	2.808993
S	-0.003241	10.896534	2.756981
S	1.597790	7.750453	5.521679
S	7.968308	10.874694	5.535484
S	4.753323	7.755516	5.534055
S	1.598071	10.881603	5.534396
S	11.151016	7.752147	5.509694
S	7.964064	7.757648	5.505642
S	4.744834	10.880498	5.556847
S	11.155024	10.877321	5.533781
S	3.228269	7.809468	8.392298
S	0.022740	10.922861	8.259410
S	6.390823	7.647302	8.208005
S	0.009831	7.660629	8.238114
S	6.397883	10.951798	8.240296
S	9.563753	7.783302	8.316701
S	9.566260	10.797410	8.341241
S	3.198068	10.771813	8.424635
S	6.320638	9.187761	11.073342
S	-0.073307	9.458882	11.099565
S	9.537356	9.257515	10.858745
C	2.634375	9.074853	11.089314
O	3.274330	10.218731	11.513946
O	2.741540	8.014275	11.678485
H	3.726110	10.006537	12.367220

CO* + H# = CHO* + #

Mo	3.211735	9.206371	0.995299
Mo	9.589681	9.394672	0.986440
Mo	-0.039797	9.216086	0.999610
Mo	6.324040	9.399143	0.990299
Mo	11.160295	9.327962	3.727233
Mo	7.964033	9.323111	3.710585
Mo	1.587567	9.329924	3.737421
Mo	4.763006	9.321140	3.738194
Mo	9.559030	9.351910	6.458253
Mo	-0.007258	9.368801	6.495286
Mo	6.368474	9.344238	6.449579
Mo	3.180309	9.366606	6.523628
Mo	4.989608	9.377249	9.223721
Mo	1.289891	9.401021	9.321104
Mo	11.269636	9.411086	9.239883
Mo	7.819437	9.423519	9.225668
S	1.580638	7.776958	-0.031783
S	4.760500	7.762255	0.064883
S	11.159621	7.774038	0.058348
S	1.586459	10.494401	-0.209484
S	7.956640	8.106024	-0.204802
S	7.956282	10.817693	-0.053975
S	4.773150	10.836715	0.050815
S	11.151914	10.827250	0.040305
S	3.177890	10.862748	2.754563
S	0.000351	7.727054	2.875335
S	6.362713	10.906376	2.846130
S	9.565119	7.771427	2.769171
S	6.359714	7.770230	2.774029
S	3.167976	7.724607	2.874636
S	9.557940	10.909501	2.834075
S	-0.002634	10.870296	2.759220
S	1.600404	7.801368	5.611400
S	7.969189	10.899822	5.529030
S	4.752294	7.778745	5.597102
S	1.606128	10.911845	5.566270
S	11.159570	7.785970	5.580673
S	7.975179	7.775442	5.551623
S	4.756745	10.907199	5.554192
S	11.155297	10.910684	5.543297
S	3.105382	7.878952	8.440576
S	-0.028971	11.041811	8.272692
S	6.434980	7.731471	8.298830
S	-0.050369	7.746648	8.317042
S	6.364628	11.032756	8.191373
S	9.561754	7.869617	8.379796
S	9.548650	10.915731	8.313907
S	3.131694	10.864605	8.476516
S	6.485223	9.907952	11.055692
S	-0.111855	9.468276	11.145652
S	9.555979	9.382198	10.911464
C	3.708981	9.186455	10.719618
O	2.695664	9.325030	11.377901
H	4.378266	8.172239	10.769424

CO* + H# = COH* + #

Mo	3.201604	9.264704	0.987457
Mo	9.586528	9.413283	0.989666
Mo	-0.054580	9.256669	0.992905
Mo	6.330627	9.406944	0.992209
Mo	11.143239	9.312594	3.735318
Mo	7.957727	9.304527	3.720248
Mo	1.580612	9.323161	3.718690
Mo	4.766302	9.314405	3.721784
Mo	9.546702	9.275454	6.483600
Mo	-0.014461	9.288806	6.472334
Mo	6.371412	9.254935	6.457371
Mo	3.171432	9.303017	6.482239
Mo	4.916104	9.212116	9.147898
Mo	1.412721	9.286085	9.245617
Mo	11.355216	9.259286	9.275802
Mo	7.783281	9.229228	9.277849
S	1.574647	7.859155	-0.076940
S	4.756516	7.817707	0.035346
S	11.158577	7.805252	0.046407
S	1.571176	10.582684	-0.174646
S	7.957919	8.107113	-0.195326
S	7.955109	10.826963	-0.055507
S	4.777424	10.867319	0.055885
S	11.131626	10.877790	0.068316
S	3.176701	10.880295	2.777246
S	-0.010825	7.737475	2.841703
S	6.368743	10.905705	2.858108
S	9.557509	7.766424	2.754102
S	6.357649	7.762981	2.757103
S	3.166431	7.738068	2.826840
S	9.545540	10.902440	2.862610
S	-0.024092	10.876967	2.784552
S	1.591482	7.751263	5.545566
S	7.959720	10.844635	5.580872
S	4.748128	7.736445	5.541352
S	1.583269	10.867181	5.571801
S	11.138730	7.727850	5.556623
S	7.977567	7.712052	5.530733
S	4.773531	10.853188	5.578019
S	11.131585	10.857933	5.590427
S	3.150878	7.731325	8.335978
S	-0.010963	10.910504	8.289908
S	6.417100	7.577967	8.250286
S	-0.019111	7.628878	8.265943
S	6.364675	10.867074	8.286259
S	9.568363	7.775242	8.391478
S	9.539740	10.741728	8.422110
S	3.181187	10.847760	8.436212
S	6.020283	9.141977	11.195242
S	0.074006	9.220637	11.146632
S	9.497057	9.234245	10.926766
C	3.203032	9.633079	10.566481
O	3.427895	10.086494	11.692352
H	4.807723	9.885822	11.821208

CHO* + O* = HCOO* + *

Mo	3.197164	9.423368	0.994838
Mo	9.586056	9.277262	0.986452
Mo	-0.060142	9.422876	1.001956
Mo	6.315708	9.286630	0.989912
Mo	11.145861	9.310746	3.745639
Mo	7.953781	9.332048	3.715262
Mo	1.572039	9.301715	3.741090
Mo	4.754473	9.322890	3.735418
Mo	9.543082	9.280991	6.479442
Mo	-0.016455	9.252136	6.514604
Mo	6.364948	9.306639	6.457099
Mo	3.164186	9.269790	6.508268
Mo	4.979932	9.303261	9.129660
Mo	1.331021	9.190626	9.357044
Mo	11.286551	9.177291	9.283126
Mo	7.801531	9.208450	9.233673
S	1.568020	8.120335	-0.193018
S	4.768251	7.832436	0.035464
S	11.127186	7.822376	0.041125
S	1.567000	10.826835	-0.063859
S	7.945558	7.913753	-0.114346
S	7.951150	10.619529	-0.158886
S	4.740850	10.904410	0.081971
S	11.160808	10.906317	0.090363
S	3.149245	10.908308	2.871675
S	-0.022916	7.767038	2.766090
S	6.347682	10.891302	2.794276
S	9.542209	7.750602	2.825625
S	6.357784	7.755334	2.826006
S	3.169704	7.773409	2.758913
S	9.562875	10.882048	2.790173
S	-0.013250	10.903702	2.885164
S	1.591911	7.716594	5.562570
S	7.976185	10.872712	5.563740
S	4.754937	7.736831	5.548588
S	1.574818	10.831308	5.613804
S	11.133314	7.719704	5.559886
S	7.951699	7.745262	5.525099
S	4.735190	10.862974	5.591514
S	11.150938	10.843352	5.612260
S	3.145195	7.763438	8.456227
S	-0.049303	10.838150	8.367868
S	6.373431	7.600388	8.178723
S	-0.014267	7.576141	8.282622
S	6.454458	10.925165	8.291115
S	9.532069	7.708871	8.330757
S	9.566909	10.725470	8.424595
S	3.086179	10.759607	8.409763
S	6.111809	8.455349	11.065318
S	-0.118441	9.066171	11.185041
S	9.429970	9.198986	10.941073
C	3.655977	9.907887	10.827039
O	2.770664	9.074755	11.181646
O	5.279905	9.954937	11.246674
H	3.539115	10.990833	11.012197

COH* + O* = COOH* + *

Mo	3.238185	9.310645	0.975751
Mo	9.578605	9.370226	0.942805
Mo	-0.016694	9.314933	0.951001
Mo	6.318067	9.371563	0.974989
Mo	11.151898	9.324962	3.648227
Mo	7.964133	9.320435	3.685522
Mo	1.594895	9.330258	3.706963
Mo	4.779078	9.323958	3.752772
Mo	9.559249	9.303221	6.398130
Mo	-0.038595	9.317422	6.395282
Mo	6.368252	9.307582	6.478438
Mo	3.179001	9.315548	6.500677
Mo	5.001103	9.292777	9.420996
Mo	1.293593	9.313180	9.124959
Mo	11.117845	9.298653	9.117942
Mo	8.201051	9.267989	9.197599
S	1.614564	7.952000	-0.147865
S	4.763537	7.778221	0.067298
S	11.170928	7.844034	-0.020166
S	1.614582	10.685430	-0.146269
S	7.942703	8.012218	-0.164220
S	7.940588	10.746863	-0.131976
S	4.791132	10.916230	0.089094
S	11.152353	10.859698	0.004918
S	3.198659	10.892089	2.805307
S	0.014285	7.754844	2.768713
S	6.364766	10.898516	2.827902
S	9.554244	7.759591	2.725442
S	6.358641	7.765182	2.780736
S	3.190604	7.763967	2.814734
S	9.546995	10.910076	2.774339
S	0.006972	10.900610	2.758253
S	1.599970	7.759176	5.544913
S	7.947527	10.869530	5.531725
S	4.759224	7.746386	5.591406
S	1.600131	10.878999	5.555882
S	11.145180	7.748607	5.455752
S	7.945117	7.750983	5.510378
S	4.764858	10.883613	5.607823
S	11.136529	10.881180	5.471912
S	3.176376	7.835771	8.460224
S	-0.129410	10.986377	8.211185
S	6.443484	7.705902	8.333183
S	-0.098551	7.640962	8.214795
S	6.450106	10.879089	8.365993
S	9.598694	7.643335	8.209855
S	9.579260	10.928853	8.238556
S	3.161509	10.772902	8.468389
S	6.685772	9.193633	11.042547
S	-0.276125	9.413789	11.004118
S	9.631133	9.252047	11.006079
C	1.901940	9.060648	10.959602
O	2.045708	8.717897	12.208625
O	3.894431	9.333204	10.854579
H	3.034912	8.731163	12.333514

HCOO* + # = CO_2* + H#

Mo	3.091114	9.444922	1.058521
Mo	9.548410	9.298352	1.050912
Mo	0.019995	9.227293	1.061684
Mo	6.315075	9.388088	1.056524
Mo	11.119156	9.311531	3.763494
Mo	7.930059	9.326873	3.727004
Mo	1.563206	9.305490	3.813502
Mo	4.741165	9.322304	3.770965
Mo	9.516620	9.303374	6.486952
Mo	-0.037031	9.282079	6.526230
Mo	6.339867	9.311568	6.480716
Mo	3.147715	9.284959	6.573386
Mo	4.980087	9.316230	9.270384
Mo	1.260122	9.296023	9.377984
Mo	11.239614	9.250556	9.257532
Mo	7.789402	9.254272	9.251888
S	1.535702	7.789894	0.114722
S	4.703441	8.121210	-0.141330
S	11.138546	7.836230	0.006144
S	1.572420	10.901215	0.145586
S	7.915311	7.966461	-0.041589
S	7.946365	10.737517	-0.020361
S	4.723355	10.859056	0.028481
S	11.169421	10.574273	-0.123691
S	3.141310	10.913427	2.945038

S	-0.034473	7.724845	2.923679
S	6.325524	10.929337	2.879741
S	9.527031	7.731449	2.847567
S	6.324078	7.761697	2.811732
S	3.147336	7.776046	2.812967
S	9.545977	10.895638	2.828515
S	-0.023140	10.861879	2.848070
S	1.581863	7.721723	5.640651
S	7.941782	10.881590	5.577758
S	4.731635	7.740039	5.600655
S	1.571538	10.853992	5.659095
S	11.111215	7.737376	5.595551
S	7.927045	7.750516	5.552791
S	4.713319	10.866548	5.635482
S	11.126845	10.862341	5.610844
S	3.104297	7.829217	8.578582
S	-0.090957	10.916188	8.340062
S	6.327165	7.642333	8.219977
S	-0.043478	7.627973	8.316394
S	6.402719	10.931973	8.322096
S	9.501769	7.746098	8.344592
S	9.519487	10.795209	8.400207
S	3.102134	10.784408	8.450041
S	6.591418	8.344861	11.166607
S	-0.232906	9.033196	11.166848
S	9.474002	9.346939	10.931454
C	3.649698	9.836362	10.799703
O	2.442068	9.572229	11.128116
O	4.440035	10.742670	11.142754
H	5.302118	8.821520	11.357718

$COOH^* + \# = CO_2^* + H^\#$

Mo	3.218245	9.477422	1.006159
Mo	9.558821	9.304120	0.992947
Mo	-0.025440	9.445120	1.002985
Mo	6.305500	9.268528	1.004399
Mo	11.145539	9.310034	3.700241
Mo	7.952978	9.307070	3.716865
Mo	1.579459	9.313458	3.731839
Mo	4.757230	9.310058	3.761953
Mo	9.556975	9.259378	6.439833
Mo	-0.028979	9.232752	6.448768
Mo	6.352447	9.252894	6.481747
Mo	3.168739	9.261236	6.531379
Mo	5.030567	9.229322	9.339213
Mo	1.336919	9.203793	9.233553
Mo	11.235226	9.154591	9.200936
Mo	7.852250	9.201045	9.218584
S	1.597648	8.195597	-0.222614
S	4.773267	7.841777	0.046870
S	11.153008	7.916377	-0.021312
S	1.583850	10.914677	-0.001410
S	7.942102	7.882112	-0.071149
S	7.927600	10.605247	-0.166758
S	4.750715	10.945104	0.114784
S	11.140919	10.878201	0.046012
S	3.170863	10.922341	2.913383
S	-0.004938	7.776369	2.734094
S	6.347870	10.873475	2.813070
S	9.544373	7.735879	2.794489
S	6.350390	7.737122	2.844714
S	3.174353	7.791312	2.740733
S	9.541963	10.887348	2.796264
S	-0.008218	10.927836	2.879375
S	1.599885	7.712417	5.541527
S	7.952312	10.835122	5.578383
S	4.734668	7.707221	5.572515
S	1.585921	10.826526	5.619404
S	11.136054	7.699605	5.491223
S	7.951369	7.712875	5.527570
S	4.744126	10.839296	5.631067
S	11.144659	10.836147	5.561465
S	3.194396	7.770998	8.501626
S	-0.065158	10.830707	8.314244
S	6.360576	7.588319	8.259447
S	-0.042226	7.533119	8.198682
S	6.399215	10.855192	8.322402
S	9.533607	7.676723	8.279051
S	9.570684	10.755017	8.348194
S	3.186669	10.709879	8.492412
S	6.563050	8.883233	11.109902
S	-0.016320	8.540376	11.086309
S	9.638453	9.354205	10.916732
C	2.588125	9.706782	10.996552
O	3.873107	9.438039	11.031814
O	2.034228	10.317488	11.937357
H	0.618776	9.660705	11.763707

$H^\# + * = H^* + \#$

Mo	3.233139	9.214054	0.968611
Mo	9.616569	9.410385	0.967486
Mo	-0.029264	9.210172	0.972572
Mo	6.349112	9.399820	0.975786
Mo	11.171972	9.328066	3.717428
Mo	7.980667	9.326253	3.707339
Mo	1.604900	9.329352	3.712025
Mo	4.784674	9.323640	3.716880
Mo	9.579001	9.335168	6.464199
Mo	0.005891	9.347962	6.465036
Mo	6.384989	9.336434	6.454165
Mo	3.188289	9.340850	6.491079
Mo	4.983128	9.345777	9.170349
Mo	1.460523	9.344840	9.171113
Mo	11.352622	9.341577	9.250743
Mo	7.798566	9.351272	9.251005
S	1.602633	7.781852	-0.061338
S	4.788774	7.766578	0.045505
S	11.177865	7.764471	0.048789
S	1.600800	10.483931	-0.247232
S	7.981565	8.114822	-0.224242
S	7.976886	10.813847	-0.084652
S	4.796719	10.836002	0.024463
S	11.166282	10.844712	0.026926
S	3.196572	10.863794	2.731932
S	0.013634	7.731565	2.852994
S	6.384809	10.910216	2.833075
S	9.577653	7.780170	2.751242
S	6.384954	7.772690	2.761633
S	3.190635	7.730532	2.844226
S	9.573955	10.911877	2.827648
S	0.010734	10.865781	2.736404
S	1.613095	7.781231	5.564876
S	7.990481	10.892091	5.541820
S	4.766525	7.775541	5.562229
S	1.610419	10.898936	5.543274
S	11.168767	7.772571	5.557755
S	7.990732	7.771014	5.545724
S	4.764442	10.892120	5.545135
S	11.163794	10.902747	5.542778
S	3.227586	7.830204	8.432558
S	-0.027793	10.995849	8.278912
S	6.415724	7.704329	8.245612
S	0.017407	7.698513	8.260520
S	6.406397	10.989048	8.231626
S	9.574052	7.851006	8.387216
S	9.577525	10.832245	8.370388
S	3.204748	10.856323	8.436790
S	6.201612	9.340956	11.098339
S	0.097313	9.493424	11.159533
S	9.582258	9.345921	10.905289
H	1.470420	8.775493	10.962130

$H^* + H^\# = H_2^* + \#$

Mo	3.233011	9.210376	0.950175
Mo	9.612495	9.400624	0.967046
Mo	-0.042484	9.217507	0.962646
Mo	6.336378	9.410851	0.963539
Mo	11.169318	9.317127	3.729450
Mo	7.976458	9.314617	3.720961
Mo	1.594249	9.324597	3.712148
Mo	4.782136	9.320416	3.714232
Mo	9.578665	9.331369	6.480503
Mo	0.013500	9.340800	6.483188
Mo	6.374905	9.328507	6.467736
Mo	3.176046	9.338375	6.470340
Mo	4.975306	9.345935	9.186101
Mo	1.494029	9.370129	9.246338
Mo	11.363405	9.356967	9.275332
Mo	7.779216	9.347851	9.260613
S	1.589442	7.797266	-0.088355
S	4.778045	7.754444	0.049116
S	11.165629	7.749595	0.063689
S	1.592075	10.492597	-0.252998
S	7.973852	8.119001	-0.233682
S	7.978861	10.819484	-0.080600
S	4.796987	10.868557	0.048358
S	11.157571	10.865853	0.055768
S	3.188275	10.854295	2.724430
S	0.007340	7.729313	2.840244
S	6.388084	10.901838	2.834799
S	9.571751	7.773027	2.761271
S	6.381564	7.774877	2.752497
S	3.182934	7.734400	2.830787
S	9.568904	10.896832	2.835357
S	-0.000050	10.859044	2.740892
S	1.599268	7.771980	5.558552
S	7.984625	10.882037	5.553237
S	4.764443	7.769898	5.553782
S	1.596772	10.894586	5.534804
S	11.170388	7.764377	5.579499
S	7.986491	7.763997	5.563791
S	4.766812	10.887434	5.538681
S	11.165475	10.893768	5.554722
S	3.222259	7.832152	8.380771
S	0.007473	10.993709	8.281501
S	6.394915	7.696176	8.262241
S	0.050081	7.717007	8.323915
S	6.394977	10.984515	8.242254
S	9.585501	7.862533	8.405428
S	9.572701	10.832731	8.381523
S	3.221169	10.861925	8.385424
S	6.215002	9.340081	11.115934
S	0.021213	9.511723	11.254289
S	9.581681	9.365925	10.911401
H	1.383218	8.935441	11.140382
H	2.745460	9.207780	10.524320

$CHO^* + * = CH^* + O^*$

Mo	3.236883	9.216176	0.959651
Mo	9.617264	9.428032	0.953165
Mo	-0.032257	9.213519	0.950003
Mo	6.345788	9.424845	0.953497
Mo	11.169772	9.335702	3.703010
Mo	7.982087	9.335775	3.699624
Mo	1.598836	9.336298	3.702950
Mo	4.789611	9.335845	3.708895
Mo	9.573031	9.345646	6.461140
Mo	0.001294	9.354519	6.468764
Mo	6.383037	9.342235	6.458314
Mo	3.190723	9.337460	6.457621
Mo	4.585959	9.340244	9.248926
Mo	1.706098	9.388447	9.206403
Mo	10.946717	9.368558	9.205623
Mo	8.138959	9.354393	9.243979
S	1.605318	7.774170	-0.060848
S	4.788087	7.767095	0.047475
S	11.173094	7.763892	0.044665
S	1.604787	10.476214	-0.270375
S	7.982049	8.146501	-0.252990
S	7.980317	10.846972	-0.089560
S	4.792670	10.866181	0.032131
S	11.166549	10.863387	0.020180
S	3.193251	10.870632	2.725178
S	0.010440	7.740586	2.832661
S	6.388746	10.920150	2.820289
S	9.573890	7.791567	2.734184
S	6.387782	7.793184	2.737321
S	3.191495	7.738961	2.842006
S	9.571732	10.923928	2.820943
S	0.009869	10.867975	2.714135
S	1.582442	7.785484	5.551079
S	7.971948	10.899895	5.537554
S	4.800115	7.777987	5.545333
S	1.591115	10.905941	5.531120
S	11.178213	7.787059	5.547622
S	7.976420	7.781602	5.539678
S	4.789405	10.903349	5.539521
S	11.179426	10.904270	5.531294
S	3.188029	7.693058	8.250855
S	-0.061916	10.889483	8.364286
S	6.378311	7.848655	8.363771
S	-0.039404	7.862459	8.400646
S	6.376916	10.846977	8.358132
S	9.552348	7.708553	8.261103
S	9.535983	11.000300	8.243887
S	3.195513	10.995696	8.249168
S	6.371244	9.360201	10.889734
S	0.335864	9.505155	11.492379
S	9.688386	9.370933	11.113264
C	1.526761	10.490022	10.963193
O	3.281514	9.198995	10.654403
H	2.070902	11.255660	11.522443

$CHO^* + H^\# = CH_2O^* + \#$

Mo	3.236908	9.219861	0.966989
Mo	9.617747	9.429269	0.928586
Mo	-0.028219	9.215398	0.948859
Mo	6.328870	9.428138	0.952252
Mo	11.174111	9.312131	3.683317
Mo	7.977556	9.310143	3.679529
Mo	1.598776	9.319482	3.737244
Mo	4.780086	9.314607	3.737740
Mo	9.571072	9.290135	6.408337
Mo	-0.007606	9.303582	6.482356
Mo	6.398022	9.290171	6.448276
Mo	3.191445	9.307468	6.522333
Mo	5.036625	9.313445	9.234987
Mo	1.298155	9.293485	9.359813
Mo	11.156546	9.251200	9.209644
Mo	8.121443	9.214922	9.156236
S	1.610893	7.793074	-0.081761
S	4.774166	7.763535	0.052626
S	11.183777	7.769526	0.026535
S	1.608679	10.491752	-0.258381
S	7.965721	8.159095	-0.272782
S	7.967970	10.849058	-0.094956
S	4.781393	10.886174	0.056092
S	11.174323	10.879582	0.033183
S	3.187699	10.855654	2.762998
S	0.026132	7.727622	2.823277
S	6.373858	10.902087	2.835898
S	9.573905	7.779357	2.693872
S	6.368971	7.782144	2.727062
S	3.184462	7.734048	2.846980
S	9.570900	10.903782	2.806887
S	0.020735	10.855060	2.734209
S	1.614010	7.755577	5.588003
S	7.976940	10.862551	5.517820
S	4.769005	7.741835	5.573361
S	1.609489	10.871516	5.595736
S	11.176215	7.742015	5.499005
S	7.970206	7.730666	5.481708
S	4.773104	10.866664	5.591678
S	11.171277	10.864898	5.518556
S	3.178729	7.854377	8.510192
S	-0.071851	10.899117	8.326898
S	6.482916	7.668237	8.261205
S	-0.023947	7.668825	8.293257
S	6.503200	10.888307	8.321940
S	9.630073	7.658897	8.212604
S	9.592277	10.856767	8.277075
S	3.147447	10.764415	8.489742
S	6.021504	8.822080	11.230296
S	12.475442	9.112386	11.127816
S	9.337747	9.173213	11.054426
C	3.753890	9.752655	10.946020
O	2.507639	9.344301	11.048335
H	3.984434	10.690659	11.494449
H	4.628076	9.150276	11.911965

$CHO^* + H^\# = CHOH^* + \#$

Mo	3.226493	9.216551	0.968978
Mo	9.607629	9.420425	0.954821
Mo	-0.032904	9.215352	0.968116
Mo	6.332181	9.417131	0.967803
Mo	11.165454	9.324792	3.701894
Mo	7.968100	9.323684	3.696633
Mo	1.594911	9.321884	3.721612
Mo	4.771342	9.320381	3.722304
Mo	9.567459	9.326553	6.436604
Mo	-0.009166	9.334681	6.467171

Mo	6.360472	9.335445	6.449252
Mo	3.185605	9.329883	6.513162
Mo	5.017608	9.345700	9.278309
Mo	1.313961	9.342106	9.249601
Mo	11.266061	9.337942	9.215001
Mo	7.812219	9.375811	9.184162
S	1.597747	7.787367	-0.067875
S	4.778523	7.769876	0.046490
S	11.171488	7.773094	0.039648
S	1.597449	10.488158	-0.250046
S	7.967298	8.143711	-0.247927
S	7.965453	10.833163	-0.088128
S	4.780496	10.859377	0.037759
S	11.165188	10.853409	0.023760
S	3.181793	10.859801	2.742901
S	0.009062	7.728005	2.843847
S	6.368981	10.911088	2.836682
S	9.566049	7.784412	2.728894
S	6.369970	7.778926	2.746080
S	3.179953	7.728476	2.844597
S	9.563472	10.912602	2.820331
S	0.010556	10.863611	2.738945
S	1.608126	7.773175	5.583369
S	7.973783	10.887317	5.529893
S	4.754858	7.765257	5.569042
S	1.612114	10.885376	5.564243
S	11.157729	7.762432	5.533233
S	7.965035	7.766939	5.531227
S	4.746830	10.887366	5.555469
S	11.161784	10.894458	5.526654
S	3.147204	7.858214	8.484362
S	-0.041143	10.991076	8.258695
S	6.378795	7.695181	8.267917
S	-0.049182	7.693864	8.260087
S	6.377154	11.007344	8.216244
S	9.546297	7.820600	8.327209
S	9.567241	10.862864	8.306712
S	3.163453	10.806848	8.482829
S	6.479481	9.697762	11.079721
S	-0.074973	9.331413	11.227104
S	9.554597	9.291325	10.869728
C	3.843560	9.129255	11.051221
O	2.555857	9.338262	11.012234
H	4.190753	8.909605	12.078939
H	1.436487	9.245402	11.636057

$CH_2O^* + * = CH_2^* + O^*$

Mo	3.228611	9.219971	0.955362
Mo	9.590023	9.432421	0.913963
Mo	-0.043951	9.210372	0.916284
Mo	6.310914	9.425191	0.958769
Mo	11.147122	9.329049	3.640866
Mo	7.954525	9.328276	3.687322
Mo	1.591781	9.336443	3.701006
Mo	4.767329	9.331923	3.753006
Mo	9.572960	9.326509	6.402474
Mo	-0.032071	9.344812	6.382579
Mo	6.367635	9.328145	6.495384
Mo	3.164266	9.328548	6.526637
Mo	4.962923	9.303831	9.464727
Mo	1.266811	9.344000	9.188452
Mo	11.126825	9.331282	9.144523
Mo	8.216051	9.315567	9.198930
S	1.604322	7.783954	-0.091585
S	4.768269	7.754646	0.059297
S	11.158803	7.768594	0.008093
S	1.603128	10.478446	-0.289766
S	7.937020	8.151694	-0.273073
S	7.937100	10.847421	-0.103926
S	4.771581	10.884499	0.049405
S	11.144565	10.866922	-0.005094
S	3.186161	10.865953	2.740740
S	0.010634	7.739643	2.798357
S	6.353757	10.914552	2.838702
S	9.539179	7.789851	2.685112
S	6.351057	7.791140	2.751957
S	3.183563	7.745991	2.844645
S	9.535487	10.919534	2.781097
S	0.004800	10.863297	2.682259
S	1.601589	7.777469	5.548049
S	7.944554	10.882941	5.529996
S	4.753264	7.769761	5.610429
S	1.609152	10.898211	5.539766
S	11.146941	7.763991	5.451056
S	7.947065	7.770856	5.520417
S	4.749655	10.891251	5.615129
S	11.145103	10.902454	5.445230
S	3.133722	7.855503	8.495473
S	-0.093940	10.984140	8.179264
S	6.455794	7.745751	8.362650
S	-0.076774	7.712739	8.209342
S	6.446816	10.895690	8.369511
S	9.626270	7.689047	8.207497
S	9.603299	10.953101	8.226805
S	3.149564	10.776238	8.538284
S	6.760529	9.425013	11.030574
S	-0.081530	9.646444	11.082890
S	9.722841	9.131557	11.005858
C	1.900940	9.111671	11.194160
O	3.968308	9.192361	10.921234
H	1.964723	8.111202	11.636019
H	2.169663	9.908985	11.891279

$CHOH^* + * = CH^* + OH^*$

Mo	3.257334	9.200965	0.946389
Mo	9.632785	9.419560	0.941057
Mo	-0.020177	9.194465	0.935924
Mo	6.355393	9.421666	0.942183
Mo	11.185034	9.356138	3.695212
Mo	7.998071	9.360210	3.703758
Mo	1.619580	9.360402	3.698048
Mo	4.806258	9.365803	3.707826
Mo	9.601886	9.405105	6.462608
Mo	0.026791	9.409402	6.452700
Mo	6.400647	9.415567	6.462845
Mo	3.214707	9.412459	6.468606
Mo	4.668393	9.474806	9.240048
Mo	1.722999	9.472228	9.150453
Mo	11.014818	9.456726	9.215922
Mo	8.197262	9.454457	9.259142
S	1.623284	7.746285	-0.057701
S	4.806994	7.733342	0.070143
S	11.184612	7.733128	0.058869
S	1.620338	10.433405	-0.310548
S	7.992072	8.140892	-0.263868
S	7.995144	10.832391	-0.111601
S	4.807099	10.854836	0.010955
S	11.181005	10.848821	0.003250
S	3.207934	10.879374	2.693740
S	0.030358	7.753260	2.844008
S	6.407625	10.934632	2.795966
S	9.583023	7.805167	2.747548
S	6.403654	7.813720	2.753438
S	3.212401	7.756070	2.854732
S	9.586483	10.933640	2.793234
S	0.026465	10.871124	2.682438
S	1.619089	7.836450	5.567590
S	7.997979	10.951093	5.519940
S	4.814965	7.837874	5.569545
S	1.618767	10.954772	5.503302
S	11.197821	7.829993	5.555562
S	7.989668	7.833708	5.569995
S	4.807646	10.963051	5.516338
S	11.200740	10.949191	5.498851
S	3.230170	7.790514	8.301776
S	-0.014820	10.969036	8.317694
S	6.409303	7.957118	8.391852
S	-0.018934	7.919077	8.378695
S	6.429661	10.937204	8.340623
S	9.594165	7.803017	8.286875
S	9.593148	11.068850	8.230097
S	3.235376	11.079038	8.263032
S	6.321558	9.503360	10.917995
S	0.311285	9.568381	11.405876
S	9.692086	9.471604	11.125270
C	1.675607	10.448911	10.981163
O	3.139457	9.282783	10.910753
H	2.136768	11.259362	11.549059
H	3.042280	8.526815	11.528706

$CH_2O^* + H^\# = CH_2OH^* + \#$

Mo	1.833563	0.030008	1.585730
Mo	3.235826	9.202233	0.988453
Mo	9.539079	9.347261	0.984549
Mo	0.013862	9.263658	0.992703
Mo	6.307949	9.415505	0.991542
Mo	11.156754	9.317491	3.662019
Mo	7.968777	9.324504	3.693713
Mo	1.584640	9.323676	3.709738
Mo	4.764531	9.330214	3.739656
Mo	9.564819	9.334538	6.417562
Mo	-0.013032	9.355488	6.428483
Mo	6.360683	9.342678	6.440681
Mo	3.183741	9.345741	6.505260
Mo	5.010717	9.308661	9.295259
Mo	1.349716	9.407410	9.218832
Mo	11.279928	9.410492	9.189300
Mo	7.803736	9.344845	9.189022
S	1.601825	7.795006	-0.045006
S	4.751687	7.749844	0.067068
S	11.141457	7.915952	-0.091853
S	1.623829	10.533768	-0.202704
S	7.917311	8.066062	-0.187043
S	7.946848	10.802053	-0.065615
S	4.793783	10.860374	0.051219
S	11.171209	10.687571	-0.102356
S	3.182922	10.865502	2.749238
S	0.004089	7.717966	2.812582
S	6.365274	10.911699	2.855610
S	9.546759	7.745290	2.759609
S	6.353560	7.775521	2.773406
S	3.179039	7.730699	2.872360
S	9.557187	10.910426	2.783204
S	0.005912	10.886702	2.752621
S	1.605171	7.782138	5.578477
S	7.967430	10.896979	5.526169
S	4.750271	7.774513	5.580406
S	1.608308	10.903176	5.541333
S	11.157210	7.768890	5.518084
S	7.964095	7.768443	5.535140
S	4.750497	10.909539	5.565815
S	11.146742	10.896376	5.485423
S	3.165167	7.876514	8.441040
S	-0.047892	11.044269	8.167329
S	6.375304	7.692455	8.245198
S	-0.032131	7.750983	8.286081
S	6.354969	10.983798	8.258779
S	9.575346	7.840882	8.328271
S	9.536054	10.873000	8.287362
S	3.192398	10.828820	8.489730
S	6.517558	9.400008	11.109301
S	-0.051520	10.098283	11.091839
S	9.607442	9.325543	10.851473
C	3.754323	9.083444	11.105333
O	2.344447	8.962290	10.918150
H	3.936665	9.975611	11.732668
H	4.098943	8.198392	11.669154
H	1.080430	9.292648	11.582670

$CHOH^* + H^\# = CH_2OH^* + \#$

Mo	3.226912	9.187956	1.006191
Mo	9.527070	9.343205	0.993070
Mo	0.004259	9.251805	1.004565
Mo	6.295261	9.406733	1.002096
Mo	11.148444	9.321057	3.668143
Mo	7.949977	9.325293	3.700808
Mo	1.580886	9.318548	3.721307
Mo	4.757649	9.321534	3.763326
Mo	9.543426	9.346297	6.403036
Mo	-0.016777	9.354975	6.432117
Mo	6.356827	9.345746	6.482061
Mo	3.177930	9.352200	6.528820
Mo	4.943727	9.384282	9.272599
Mo	1.280144	9.404288	9.244217
Mo	11.269427	9.393254	9.145877
Mo	7.828235	9.366957	9.179263
S	1.592426	7.775980	-0.021979
S	4.742099	7.733038	0.088540
S	11.130240	7.902984	-0.073699
S	1.616882	10.512148	-0.197531
S	7.906831	8.062606	-0.180662
S	7.931914	10.799790	-0.053119
S	4.777358	10.847296	0.061192
S	11.161514	10.678984	-0.091968
S	3.179257	10.856381	2.762954
S	-0.005735	7.714327	2.829377
S	6.345468	10.907494	2.864110
S	9.535009	7.747326	2.772045
S	6.342025	7.769441	2.787381
S	3.173676	7.720531	2.895718
S	9.543477	10.910168	2.787949
S	0.004014	10.882253	2.756315
S	1.608295	7.782849	5.594141
S	7.941834	10.901765	5.525350
S	4.754081	7.774053	5.621719
S	1.612667	10.900739	5.548280
S	11.143284	7.776719	5.520586
S	7.940121	7.773893	5.545278
S	4.754711	10.904861	5.588940
S	11.142548	10.902207	5.485813
S	3.121149	7.905060	8.510007
S	-0.053157	11.040561	8.185560
S	6.379419	7.685855	8.343848
S	-0.044975	7.726476	8.244486
S	6.394703	11.054311	8.291621
S	9.551747	7.843667	8.292071
S	9.538846	10.895911	8.258972
S	3.137215	10.858727	8.471822
S	6.625207	9.456984	11.201260
S	-0.192122	9.493634	11.073712
S	9.549223	9.361870	10.820590
C	3.900304	9.426479	10.982485
O	2.500667	9.422994	10.983219
H	4.230737	9.456211	12.029855
H	5.786009	8.342136	10.998704
H	2.059770	9.449261	11.861253

$CH_2OH^* + * = CH_2^* + OH^*$

Mo	3.226861	9.218275	0.957707
Mo	9.527074	9.366156	0.946724
Mo	0.003267	9.279374	0.954043
Mo	6.293839	9.432993	0.964338
Mo	11.144662	9.340472	3.622219
Mo	7.950358	9.346212	3.660627
Mo	1.581427	9.339990	3.675610
Mo	4.751053	9.344327	3.721898
Mo	9.556652	9.354147	6.368934
Mo	-0.018820	9.353454	6.368585
Mo	6.346888	9.347626	6.430332
Mo	3.161820	9.353702	6.502622
Mo	5.052912	9.330813	9.322360
Mo	1.283318	9.345954	9.207734
Mo	11.289451	9.349888	9.112851
Mo	7.846579	9.335814	9.139100
S	1.592787	7.804770	-0.071326
S	4.744356	7.762814	0.041139
S	11.130407	7.916448	-0.110217
S	1.617444	10.541172	-0.246626
S	7.903130	8.084366	-0.219114
S	7.928896	10.820288	-0.098299
S	4.780118	10.876615	0.020306
S	11.158290	10.696276	-0.148488
S	3.177016	10.882135	2.720173
S	-0.005721	7.739377	2.777612
S	6.343582	10.930785	2.831623
S	9.531198	7.768485	2.723043
S	6.337501	7.794023	2.746599
S	3.172652	7.746351	2.841624
S	9.541741	10.931530	2.744817
S	0.001154	10.904390	2.712911
S	1.606224	7.789986	5.534382
S	7.945171	10.912224	5.498274
S	4.729957	7.785907	5.568860
S	1.608250	10.910632	5.516142
S	11.138988	7.782197	5.460318
S	7.946122	7.788859	5.496517
S	4.727524	10.914182	5.562855
S	11.143179	10.916891	5.446940
S	3.177825	7.903259	8.506248
S	-0.037265	11.007716	8.165927
S	6.372924	7.691168	8.222814

S	-0.027101	7.690945	8.163189
S	6.371503	10.981286	8.255705
S	9.570537	7.820618	8.241053
S	9.566760	10.881847	8.245665
S	3.165487	10.791275	8.506530
S	6.649176	9.093837	11.070323
S	-0.175398	9.296305	11.114893
S	9.609920	9.428632	10.793323
C	1.877314	9.209237	11.207647
O	3.974139	9.449614	11.005630
H	2.066560	8.225810	11.651006
H	2.023135	10.045806	11.892404
H	4.480083	9.334548	11.833384

$CH^* + H^# = CH_2^* + #$

Mo	3.225618	9.220936	0.930095
Mo	9.602418	9.428051	0.966497
Mo	-0.060445	9.225624	0.949547
Mo	6.335027	9.432572	0.945805
Mo	11.152261	9.323855	3.736653
Mo	7.962383	9.315794	3.731854
Mo	1.586547	9.329487	3.682529
Mo	4.781130	9.324575	3.684551
Mo	9.558799	9.309275	6.489186
Mo	-0.002582	9.314733	6.463063
Mo	6.358795	9.306966	6.480751
Mo	3.188217	9.314729	6.417485
Mo	4.643093	9.272763	9.215350
Mo	1.782396	9.294308	9.218058
Mo	11.417207	9.296428	9.303585
Mo	7.746121	9.304274	9.298531
S	1.576550	7.807526	-0.102566
S	4.774867	7.771536	0.025608
S	11.148989	7.765424	0.051990
S	1.576871	10.498268	-0.269296
S	7.974339	8.153868	-0.257363
S	7.975821	10.854667	-0.081047
S	4.793269	10.882984	0.031697
S	11.139076	10.891172	0.059050
S	3.181866	10.864964	2.705223
S	-0.012077	7.742119	2.824735
S	6.389680	10.911342	2.826978
S	9.557094	7.787266	2.755840
S	6.381667	7.786055	2.722529
S	3.176601	7.739126	2.801967
S	9.551571	10.905370	2.853857
S	-0.017413	10.863885	2.733817
S	1.576734	7.762697	5.505885
S	7.960837	10.871542	5.588445
S	4.796644	7.754582	5.502795
S	1.578342	10.880202	5.515981
S	11.145232	7.748278	5.569333
S	7.965332	7.748096	5.570929
S	4.792347	10.878264	5.519346
S	11.148064	10.883996	5.583778
S	3.183233	7.676226	8.208900
S	0.075473	10.903625	8.332563
S	6.328991	7.675684	8.331800
S	0.062132	7.697745	8.307107
S	6.310016	10.910994	8.357163
S	9.568570	7.831872	8.403202
S	9.569878	10.775824	8.412611
S	3.201197	10.916899	8.237590
S	6.261800	9.254106	11.198856
S	0.114796	9.261550	11.089700
S	9.535643	9.315067	10.894453
C	3.174196	9.344515	10.706932
H	3.151179	9.279941	11.803527
H	4.818710	9.825664	11.029223

$CH_2^* + H^# = CH_3^* + #$

Mo	3.231664	9.221194	0.981844
Mo	9.609275	9.402022	0.986361
Mo	-0.026014	9.226638	0.987799
Mo	6.351350	9.403099	0.988096
Mo	11.171051	9.318972	3.726660
Mo	7.981982	9.319446	3.719271
Mo	1.597666	9.318443	3.715916
Mo	4.784299	9.318182	3.722028
Mo	9.583322	9.314925	6.473581
Mo	0.006711	9.315048	6.480795
Mo	6.383611	9.317402	6.456349
Mo	3.190592	9.326738	6.479951
Mo	4.942286	9.325403	9.244989
Mo	1.460195	9.299199	9.246063
Mo	11.349179	9.310254	9.268517
Mo	7.802841	9.310904	9.261758
S	1.599675	7.794436	-0.048338
S	4.786313	7.776599	0.051314
S	11.174566	7.780311	0.051657
S	1.601918	10.510838	-0.215431
S	7.980582	8.110450	-0.207612
S	7.980210	10.826420	-0.053236
S	4.799137	10.842776	0.043768
S	11.164320	10.843132	0.043910
S	3.192898	10.863224	2.751365
S	0.007793	7.724800	2.851160
S	6.386438	10.907942	2.849434
S	9.576088	7.770402	2.763150
S	6.384146	7.769836	2.765613
S	3.189108	7.725569	2.847451
S	9.573845	10.908135	2.845546
S	0.006114	10.867766	2.759420
S	1.604360	7.763562	5.563633
S	7.994126	10.877783	5.562904
S	4.775999	7.759326	5.557196
S	1.601334	10.879693	5.553280
S	11.166040	7.752235	5.560335
S	7.990958	7.754572	5.552067
S	4.774921	10.882947	5.554060
S	11.174263	10.882376	5.565838
S	3.193683	7.801323	8.376579
S	0.036617	10.944663	8.309285
S	6.378358	7.692905	8.266091
S	-0.004708	7.664432	8.286180
S	6.385393	10.938179	8.265504
S	9.578749	7.820850	8.383154
S	9.586991	10.800932	8.390724
S	3.192048	10.842108	8.377642
S	6.321745	9.303864	11.123787
S	0.031119	9.122305	11.261129
S	9.608559	9.311470	10.921500
C	3.215568	9.410196	10.637588
H	3.180771	8.551466	11.331287
H	3.311131	10.348061	11.212770
H	1.241358	9.887772	11.168714

$CH_3^* + H^# = CH_4^* + #$

Mo	3.218359	9.370989	0.958475
Mo	9.591178	9.371770	0.958590
Mo	-0.054520	9.272543	0.961983
Mo	6.317788	9.274936	0.964548
Mo	11.148703	9.319027	3.716600
Mo	7.945521	9.318515	3.725221
Mo	1.588348	9.320894	3.722606
Mo	4.767682	9.322159	3.732385
Mo	9.546484	9.319612	6.457916
Mo	-0.013879	9.315738	6.467866
Mo	6.345944	9.319826	6.500535
Mo	3.196646	9.317914	6.500995
Mo	4.952219	9.316766	9.341077
Mo	1.323470	9.310126	9.201298
Mo	11.310016	9.319827	9.213364
Mo	7.797738	9.317770	9.246311
S	1.605488	7.965448	-0.160767
S	4.804167	7.761545	0.060559
S	11.181653	7.764793	0.059817
S	1.557404	10.675502	-0.163574
S	7.975879	7.971323	-0.163198
S	7.930401	10.679115	-0.160042
S	4.733314	10.888605	0.066690
S	11.111021	10.885379	0.068400
S	3.169845	10.891238	2.816162
S	-0.000885	7.748826	2.817312
S	6.357138	10.877276	2.775728
S	9.548130	7.769420	2.767035
S	6.363545	7.749228	2.819767
S	3.180973	7.768505	2.767661
S	9.537856	10.886993	2.818085
S	-0.012199	10.875105	2.771353
S	1.615838	7.764654	5.561633
S	7.944134	10.879167	5.561424
S	4.758574	7.754597	5.567990
S	1.608790	10.870343	5.566416
S	11.137636	7.754249	5.540808
S	7.943188	7.757952	5.563372
S	4.762980	10.883800	5.573501
S	11.141725	10.881717	5.542333
S	3.161288	7.832985	8.444783
S	-0.041528	10.973319	8.231784
S	6.323460	7.679146	8.325714
S	-0.045024	7.654291	8.232812
S	6.349944	10.956622	8.312182
S	9.540180	7.815342	8.346505
S	9.546351	10.825305	8.345626
S	3.157532	10.782759	8.480539
S	6.551740	9.376184	11.272846
S	0.031229	9.353506	11.097842
S	9.576988	9.325985	10.882991
C	3.556037	9.217706	11.201627
H	3.515599	10.276005	11.502813
H	2.525164	8.845421	11.017535
H	3.806998	8.633734	12.108856
H	5.192863	8.799907	11.192766

8. Transition state of elementary reaction on S edge

$H_2O^* + # = OH^* + H^#$

Mo	4.822641	3.123676	0.184381
Mo	7.972391	3.118742	0.157915
Mo	11.133598	3.120911	0.159387
Mo	1.569074	3.121924	0.188654
Mo	6.384808	3.093356	2.779753
Mo	9.559861	3.093831	2.788598
Mo	3.191501	3.101379	2.727355
Mo	-0.008581	3.102082	2.741649
Mo	1.595312	3.059541	5.503588
Mo	4.766722	3.094313	5.511323
Mo	11.179070	3.094977	5.520922
Mo	7.973631	3.034938	5.547840
Mo	6.291273	3.042495	8.132074
Mo	3.257265	3.096969	8.105463
Mo	-0.056431	3.097769	8.111284
Mo	9.660020	3.042717	8.137704
S	6.401542	1.506551	0.904345
S	-0.033898	1.500882	0.862393
S	6.405956	4.719218	0.936864
S	3.198447	4.732724	0.855558
S	9.553471	1.521392	0.913198
S	3.198925	1.502474	0.828212
S	-0.035628	4.732278	0.886910
S	9.549600	4.702459	0.942909
S	1.595783	4.644345	3.670806
S	7.970478	1.512945	3.692769
S	1.595274	1.531649	3.639665
S	7.970509	4.632988	3.736989
S	11.160891	4.657530	3.688496
S	4.780249	4.656864	3.677445
S	4.770706	1.539725	3.665071
S	11.170601	1.540292	3.677358
S	3.235328	1.471992	6.423189
S	6.406911	4.649108	6.494902
S	9.638091	1.451321	6.458194
S	9.538998	4.649234	6.501893
S	0.028142	4.679011	6.428359
S	3.165238	4.678404	6.422624
S	-0.042423	1.473836	6.429583
S	6.307929	1.451511	6.450542
S	1.601280	1.693961	9.267167
S	4.761865	3.927213	9.619310
S	7.972874	2.159215	9.447787
S	11.193182	3.914947	9.630163
O	1.613972	4.291900	9.192627
H	1.640512	5.199045	9.559432
H	1.610502	3.192464	9.835745

$OH^* + # = O^* + H^#$

Mo	4.815562	3.084688	0.166395
Mo	7.969334	3.081789	0.161518
Mo	11.123195	3.083291	0.174720
Mo	1.599675	3.087328	0.191095
Mo	6.383458	3.097400	2.780019
Mo	9.559374	3.097188	2.777592
Mo	3.187774	3.107922	2.740007
Mo	-0.000022	3.108809	2.735855
Mo	1.594182	3.126594	5.482387
Mo	4.777660	3.150837	5.543539
Mo	11.166966	3.152521	5.541924
Mo	7.972041	3.079032	5.520360
Mo	6.423081	3.097365	8.149768
Mo	3.147514	3.234437	8.171541
Mo	0.044061	3.236657	8.171873
Mo	9.522801	3.098150	8.148758
S	6.389531	1.488690	0.932684
S	-0.021682	1.477424	0.869018
S	6.394706	4.686075	0.914126
S	3.215140	4.706213	0.849802
S	9.547242	1.483702	0.930546
S	3.213616	1.478490	0.877493
S	-0.023601	4.706808	0.838689
S	9.543059	4.689830	0.911353
S	1.592794	4.678041	3.635706
S	7.972150	1.525676	3.695967
S	1.592647	1.548649	3.668072
S	7.972040	4.654986	3.699807
S	11.160528	4.672250	3.671297
S	4.782973	4.671766	3.674051
S	4.767435	1.569789	3.715354
S	11.176533	1.570409	3.713265
S	3.206595	1.588134	6.485358
S	6.439964	4.709989	6.482800
S	9.616467	1.514968	6.472540
S	9.504307	4.710326	6.481491
S	0.021585	4.754443	6.400781
S	3.167465	4.753631	6.401124
S	-0.018476	1.590016	6.486870
S	6.328374	1.514196	6.473886
S	1.595263	1.718622	9.307600
S	4.821105	3.980390	9.555763
S	7.973457	2.105516	9.512312
S	11.124657	3.982383	9.554148
O	1.596395	4.353630	8.918161
H	1.596120	3.208978	9.732526

$CO^* + O^* = CO_2 + 2^*$

Mo	4.864534	3.058175	0.135697
Mo	8.023336	3.058635	0.102028
Mo	11.177124	3.075937	0.108227
Mo	1.585997	3.075138	0.138552
Mo	6.421743	3.057616	2.714775
Mo	9.597740	3.090502	2.732156
Mo	3.226307	3.080138	2.673805
Mo	0.033262	3.115003	2.717616
Mo	1.665503	3.150769	5.452644
Mo	4.819449	3.060714	5.474613
Mo	11.174637	3.169180	5.478938
Mo	8.009595	3.059360	5.480129

Mo	6.418422	2.936627	8.067781
Mo	3.308706	3.170649	8.180846
Mo	0.053563	3.271232	8.181103
Mo	9.582850	3.085242	8.119998
S	6.450731	1.446740	0.857734
S	-0.001519	1.479234	0.880097
S	6.450317	4.666238	0.854907
S	3.234515	4.681342	0.770297
S	9.608447	1.485333	0.890914
S	3.218756	1.458071	0.788099
S	-0.001294	4.698270	0.833746
S	9.589355	4.663958	0.862782
S	1.663841	4.675370	3.591475
S	8.020395	1.506974	3.644430
S	1.627820	1.554745	3.640634
S	7.988255	4.629555	3.656080
S	11.180154	4.682951	3.619179
S	4.826191	4.617116	3.625288
S	4.801716	1.507921	3.621068
S	11.210277	1.567136	3.675040
S	3.185721	1.538064	6.435412
S	6.417639	4.623489	6.456170
S	9.665321	1.509514	6.431381
S	9.516538	4.703736	6.451143
S	0.044755	4.741299	6.328966
S	3.302728	4.714613	6.382130
S	0.014061	1.652772	6.439119
S	6.406704	1.410831	6.386730
S	1.532819	1.955676	9.293960
S	4.829735	2.219765	9.585097
S	8.051803	2.101228	9.482743
S	11.126037	3.872127	9.636095
C	2.394020	4.546536	9.645298
O	1.355109	4.774840	8.816076
O	2.736747	5.158743	10.620391

CO* + OH* = COOH* + *

Mo	4.831953	3.158642	0.212727
Mo	8.002253	3.145825	0.185569
Mo	11.152041	3.144439	0.195096
Mo	1.542043	3.154476	0.217591
Mo	6.390598	3.126351	2.785210
Mo	9.566868	3.102756	2.827938
Mo	3.196186	3.140999	2.751457
Mo	-0.005856	3.116856	2.799048
Mo	1.601046	3.115210	5.547538
Mo	4.805148	3.133823	5.519607
Mo	11.165214	3.072656	5.579783
Mo	7.957563	3.038502	5.567413
Mo	6.302407	3.013449	8.152950
Mo	3.240140	3.073786	8.158105
Mo	0.006211	3.216942	8.250302
Mo	9.525319	2.839001	8.206722
S	6.415561	1.532805	0.905642
S	-0.029291	1.526213	0.925064
S	6.429835	4.756451	0.938975
S	3.187226	4.763389	0.865017
S	9.573715	1.544216	0.945747
S	3.189175	1.545846	0.847176
S	-0.040450	4.752954	0.963689
S	9.573988	4.717984	0.994869
S	1.600595	4.676893	3.703603
S	7.956134	1.527968	3.696344
S	1.614589	1.569289	3.693093
S	7.982118	4.649907	3.774569
S	11.151747	4.652242	3.763485
S	4.794179	4.697838	3.691603
S	4.777932	1.573839	3.672930
S	11.177177	1.538496	3.723030
S	3.259217	1.516973	6.439466
S	6.433186	4.666549	6.537247
S	9.556102	1.394068	6.447889
S	9.547006	4.566263	6.624384
S	-0.015097	4.699138	6.400178
S	3.186003	4.693696	6.497607
S	0.042387	1.536949	6.510716
S	6.298739	1.448491	6.446897
S	1.684712	1.925553	9.359480
S	4.793252	3.890618	9.636592
S	7.837863	2.094356	9.588810
S	11.188955	1.956344	9.504171
C	0.876017	4.836769	9.200304
O	1.578922	5.624878	9.720243
O	11.925178	4.970088	9.348383
H	11.682061	4.704496	10.261645

CO* + H# = CHO* + #

Mo	4.847387	3.069378	0.183767
Mo	7.987732	3.070834	0.157417
Mo	11.155656	3.080126	0.160927
Mo	1.543382	3.075615	0.188753
Mo	6.392329	3.090598	2.770832
Mo	9.571606	3.098983	2.795620
Mo	3.194139	3.111125	2.723432
Mo	-0.001001	3.120018	2.771735
Mo	1.619478	3.153901	5.494024
Mo	4.794932	3.152142	5.518853
Mo	11.153021	3.163599	5.543489
Mo	7.977253	3.098129	5.534112
Mo	6.302915	3.147294	8.115623
Mo	3.290183	3.279403	8.150461
Mo	0.030522	3.188660	8.198915
Mo	9.527199	3.141416	8.175573
S	6.421284	1.461709	0.926493
S	-0.035166	1.476198	0.936839
S	6.422941	4.688110	0.897847
S	3.199203	4.686764	0.800521
S	9.575181	1.499179	0.948565
S	3.193388	1.477272	0.851950
S	-0.033102	4.704716	0.888268
S	9.566578	4.664860	0.922139
S	1.611954	4.691348	3.637361
S	7.979288	1.529839	3.714653
S	1.606391	1.567650	3.684412
S	7.974714	4.655464	3.694394
S	11.156650	4.686392	3.684926
S	4.793245	4.673455	3.640822
S	4.772426	1.560715	3.695435
S	11.178290	1.568045	3.735967
S	3.186981	1.598007	6.489451
S	6.430542	4.738631	6.447994
S	9.607668	1.541029	6.509228
S	9.505983	4.732534	6.490452
S	-0.002582	4.738933	6.425978
S	3.242321	4.787278	6.383915
S	0.022631	1.615585	6.447064
S	6.338737	1.513017	6.490450
S	1.583559	1.978098	9.370205
S	4.984990	3.549438	9.945830
S	7.948503	2.134437	9.442762
S	11.136098	3.910786	9.650164
C	1.664105	4.589050	8.700490
O	1.609048	5.669816	9.198345
H	3.344126	3.659550	9.888418

CO* + H# = COH* + #

Mo	4.827195	3.094354	0.171481
Mo	7.963794	3.094020	0.161676
Mo	11.118833	3.087176	0.171810
Mo	1.681207	3.091271	0.173999
Mo	6.401474	3.132413	2.820774
Mo	9.574259	3.125926	2.760461
Mo	3.223172	3.128464	2.763972
Mo	0.020217	3.115594	2.695995
Mo	1.599391	3.107016	5.474375
Mo	4.801501	3.174923	5.566770
Mo	11.185431	3.153521	5.447031
Mo	8.009915	3.168656	5.572411
Mo	6.394149	3.219890	8.204579
Mo	3.163809	3.162428	8.200079
Mo	-0.151804	3.066858	8.020458
Mo	9.811833	3.325617	8.109259
S	6.399111	1.520930	0.982842
S	0.022090	1.490715	0.815866
S	6.398028	4.691776	0.936455
S	3.252277	4.718191	0.886284
S	9.535175	1.489193	0.921452
S	3.256699	1.488122	0.927877
S	0.020868	4.699556	0.781975
S	9.542177	4.712346	0.879330
S	1.604268	4.679474	3.640882
S	7.999106	1.584849	3.763757
S	1.617983	1.557960	3.637011
S	7.999469	4.697235	3.706957
S	11.195617	4.699269	3.600811
S	4.797457	4.705221	3.708178
S	4.805132	1.589220	3.750861
S	11.179153	1.562738	3.641396
S	3.210277	1.579567	6.456027
S	6.420330	4.780304	6.516502
S	9.654005	1.620086	6.551767
S	9.618822	4.820563	6.397523
S	0.008757	4.707886	6.396602
S	3.157635	4.728132	6.469386
S	0.004837	1.472212	6.319945
S	6.387388	1.599784	6.567201
S	1.553913	1.935546	9.354844
S	4.740670	3.836760	9.723452
S	8.127690	2.523885	9.518162
S	11.348881	3.834540	9.933586
C	1.412565	4.194396	8.911354
O	1.190586	5.099112	9.733960
H	-0.224646	4.804375	9.954061

CHO* + O* = HCOO* + *

Mo	4.779043	3.146123	0.196951
Mo	7.916002	3.149709	0.203788
Mo	11.189953	3.168674	0.202767
Mo	1.657242	3.162444	0.182960
Mo	6.387185	3.102277	2.809278
Mo	9.569894	3.130866	2.739265
Mo	3.195491	3.132035	2.809980
Mo	0.008172	3.160778	2.749276
Mo	1.598390	3.156869	5.539135
Mo	4.788000	3.073790	5.607285
Mo	11.144302	3.155879	5.503757
Mo	8.002784	3.017261	5.547673
Mo	6.449347	2.706868	8.230876
Mo	3.139848	3.357988	8.276087
Mo	-0.087658	3.279121	8.256348
Mo	9.677915	2.966665	8.142887
S	6.348498	1.526038	0.932761
S	0.045710	1.556255	0.875847
S	6.349772	4.739367	0.984602
S	3.223507	4.747657	0.978025
S	9.560844	1.540946	0.826535
S	3.203328	1.547536	0.954540
S	0.050592	4.777104	0.882079
S	9.542453	4.763378	0.866364
S	1.597755	4.709725	3.696070
S	8.009696	1.526248	3.659312
S	1.575017	1.591310	3.715691
S	7.977100	4.642470	3.758374
S	11.142765	4.711145	3.664340
S	4.818106	4.647699	3.780501
S	4.772078	1.555513	3.737131
S	11.184388	1.591616	3.661001
S	3.137540	1.570969	6.528181
S	6.428379	4.505926	6.699850
S	9.683616	1.434320	6.392120
S	9.507815	4.640669	6.540877
S	-0.024830	4.753187	6.424509
S	3.224315	4.741315	6.381506
S	-0.038532	1.634030	6.515287
S	6.402006	1.350084	6.402923
S	1.449281	1.991344	9.325809
S	4.823973	1.805337	9.430752
S	8.167715	1.804203	9.440648
S	11.016409	3.780352	9.792127
C	2.014208	5.073073	8.851636
O	0.832349	4.985591	9.301332
O	3.666154	4.427500	9.682960
H	2.485828	6.069584	8.838304

COH* + O* = COOH* + *

Mo	4.764558	3.132041	0.178226
Mo	7.919760	3.143982	0.187909
Mo	11.061512	3.132275	0.208101
Mo	1.599249	3.115588	0.205856
Mo	6.333929	3.138528	2.820242
Mo	9.511658	3.138461	2.797253
Mo	3.154742	3.099298	2.783946
Mo	-0.038261	3.095441	2.735198
Mo	1.538263	3.058054	5.494591
Mo	4.760383	3.101277	5.579188
Mo	11.121393	3.096379	5.556193
Mo	7.911892	3.166710	5.562282
Mo	6.394174	3.151116	8.202393
Mo	3.010290	3.061188	8.292132
Mo	0.073105	3.131763	8.269204
Mo	9.497720	3.086241	8.175674
S	6.344943	1.554147	0.962503
S	-0.054892	1.505566	0.823787
S	6.332197	4.726644	0.962178
S	3.180871	4.727263	0.934245
S	9.481063	1.526995	0.941259
S	3.195892	1.504954	0.906373
S	-0.041833	4.726060	0.858006
S	9.493806	4.752982	0.942726
S	1.545250	4.643848	3.682345
S	7.923897	1.587876	3.739026
S	1.546798	1.516622	3.646551
S	7.928017	4.713824	3.726125
S	11.142934	4.657843	3.705241
S	4.719678	4.668186	3.743069
S	4.755606	1.556309	3.733326
S	11.109050	1.562726	3.689616
S	3.160047	1.531774	6.473959
S	6.295424	4.743039	6.530276
S	9.440630	1.523628	6.465565
S	9.571811	4.706278	6.519057
S	-0.015311	4.649588	6.423110
S	3.118749	4.620467	6.461541
S	-0.067045	1.479713	6.418979
S	6.398967	1.533177	6.545001
S	1.580213	1.538145	9.250663
S	4.780817	2.289320	9.599249
S	7.969002	3.974934	9.651767
S	11.027275	1.940531	9.372507
C	0.006985	4.398918	9.700734
O	1.716978	4.370934	8.951013
O	-0.023110	5.210247	10.692050
H	12.361004	6.093160	10.461611

HCOO* + # = CO_2 + * + H#

Mo	4.753242	3.150895	0.163071
Mo	7.900536	3.151707	0.189408
Mo	11.194229	3.164363	0.197801
Mo	1.585705	3.162819	0.167016
Mo	6.352731	3.081233	2.778780
Mo	9.542586	3.104824	2.735023
Mo	3.172937	3.105135	2.804718
Mo	-0.011947	3.127056	2.779151
Mo	1.578165	3.080669	5.563375
Mo	4.770940	3.009489	5.547968
Mo	11.118468	3.093855	5.518734
Mo	7.955337	2.985820	5.520483
Mo	6.290228	2.812862	8.112212
Mo	3.400732	2.988455	8.193727
Mo	-0.096810	3.160854	8.217930
Mo	9.582262	2.953946	8.137258
S	6.321810	1.519108	0.875507
S	0.016645	1.542192	0.896380
S	6.323009	4.738784	0.960471
S	3.176904	4.723002	0.972572
S	9.552166	1.539041	0.805945
S	3.163542	1.560351	0.911021
S	0.019605	4.767379	0.942465
S	9.538618	4.750470	0.873824
S	1.586132	4.662417	3.742067
S	7.970147	1.501100	3.626861
S	1.562897	1.550409	3.703777
S	7.946699	4.615640	3.733274
S	11.116889	4.665879	3.692914
S	4.780512	4.626492	3.760842
S	4.752785	1.503760	3.665897
S	11.145488	1.552418	3.656600
S	3.155225	1.429754	6.471675
S	6.386026	4.542860	6.577939
S	9.615697	1.404671	6.406527
S	9.468531	4.609174	6.513933

S	-0.034886	4.661697	6.436277
S	3.219424	4.610611	6.530592
S	-0.070803	1.534381	6.483503
S	6.332482	1.311871	6.390558
S	1.487019	1.804719	9.278001
S	4.918125	2.810333	9.948881
S	8.015733	1.849538	9.366581
S	11.012593	3.753862	9.730375
C	2.231811	4.719236	9.313456
O	0.955427	4.768196	9.179075
O	3.053066	5.533757	9.691536
H	2.326507	3.224547	9.706459

$COOH^* + \# = CO_2 + * + H^\#$

Mo	4.801490	3.131162	0.194106
Mo	7.966617	3.117159	0.175992
Mo	11.158195	3.117911	0.179986
Mo	1.555603	3.132195	0.187817
Mo	6.378778	3.126131	2.813551
Mo	9.560147	3.102272	2.831156
Mo	3.182944	3.151876	2.796222
Mo	-0.010665	3.124029	2.819710
Mo	1.592104	3.153890	5.571784
Mo	4.796773	3.178535	5.564751
Mo	11.151662	3.086978	5.572882
Mo	7.968490	3.081329	5.593947
Mo	6.309557	3.108827	8.220382
Mo	3.212679	3.270743	8.256926
Mo	-0.207799	3.075212	8.208511
Mo	9.675329	3.021374	8.184458
S	6.381404	1.527232	0.940649
S	-0.014776	1.530872	0.950792
S	6.394758	4.721537	0.936062
S	3.177111	4.730078	0.895467
S	9.560593	1.535779	0.946086
S	3.177085	1.549276	0.920392
S	-0.029642	4.719142	0.950892
S	9.559646	4.687589	0.961488
S	1.578631	4.701440	3.723758
S	7.953024	1.545919	3.742924
S	1.607191	1.588806	3.739854
S	7.976556	4.658670	3.769057
S	11.143050	4.666380	3.755930
S	4.793619	4.707956	3.707143
S	4.764349	1.595273	3.740446
S	11.166128	1.538706	3.729863
S	3.230605	1.626167	6.545832
S	6.437112	4.714205	6.558335
S	9.585403	1.455802	6.525202
S	9.557154	4.663678	6.590399
S	-0.058266	4.685099	6.520780
S	3.190432	4.760221	6.457157
S	0.035872	1.521730	6.489132
S	6.303773	1.523581	6.521065
S	1.637915	1.989670	9.349647
S	4.840175	3.917719	9.771491
S	7.925198	2.127020	9.486128
S	11.083366	2.960187	10.153728
C	0.859867	4.699918	9.177945
O	-0.030713	5.366506	9.778618
O	2.104725	4.940714	9.132776
H	11.698789	4.320000	10.098218

$H^\# + * = H^* + \#$

Mo	4.711573	3.090619	0.221626
Mo	8.060579	3.094098	0.215718
Mo	11.170584	3.106576	0.209265
Mo	1.599265	3.104019	0.202752
Mo	6.386929	3.107590	2.759891
Mo	9.583526	3.134700	2.811887
Mo	3.194035	3.115664	2.806310
Mo	0.005975	3.145210	2.845286
Mo	1.618093	3.142970	5.616762
Mo	4.796182	3.134697	5.507205
Mo	11.159343	3.202109	5.566591
Mo	7.976354	3.146857	5.563700
Mo	6.202874	3.251850	8.102071
Mo	3.552851	3.122480	8.142000
Mo	-0.092907	3.217729	8.196118
Mo	9.648266	3.219774	8.166505
S	6.391093	1.501778	0.864450
S	0.006730	1.541075	1.007360
S	6.387133	4.688532	0.841578
S	3.159138	4.725599	0.938466
S	9.618806	1.489151	0.978159
S	3.145879	1.479903	0.964732
S	0.011792	4.695659	0.961844
S	9.608177	4.733326	0.933340
S	1.623845	4.685933	3.756176
S	7.983448	1.573109	3.734567
S	1.592659	1.587101	3.779883
S	7.963847	4.680798	3.692760
S	11.162264	4.728250	3.713730
S	4.801412	4.684452	3.663190
S	4.799316	1.547229	3.692711
S	11.166992	1.596794	3.772867
S	3.203545	1.503361	6.465392
S	6.376281	4.799000	6.420912
S	9.619411	1.582638	6.526794
S	9.532007	4.789806	6.487697
S	0.046883	4.782391	6.521965
S	3.264448	4.736279	6.517838
S	-0.060284	1.594239	6.540382
S	6.354567	1.559193	6.533945
S	1.605822	2.345883	9.419515
S	4.854722	3.590771	9.995776
S	7.951720	2.388029	9.460092
S	11.143460	4.127845	9.666664
H	3.304707	4.356654	9.441878

$2H^* = H_2 + 2*$

Mo	4.869354	3.077717	0.221805
Mo	7.995732	3.093084	0.205739
Mo	11.151702	3.100952	0.203229
Mo	1.550115	3.081741	0.215657
Mo	6.402518	3.116772	2.820729
Mo	9.577449	3.148081	2.847384
Mo	3.203192	3.113173	2.746507
Mo	-0.000284	3.144463	2.791927
Mo	1.621853	3.150546	5.536190
Mo	4.785990	3.148568	5.522072
Mo	11.177575	3.220672	5.562730
Mo	7.988407	3.164620	5.625898
Mo	6.149494	3.234265	8.146641
Mo	3.352721	3.204467	8.103782
Mo	0.027365	3.177507	8.181787
Mo	9.704981	3.270547	8.221633
S	6.442610	1.480366	0.985432
S	-0.036767	1.490070	0.963749
S	6.429044	4.707759	0.943515
S	3.210649	4.689531	0.828534
S	9.577188	1.529756	1.016386
S	3.206993	1.482741	0.871325
S	-0.021022	4.724721	0.899284
S	9.570158	4.696805	0.958481
S	1.622821	4.691901	3.671567
S	7.998007	1.588823	3.808878
S	1.597693	1.582789	3.705627
S	7.973440	4.696270	3.757153
S	11.180536	4.738461	3.701954
S	4.785784	4.686611	3.664397
S	4.789687	1.560304	3.707501
S	11.174367	1.609182	3.773946
S	3.196037	1.539002	6.444813
S	6.362008	4.786374	6.489378
S	9.649043	1.622697	6.597199
S	9.562934	4.815477	6.528846
S	0.074771	4.768804	6.484120
S	3.233180	4.770606	6.407288
S	-0.047606	1.599973	6.480372
S	6.363031	1.568912	6.572510
S	1.616913	1.969118	9.298651
S	4.804320	3.646269	10.039804
S	7.983630	2.602185	9.551663
S	11.304226	4.136512	9.644002
H	2.274190	4.419096	8.722137
H	3.393785	4.182045	9.704285

$CHO^* + * = CH^* + O^*$

Mo	4.831016	3.067758	0.147893
Mo	8.030958	3.058027	0.117082
Mo	11.157889	3.063898	0.123232
Mo	1.569640	3.073088	0.146150
Mo	6.401974	3.106406	2.702336
Mo	9.585376	3.095784	2.747713
Mo	3.209389	3.123392	2.672144
Mo	0.019036	3.114118	2.721188
Mo	1.626614	3.167811	5.465230
Mo	4.828157	3.185637	5.442312
Mo	11.176217	3.150437	5.522508
Mo	7.982309	3.129833	5.515513
Mo	6.387121	3.256750	8.144636
Mo	3.303021	3.292262	8.235440
Mo	0.140438	3.290265	8.372192
Mo	9.572286	3.059610	8.162828
S	6.433810	1.465532	0.868162
S	-0.012958	1.472367	0.895212
S	6.441036	4.683112	0.813277
S	3.201483	4.704731	0.748393
S	9.596073	1.474726	0.923232
S	3.198792	1.467593	0.817966
S	-0.021878	4.689736	0.840704
S	9.588733	4.667238	0.875621
S	1.621306	4.692254	3.596306
S	7.976354	1.554836	3.689932
S	1.627524	1.581821	3.655881
S	7.992207	4.660541	3.650235
S	11.176383	4.666985	3.656709
S	4.810926	4.698988	3.572133
S	4.793693	1.579845	3.642052
S	11.192854	1.573609	3.702583
S	3.236763	1.634679	6.391220
S	6.456022	4.782640	6.387236
S	9.583581	1.524160	6.475677
S	9.565789	4.709284	6.500016
S	0.026517	4.713313	6.402936
S	3.229881	4.738250	6.348685
S	0.033786	1.623336	6.444135
S	6.325759	1.598063	6.492681
S	1.707050	1.808119	9.215499
S	4.949974	4.400809	9.517885
S	7.894768	2.413112	9.622767
S	11.164307	2.310003	9.635524
C	2.715462	4.712317	9.341463
O	0.637982	4.708315	9.323231
H	2.613399	5.662764	9.874316

$CHO^* + H^\# = CH_2O^* + \#$

Mo	4.755516	3.105000	0.144957
Mo	7.924638	3.089541	0.169658
Mo	11.214529	3.106234	0.175222
Mo	1.606722	3.116861	0.150698
Mo	6.370893	3.100436	2.742118
Mo	9.561620	3.098185	2.707381
Mo	3.184497	3.133385	2.781368
Mo	0.004590	3.133321	2.764190
Mo	1.596375	3.164178	5.538164
Mo	4.793203	3.147605	5.528862
Mo	11.129192	3.140157	5.502194
Mo	7.971815	3.050763	5.481411
Mo	6.448880	3.078260	8.135130
Mo	3.277009	3.291958	8.272013
Mo	-0.106830	3.254052	8.217645
Mo	9.585121	3.038866	8.115408
S	6.327178	1.485461	0.884618
S	0.041678	1.508983	0.919455
S	6.343427	4.709840	0.879463
S	3.188206	4.707559	0.912890
S	9.576015	1.487606	0.811625
S	3.177101	1.530705	0.939150
S	0.032340	4.729448	0.895128
S	9.561097	4.705546	0.810935
S	1.590467	4.704281	3.683350
S	7.973758	1.521353	3.628357
S	1.590980	1.587657	3.726400
S	7.975990	4.642548	3.659205
S	11.126793	4.680747	3.647427
S	4.804976	4.684306	3.676228
S	4.767251	1.571687	3.705341
S	11.164675	1.567981	3.668524
S	3.191547	1.626670	6.520907
S	6.463386	4.687038	6.447203
S	9.618418	1.465605	6.408903
S	9.488975	4.677848	6.471264
S	-0.038425	4.728901	6.407218
S	3.213724	4.748128	6.430860
S	-0.046986	1.612085	6.491306
S	6.323221	1.495249	6.431351
S	1.498135	1.928342	9.295490
S	5.019862	4.097165	9.581039
S	7.996405	2.001520	9.420086
S	10.983971	3.781406	9.747901
C	2.151209	4.820342	9.197776
O	0.882531	4.860471	9.221073
H	2.639584	5.689887	9.681140
H	2.354961	3.222772	9.883298

$CHO^* + H^\# = CHOH^* + \#$

Mo	4.802475	3.050922	0.167426
Mo	8.014464	3.060717	0.140670
Mo	11.130056	3.064454	0.159658
Mo	1.522008	3.057579	0.164655
Mo	6.374606	3.107339	2.723738
Mo	9.559937	3.124943	2.787111
Mo	3.171209	3.104987	2.692540
Mo	-0.019115	3.121234	2.764391
Mo	1.593467	3.167239	5.524982
Mo	4.763304	3.166037	5.420833
Mo	11.155553	3.196705	5.532558
Mo	7.949730	3.189632	5.539727
Mo	6.076992	3.283081	8.049568
Mo	3.485356	3.244064	8.004019
Mo	-0.239898	3.187263	8.153694
Mo	9.682105	3.293851	8.145156
S	6.419173	1.464196	0.892338
S	-0.053637	1.470969	0.947135
S	6.409695	4.674689	0.824620
S	3.162056	4.678362	0.766399
S	9.567395	1.487168	0.974817
S	3.156368	1.454286	0.834245
S	-0.047144	4.687242	0.872536
S	9.564323	4.677341	0.899316
S	1.592760	4.680591	3.643184
S	7.959405	1.588711	3.744906
S	1.587080	1.582775	3.707372
S	7.946986	4.690749	3.658237
S	11.160769	4.710962	3.667431
S	4.763378	4.690600	3.561528
S	4.765380	1.553206	3.634129
S	11.150915	1.587651	3.744053
S	3.218072	1.558638	6.450200
S	6.312834	4.822768	6.382729
S	9.582111	1.633595	6.553089
S	9.542300	4.840159	6.456190
S	0.016370	4.775738	6.513180
S	3.223580	4.804017	6.325268
S	-0.027460	1.569981	6.488930
S	6.330731	1.608221	6.498119
S	1.581101	2.200064	9.428208
S	4.734840	3.391823	10.077975
S	7.901239	2.649579	9.471576
S	11.099163	3.562165	9.944703
C	1.326890	3.956891	9.646788
O	2.385800	4.706875	9.203946
H	3.623799	4.407249	9.926605
H	0.900215	4.287883	10.602606

$CH_2O^* + * = CH_2^* + O^*$

Mo	4.807004	3.137511	0.180814
Mo	7.955040	3.139568	0.176155
Mo	11.104184	3.152124	0.191139
Mo	1.656760	3.148470	0.191858
Mo	6.384953	3.101584	2.822598
Mo	9.560065	3.121552	2.781393
Mo	3.199019	3.109826	2.777246
Mo	0.000045	3.125128	2.723181
Mo	1.587411	3.091998	5.507909
Mo	4.788254	3.057939	5.576959
Mo	11.153868	3.118366	5.504932
Mo	7.995646	3.056055	5.581744
Mo	6.354773	2.898676	8.217243

Mo	3.095054	3.219533	8.345091
Mo	-0.122693	3.044080	8.194430
Mo	9.646357	3.089710	8.163649
S	6.383173	1.541018	0.941998
S	-0.000161	1.540312	0.810456
S	6.382032	4.711343	0.985607
S	3.238912	4.746910	0.941137
S	9.533158	1.527732	0.906984
S	3.226639	1.519181	0.900423
S	0.004722	4.750560	0.841082
S	9.521716	4.750849	0.938307
S	1.592178	4.665503	3.679365
S	7.993931	1.534113	3.715889
S	1.584308	1.553794	3.652236
S	7.968533	4.648556	3.768619
S	11.166554	4.681988	3.674856
S	4.792022	4.640695	3.757646
S	4.778368	1.536834	3.710973
S	11.173464	1.562601	3.655210
S	3.164018	1.515192	6.470853
S	6.394780	4.591083	6.610284
S	9.651272	1.479678	6.488318
S	9.538954	4.687899	6.496406
S	0.004953	4.639860	6.479275
S	3.190464	4.637624	6.417766
S	-0.028470	1.491277	6.350056
S	6.390778	1.413065	6.489153
S	1.464023	1.705570	9.215269
S	4.752021	2.160005	9.670032
S	8.098944	2.196416	9.580713
S	11.139258	4.022122	9.710021
C	0.514400	4.629179	9.493097
O	2.558919	4.608583	9.309578
H	0.447421	5.692984	9.237367
H	0.736743	4.450819	10.549817

CHOH* + * = CH* + OH*

Mo	4.722195	3.168437	0.190372
Mo	8.035036	3.159766	0.180862
Mo	11.232183	3.182224	0.170451
Mo	1.586743	3.186989	0.182359
Mo	6.393686	3.072340	2.708265
Mo	9.591222	3.101052	2.747451
Mo	3.197400	3.116239	2.794886
Mo	0.020617	3.136036	2.817183
Mo	1.608220	3.097268	5.615895
Mo	4.821717	3.013484	5.500289
Mo	11.174736	3.075999	5.542221
Mo	7.988634	2.958618	5.470917
Mo	6.321468	2.800852	8.063233
Mo	3.601388	3.163624	8.178261
Mo	-0.179447	3.048110	8.236680
Mo	9.500818	2.946050	8.113722
S	6.374892	1.534310	0.752815
S	0.031031	1.577300	0.937705
S	6.384473	4.743696	0.867904
S	3.164559	4.770396	0.979465
S	9.644910	1.544090	0.842557
S	3.145853	1.553981	0.904593
S	0.025388	4.765970	0.998767
S	9.622231	4.760430	0.929426
S	1.616892	4.664859	3.784963
S	7.997011	1.480197	3.574995
S	1.607930	1.570392	3.752461
S	7.970214	4.602574	3.704512
S	11.155386	4.665620	3.741449
S	4.840275	4.624334	3.710060
S	4.786968	1.504781	3.619629
S	11.188850	1.548791	3.680013
S	3.222180	1.493783	6.555529
S	6.442980	4.529519	6.532813
S	9.647786	1.395883	6.383196
S	9.482185	4.593642	6.470264
S	0.019920	4.659450	6.598212
S	3.288261	4.681744	6.432161
S	-0.007703	1.456979	6.483883
S	6.368186	1.291814	6.336764
S	1.682775	2.024254	9.434690
S	5.018498	2.826049	9.970547
S	8.018641	1.813129	9.379359
S	10.918658	3.953829	9.587818
C	0.938714	3.524488	9.813540
O	2.818828	4.722823	9.287137
H	3.234825	4.720531	10.171583
H	0.962671	4.023704	10.783540

$CH_2O^* + H^\# = CH_2OH^* + \#$

Mo	4.761621	3.229726	0.217395
Mo	7.858425	3.214847	0.226288
Mo	11.220684	3.218653	0.231727
Mo	1.565176	3.233851	0.218169
Mo	6.346566	3.148524	2.829853
Mo	9.538914	3.135170	2.770478
Mo	3.163932	3.174666	2.859314
Mo	-0.019596	3.159411	2.830632
Mo	1.571967	3.110030	5.620274
Mo	4.765134	3.098230	5.613557
Mo	11.116028	3.063415	5.544908
Mo	7.952682	3.030342	5.552440
Mo	6.324717	2.926826	8.159471
Mo	3.349065	3.104423	8.268211
Mo	-0.230955	3.036067	8.178976
Mo	9.622988	2.937460	8.140397
S	6.304074	1.581398	0.930381
S	0.021842	1.587347	0.935481
S	6.318918	4.820209	1.021952
S	3.164865	4.789351	1.031403
S	9.539984	1.605210	0.813561
S	3.160670	1.643400	0.959172
S	0.008145	4.828484	1.017345
S	9.536438	4.782601	0.915362
S	1.561770	4.704640	3.809588
S	7.950322	1.546873	3.657597
S	1.577440	1.595159	3.746454
S	7.961211	4.663341	3.772322
S	11.109271	4.678954	3.754246
S	4.773760	4.699576	3.812149
S	4.746297	1.584465	3.731793
S	11.137154	1.555836	3.658763
S	3.197727	1.505032	6.559162
S	6.414935	4.621677	6.584767
S	9.581452	1.390301	6.440031
S	9.506709	4.618678	6.561865
S	-0.099059	4.645805	6.516380
S	3.171097	4.678866	6.598305
S	-0.021486	1.470701	6.460327
S	6.309065	1.398007	6.435840
S	1.563239	1.729952	9.304830
S	4.947486	3.378621	9.925591
S	7.973656	1.847629	9.353469
S	11.063848	3.059685	9.957872
C	1.039069	4.714601	9.228425
O	2.268278	4.277107	9.725052
H	1.182477	5.540697	8.520406
H	0.384660	5.019042	10.061576
H	1.905381	3.020100	10.068562

$CHOH^* + H^\# = CH_2OH^* + \#$

Mo	4.848868	3.211462	0.244509
Mo	8.025583	3.201351	0.201937
Mo	11.198187	3.209083	0.211838
Mo	1.566300	3.220745	0.237040
Mo	6.414952	3.109835	2.792697
Mo	9.602643	3.101114	2.829310
Mo	3.208929	3.140781	2.787790
Mo	0.021911	3.130373	2.835417
Mo	1.621676	3.063109	5.594455
Mo	4.828461	3.061290	5.552754
Mo	11.170275	3.047472	5.585292
Mo	7.993824	2.956228	5.555911
Mo	6.376795	2.876206	8.137425
Mo	3.338610	3.056255	8.210364
Mo	-0.079227	3.131622	8.346063
Mo	9.552769	2.886418	8.193817
S	6.440623	1.563378	0.871906
S	0.006986	1.580791	0.928303
S	6.452072	4.794447	0.990861
S	3.208572	4.804648	0.940823
S	9.615276	1.587585	0.911560
S	3.200692	1.591828	0.845963
S	-0.004820	4.802974	1.031109
S	9.604886	4.759636	1.034186
S	1.622161	4.666058	3.782305
S	7.996602	1.493412	3.654879
S	1.629214	1.558118	3.712550
S	8.002360	4.612989	3.798409
S	11.173649	4.654976	3.799091
S	4.825892	4.661452	3.748912
S	4.793912	1.551765	3.664029
S	11.208751	1.532952	3.714414
S	3.276305	1.465971	6.479376
S	6.474987	4.568937	6.559487
S	9.649333	1.360960	6.432462
S	9.515737	4.552148	6.568578
S	0.004544	4.612393	6.544824
S	3.227952	4.624571	6.509926
S	0.007439	1.494214	6.540018
S	6.334384	1.341514	6.402837
S	1.725785	1.646373	9.257210
S	4.968720	3.679776	9.745244
S	7.956354	1.788182	9.413034
S	10.920520	3.887488	9.686994
C	0.876059	4.448519	9.587188
O	2.242823	4.624612	9.464726
H	2.682629	5.084802	10.214269
H	0.473058	5.098134	10.378025
H	1.006266	2.862302	9.972970

$CH_2OH^* + * = CH_2^* + OH^*$

Mo	4.838816	3.276859	0.218679
Mo	7.999145	3.267688	0.214307
Mo	11.154137	3.271597	0.247958
Mo	1.679491	3.283495	0.242741
Mo	6.416864	3.128131	2.843842
Mo	9.594954	3.112796	2.823907
Mo	3.234845	3.155231	2.820245
Mo	0.033857	3.137967	2.777193
Mo	1.615462	3.007096	5.568229
Mo	4.843387	3.033063	5.574197
Mo	11.199066	2.955663	5.548483
Mo	8.013288	2.945257	5.604880
Mo	6.317321	2.855558	8.230682
Mo	3.229964	3.042717	8.311470
Mo	-0.230816	2.784847	8.191103
Mo	9.728138	2.827070	8.155644
S	6.415016	1.644698	0.903150
S	0.046354	1.635410	0.800412
S	6.427192	4.814202	1.072772
S	3.266392	4.856127	1.041473
S	9.570486	1.616930	0.872751
S	3.260063	1.637722	0.885343
S	0.034208	4.851121	0.977462
S	9.567559	4.832625	1.062319
S	1.610435	4.653844	3.801499
S	8.003894	1.505199	3.680408
S	1.635365	1.552560	3.649273
S	8.018250	4.613450	3.860565
S	11.195558	4.626330	3.809159
S	4.836044	4.665614	3.815702
S	4.807198	1.543797	3.684832
S	11.212250	1.508462	3.618490
S	3.260167	1.462985	6.480064
S	6.468779	4.528159	6.647258
S	9.646111	1.285612	6.437097
S	9.601455	4.508625	6.605798
S	-0.008255	4.483760	6.624716
S	3.216713	4.553886	6.507950
S	0.051258	1.294805	6.351414
S	6.349947	1.343852	6.464103
S	1.645041	1.627936	9.199831
S	4.875388	3.570698	9.859746
S	8.010739	1.869591	9.414017
S	11.139880	3.243540	10.019075
C	0.234232	4.198201	9.743519
O	2.243304	4.665565	9.159217
H	-0.033388	5.256882	9.655999
H	0.681105	3.924404	10.702875
H	2.753306	5.098431	9.872410

$CH^* + H^\# = CH_2^* + \#$

Mo	4.841717	3.066655	0.160415
Mo	7.954271	3.070870	0.133483
Mo	11.142154	3.065842	0.129791
Mo	1.516040	3.060517	0.148621
Mo	6.373659	3.114359	2.747473
Mo	9.555378	3.106991	2.777195
Mo	3.176820	3.096284	2.686357
Mo	-0.027925	3.091214	2.732268
Mo	1.593448	3.088708	5.488610
Mo	4.744007	3.164352	5.461668
Mo	11.160937	3.129037	5.486379
Mo	7.948962	3.164706	5.540720
Mo	6.218362	3.314256	8.082773
Mo	3.308738	3.147740	8.049461
Mo	-0.168500	3.080891	8.070486
Mo	9.768056	3.196889	8.092576
S	6.406807	1.462373	0.920077
S	-0.055712	1.450616	0.889710
S	6.402097	4.703091	0.863671
S	3.171950	4.672177	0.767365
S	9.545290	1.504306	0.932450
S	3.178608	1.470896	0.809994
S	-0.048828	4.690270	0.854448
S	9.551825	4.655605	0.886837
S	1.581324	4.642741	3.628809
S	7.950783	1.574699	3.734950
S	1.588727	1.541754	3.635670
S	7.961422	4.681611	3.667141
S	11.163462	4.679198	3.648260
S	4.748416	4.688432	3.594359
S	4.769817	1.563095	3.654676
S	11.142455	1.540831	3.681503
S	3.215452	1.499484	6.389092
S	6.354441	4.818259	6.373853
S	9.567889	1.560593	6.507735
S	9.585952	4.779280	6.447602
S	0.003941	4.711706	6.443930
S	3.131290	4.731931	6.384287
S	-0.027934	1.478977	6.406317
S	6.309976	1.613494	6.516208
S	1.615932	2.108344	9.468549
S	4.738608	4.030730	9.785054
S	7.915769	2.668513	9.483531
S	11.210013	3.182490	9.919170
C	1.546772	3.836271	9.205451
H	3.256351	4.369517	9.452015
H	1.430673	4.518364	10.057516

$CH_2^* + H^\# = CH_3^* + \#$

Mo	4.848188	3.141459	0.193717
Mo	8.000400	3.130483	0.173626
Mo	11.151602	3.134904	0.162417
Mo	1.553293	3.144606	0.188204
Mo	6.395527	3.102018	2.772392
Mo	9.583186	3.101172	2.802574
Mo	3.192562	3.131772	2.729491
Mo	0.011037	3.128888	2.768286
Mo	1.598110	3.104330	5.480584
Mo	4.814566	3.104354	5.524805
Mo	11.175713	3.098756	5.569541
Mo	7.989487	3.022835	5.536799
Mo	6.475369	2.981659	8.136327
Mo	3.173261	3.070828	8.227815
Mo	0.056553	3.150934	8.262282
Mo	9.476469	3.005314	8.140570
S	6.421942	1.510893	0.897127
S	-0.025699	1.524818	0.900330
S	6.432446	4.738371	0.938204
S	3.201585	4.748566	0.838612
S	9.583826	1.534283	0.928383
S	3.198389	1.534001	0.821751
S	-0.035461	4.748909	0.916822
S	9.576815	4.709542	0.966841
S	1.609889	4.692814	3.672522
S	7.984161	1.513410	3.672297
S	1.610142	1.554806	3.646165
S	7.984316	4.634295	3.740154
S	11.170042	4.664864	3.736612
S	4.799847	4.668390	3.690311
S	4.770962	1.560377	3.664664
S	11.199436	1.557659	3.710983

S	3.197405	1.558379	6.401191
S	6.468466	4.648098	6.521080
S	9.632857	1.437413	6.456513
S	9.506360	4.657289	6.511325
S	0.019654	4.680919	6.475815
S	3.213775	4.647645	6.453927
S	0.025272	1.535821	6.475752
S	6.346791	1.433899	6.438269
S	1.707756	1.663190	9.256150
S	4.900912	3.838215	9.578425
S	7.981172	2.062367	9.602428
S	11.029451	3.999058	9.493264
C	1.678407	4.478968	8.880757
H	2.015466	4.493037	9.932313
H	1.608751	5.504613	8.502744
H	0.448012	3.498994	9.882725

CH_3* + H* = CH_4* + #

Mo	4.762426	3.143187	0.249956
Mo	8.070266	3.139929	0.245976
Mo	11.197647	3.143695	0.221886
Mo	1.621982	3.144454	0.219385
Mo	6.415306	3.114842	2.794203
Mo	9.602383	3.117329	2.834988
Mo	3.218816	3.125629	2.824400
Mo	0.031267	3.126670	2.848951
Mo	1.627966	3.088181	5.597215
Mo	4.815564	3.108479	5.569681
Mo	11.200807	3.114268	5.600763
Mo	8.001416	3.044288	5.582370
Mo	6.353537	3.013173	8.183700
Mo	3.284891	3.081058	8.190955
Mo	-0.059366	3.159065	8.235531
Mo	9.639780	3.046100	8.199284
S	6.415862	1.532449	0.875966
S	0.032309	1.556745	0.980571
S	6.419076	4.736852	0.909724
S	3.187704	4.757029	0.976452
S	9.639933	1.518458	0.962149
S	3.186107	1.521331	0.955986
S	0.032159	4.721670	1.001559
S	9.634891	4.751402	0.993234
S	1.632182	4.672320	3.773814
S	8.000160	1.533015	3.712529
S	1.630262	1.556128	3.746641
S	7.996313	4.650650	3.770630
S	11.184889	4.680363	3.772650
S	4.832405	4.676275	3.738418
S	4.819064	1.559620	3.715698
S	11.198421	1.562535	3.756619
S	3.272596	1.491043	6.490736
S	6.449564	4.649393	6.560029
S	9.658065	1.463419	6.506842
S	9.546800	4.662404	6.559827
S	0.041162	4.702246	6.514112
S	3.215525	4.681540	6.518615
S	0.000870	1.516225	6.528182
S	6.346537	1.445576	6.483764
S	1.632362	1.739358	9.344320
S	4.841035	3.817771	9.711924
S	8.003263	2.075045	9.494081
S	11.122214	3.843207	9.766831
C	1.272099	4.722102	9.464343
H	2.373312	4.823536	9.272245
H	0.818589	5.617354	9.020588
H	1.168374	4.788167	10.560812
H	1.247641	3.179547	9.743536