

## XYZ Coordinates for the configurations

### 1. Surface

# Fe<sub>2</sub>C(111)

1.000000000000

10.94560000 0.00000000 0.00000000

2.91646064 9.85136200 0.00000000

0.00000004 0.00000003 22.33820000

C Fe

44 80

Cart

8.75428253 8.56045134 11.06790422

7.29605221 3.63477033 11.06790422

3.28148253 8.56045134 11.06790422

1.82325221 3.63477033 11.06790422

6.02868044 8.46772381 10.88273308

4.57045013 3.54204280 10.88273308

11.50148044 8.46772381 10.88273308

10.04325013 3.54204280 10.88273308

8.71629626 6.41309755 9.69072998

7.25806595 1.48741655 9.69072998

3.24349626 6.41309755 9.69072998

1.78526595 1.48741655 9.69072998

7.42287539 9.60750802 8.64319703

5.96464507 4.68182701 8.64319703

12.89567539 9.60750802 8.64319703

11.43744507 4.68182701 8.64319703

8.69960883 2.82528651 7.59376644

4.68503914 7.75096752 7.59376644

3.22680883 2.82528651 7.59376644

10.15783914 7.75096752 7.59376644

7.44045385 5.86758695 6.53346587

5.98222353 0.94190595 6.53346587

1.96765385 5.86758695 6.53346587

0.50942353 0.94190595 6.53346587

6.18124440 8.91008113 5.47339490

4.72301409 3.98440012 5.47339490

11.65404440 8.91008113 5.47339490

10.19581409 3.98440012 5.47339490

8.91616173 7.05424482 4.42384453

7.45793141 2.12856381 4.42384453

3.44336172 7.05424482 4.42384453

1.98513141 2.12856381 4.42384453

6.16477817	5.32385880	3.37705773
4.70654786	0.39817779	3.37705773
11.63757817	5.32385880	3.37705773
10.17934786	0.39817779	3.37705773
8.85213564	3.26925706	2.18423498
4.83756595	8.19493807	2.18423498
3.37933564	3.26925706	2.18423498
10.31036595	8.19493807	2.18423498
7.58465674	8.10247454	1.99986387
6.12642643	3.17679353	1.99986387
13.05745674	8.10247454	1.99986387
11.59922643	3.17679353	1.99986387
7.41517833	7.19804643	10.85070551
5.95694802	2.27236543	10.85070551
12.88797833	7.19804643	10.85070551
11.42974802	2.27236543	10.85070551
8.64758887	2.26380259	10.84205292
4.63301918	7.18948360	10.84205292
3.17478887	2.26380259	10.84205292
10.10581918	7.18948360	10.84205292
8.68298402	4.77492230	10.61960547
4.66841434	9.70060330	10.61960547
3.21018402	4.77492230	10.61960547
10.14121434	9.70060330	10.61960547
7.40085242	9.73209893	10.52574638
5.94262210	4.80641793	10.52574638
12.87365242	9.73209893	10.52574638
11.41542210	4.80641793	10.52574638
8.78975245	8.23400849	8.86474812
7.33152214	3.30832749	8.86474812
3.31695245	8.23400849	8.86474812
1.85872214	3.30832749	8.86474812
6.06064062	8.25610073	8.86140783
4.60241031	3.33041973	8.86140783
11.53344062	8.25610073	8.86140783
10.07521031	3.33041973	8.86140783
7.32388407	6.01742230	8.44636323
5.86565376	1.09174129	8.44636323
1.85108407	6.01742230	8.44636323
0.39285376	1.09174129	8.44636323
8.61764163	1.09771184	8.42932316
4.60307195	6.02339284	8.42932316
3.14484163	1.09771184	8.42932316
10.07587195	6.02339284	8.42932316

7.54826274	9.44966250	6.72802327
6.09003243	4.52398149	6.72802327
13.02106274	9.44966250	6.72802327
11.56283243	4.52398149	6.72802327
8.82109357	4.51898944	6.70537141
4.80652388	9.44467045	6.70537141
3.34829357	4.51898944	6.70537141
10.27932388	9.44467045	6.70537141
6.05979860	7.21628821	6.36197433
4.60156828	2.29060720	6.36197433
11.53259860	7.21628821	6.36197433
10.07436828	2.29060720	6.36197433
8.79067986	7.21139122	6.33930088
7.33244954	2.28571021	6.33930088
3.31787986	7.21139122	6.33930088
1.85964954	2.28571021	6.33930088
8.81911022	0.78674274	4.63805664
4.80454053	5.71242375	4.63805664
3.34631022	0.78674274	4.63805664
10.27734053	5.71242375	4.63805664
7.55727780	5.71838543	4.62066149
6.09904749	0.79270443	4.62066149
2.08447780	5.71838543	4.62066149
0.62624749	0.79270443	4.62066149
8.82021301	3.47978425	4.20587525
4.80564333	8.40546526	4.20587525
3.34741301	3.47978425	4.20587525
10.27844332	8.40546526	4.20587525
7.54940773	8.42789950	4.20249926
6.09117742	3.50221850	4.20249926
13.02220773	8.42789950	4.20249926
11.56397742	3.50221850	4.20249926
8.93827423	6.93054899	2.54134577
7.48004392	2.00486799	2.54134577
3.46547423	6.93054899	2.54134577
2.00724392	2.00486799	2.54134577
6.19786617	6.96187760	2.44749202
4.73963586	2.03619660	2.44749202
11.67066617	6.96187760	2.44749202
10.21243586	2.03619660	2.44749202
6.23309397	9.47347000	2.22578799
4.77486366	4.54778900	2.22578799
11.70589397	9.47347000	2.22578799
10.24766366	4.54778900	2.22578799

8.92396109	9.46470958	2.21652769
7.46573078	4.53902858	2.21652769
3.45116109	9.46470958	2.21652769
1.99293078	4.53902858	2.21652769

# Fe<sub>7</sub>C<sub>3</sub>(071)

1.000000000000

9.92520000	0.00000000	0.00000000
0.00000006	35.68530000	0.00000000
0.00000004	0.00000004	22.83590000

C	Fe
104	224

Cart

8.26336538	21.24066367	7.59172788
3.30076538	21.24066367	7.59172788
5.94963745	3.41179813	7.59134295
0.98703745	3.41179813	7.59134295
9.04369778	34.01738290	7.48923946
4.08109778	34.01738290	7.48923946
5.16726094	16.14089067	7.44290395
0.20466095	16.14089067	7.44290395
9.01996622	23.89403096	7.43125701
4.05736622	23.89403096	7.43125701
5.19082608	6.05212919	7.36365754
0.22822608	6.05212919	7.36365754
5.98502975	28.92987343	7.33153213
1.02242975	28.92987343	7.33153213
8.23079223	11.06439611	7.24218480
3.26819223	11.06439611	7.24218480
7.71638684	18.65732592	6.61879414
2.75378684	18.65732592	6.61879414
6.49400736	0.82865618	6.61444674
1.53140736	0.82865618	6.61444674
8.49745900	31.40970482	6.38747464
3.53485900	31.40970482	6.38747464
6.51710079	26.23850534	6.35420596
1.55450079	26.23850534	6.35420596
5.71483196	13.54794023	6.31751887
0.75223195	13.54794023	6.31751887
7.69785709	8.37875306	6.25799731
2.73525709	8.37875306	6.25799731
8.94135981	2.34696426	5.77013822
3.97875981	2.34696426	5.77013822

5.27037859	20.17525213	5.76936190
0.30777859	20.17525213	5.76936190
6.03823606	32.94860877	5.65820369
1.07563606	32.94860877	5.65820369
8.17389662	15.07676733	5.59833441
3.21129662	15.07676733	5.59833441
8.98212214	27.78034703	5.42706081
4.01952214	27.78034703	5.42706081
5.23318172	9.91703369	5.33412877
0.27058172	9.91703369	5.33412877
7.74798269	22.76644283	4.53934559
2.78538269	22.76644283	4.53934559
6.46404511	4.90274983	4.46615249
1.50144511	4.90274983	4.46615249
8.52568972	35.47055436	4.27843838
3.56308972	35.47055436	4.27843838
5.68627566	17.62737041	4.27591615
0.72367566	17.62737041	4.27591615
6.47025795	30.29454763	4.06855897
1.50765795	30.29454763	4.06855897
7.74533481	12.43760244	3.99355861
2.78273481	12.43760244	3.99355861
5.26389769	24.27008098	3.84194806
0.30129769	24.27008098	3.84194806
8.95161105	6.41329904	3.76923447
3.98901105	6.41329904	3.76923447
6.04443627	1.23642718	3.56092490
1.08183627	1.23642718	3.56092490
8.16751626	19.07971660	3.55939224
3.20491626	19.07971660	3.55939224
8.94525255	31.80489869	3.37275897
3.98265255	31.80489869	3.37275897
5.26688885	13.94100003	3.29653154
0.30428885	13.94100003	3.29653154
7.71447398	26.79121873	2.50218212
2.75187398	26.79121873	2.50218212
6.50074765	8.92696367	2.40929494
1.53814765	8.92696367	2.40929494
5.69244858	21.63088854	2.23776017
0.72984858	21.63088854	2.23776017
8.51956025	3.75842252	2.18092976
3.55696025	3.75842252	2.18092976
6.46011556	34.36037323	2.06877628
1.49751556	34.36037323	2.06877628

7.75174215	16.53184786	2.06607582
2.78914215	16.53184786	2.06607582
5.21651826	28.32942525	1.57859967
0.25391826	28.32942525	1.57859967
8.19594949	23.15982144	1.51816510
3.23334949	23.15982144	1.51816510
8.99840217	10.46855759	1.48157489
4.03580217	10.46855759	1.48157489
6.01616274	5.29777343	1.45159515
1.05356274	5.29777343	1.45159515
8.97540140	0.19396098	1.22511777
4.01280140	0.19396098	1.22511777
5.23507690	18.04988382	1.21666097
0.27247690	18.04988382	1.21666097
5.74937142	25.64377628	0.59408316
0.78677142	25.64377628	0.59408316
8.46630186	7.77666259	0.50537537
3.50370186	7.77666259	0.50537537
7.67208009	30.65644344	0.47405166
2.70948009	30.65644344	0.47405166
6.53864023	12.81296917	0.40425393
1.57604023	12.81296917	0.40425393
7.64847389	20.56662211	0.39356358
2.68587389	20.56662211	0.39356358
6.56241686	2.68989851	0.35016159
1.59981686	2.68989851	0.35016159
8.43080506	33.29645583	0.24890513
3.46820506	33.29645583	0.24890513
5.78209034	15.46652774	0.24363810
0.81949034	15.46652774	0.24363810
9.19501216	19.67425369	7.31575829
4.23241216	19.67425369	7.31575829
5.01875478	1.84743037	7.31215532
0.05615478	1.84743037	7.31215532
9.90761336	22.20114239	7.31149161
4.94501336	22.20114239	7.31149161
9.26878777	4.35800617	7.26334073
4.30618777	4.35800617	7.26334073
5.71655837	24.72257107	7.25507708
0.75395837	24.72257107	7.25507708
8.49554940	6.87495425	7.17997263
3.53294940	6.87495425	7.17997263
4.98343754	32.41577265	7.16798640
0.02083754	32.41577265	7.16798640

9.22724984	14.54400424	7.10580140
4.26464984	14.54400424	7.10580140
7.43989589	22.86425793	7.08924902
2.47729589	22.86425793	7.08924902
6.73910809	20.28941580	7.07404062
1.77650809	20.28941580	7.07404062
7.46891501	2.46220705	7.06500679
2.50631501	2.46220705	7.06500679
5.03934465	27.33259306	7.06231826
0.07674465	27.33259306	7.06231826
6.77203487	5.02233299	7.04625858
1.80943487	5.02233299	7.04625858
9.28043798	29.79919061	7.04369238
4.31783798	29.79919061	7.04369238
9.17630291	9.46967993	6.97008982
4.21370291	9.46967993	6.97008982
9.89923058	11.92996550	6.95466227
4.93663057	11.92996550	6.95466227
5.72401444	34.80235612	6.94897921
0.76141444	34.80235612	6.94897921
8.48401641	16.93836661	6.92744520
3.52141641	16.93836661	6.92744520
7.53771637	33.04879171	6.91229316
2.57511637	33.04879171	6.91229316
8.23284331	25.49358588	6.86693585
3.27024331	25.49358588	6.86693585
6.67523959	15.17922090	6.85526089
1.71263959	15.17922090	6.85526089
8.20754158	35.56521395	6.82652550
3.24494158	35.56521395	6.82652550
7.51193947	27.95494682	6.81795081
2.54933947	27.95494682	6.81795081
6.00523440	17.69898686	6.80747346
1.04263440	17.69898686	6.80747346
6.78008789	30.54832747	6.80112944
1.81748789	30.54832747	6.80112944
5.98167538	7.64257308	6.78575303
1.01907539	7.64257308	6.78575303
6.70373881	10.09324148	6.72500601
1.74113881	10.09324148	6.72500601
7.43412574	12.68162805	6.71482518
2.47152574	12.68162805	6.71482518
9.20237203	23.70755159	5.40883292
4.23977203	23.70755159	5.40883292

5.01308409	5.84924183	5.34079770
0.05048409	5.84924183	5.34079770
8.51906088	21.15058790	5.31551985
3.55646088	21.15058790	5.31551985
5.69214006	3.30105448	5.27256198
0.72954006	3.30105448	5.27256198
5.69756799	28.84294734	5.15830260
0.73496799	28.84294734	5.15830260
9.19456437	18.62646459	5.14401833
4.23196437	18.62646459	5.14401833
5.01407532	0.79063028	5.14372568
0.05147532	0.79063028	5.14372568
6.76620888	24.38803935	5.09559788
1.80360888	24.38803935	5.09559788
8.51767395	10.97877432	5.06713038
3.55507395	10.97877432	5.06713038
6.04738790	21.81046530	5.03561645
1.08478790	21.81046530	5.03561645
7.44646670	6.52852373	5.02240202
2.48386670	6.52852373	5.02240202
4.99213186	26.09685947	5.01962713
0.02953186	26.09685947	5.01962713
9.29808661	33.84390270	5.00723842
4.33548661	33.84390270	5.00723842
8.16216096	3.96219150	4.99311053
3.19956096	3.96219150	4.99311053
9.87730749	15.99081977	4.98028184
4.91470749	15.99081977	4.98028184
5.02290261	31.37835041	4.97056882
0.06030261	31.37835041	4.97056882
9.22343633	8.23339209	4.92743347
4.26083633	8.23339209	4.92743347
6.73236597	19.14408188	4.92022572
1.76976597	19.14408188	4.92022572
7.48115977	1.30721115	4.91817255
2.51855977	1.30721115	4.91817255
9.19301749	13.51872762	4.89841728
4.23041749	13.51872762	4.89841728
8.17385672	29.48135796	4.78835126
3.21125672	29.48135796	4.78835126
7.48259254	31.90981063	4.73331811
2.51999254	31.90981063	4.73331811
6.04087025	11.61688293	4.69608790
1.07827025	11.61688293	4.69608790



7.44944627	26.80861236	4.67166383
2.48684627	26.80861236	4.67166383
6.72851437	14.05093327	4.66445448
1.76591437	14.05093327	4.66445448
6.82729959	34.44319555	4.65723262
1.86469959	34.44319555	4.65723262
7.38339249	16.58570119	4.62418127
2.42079249	16.58570119	4.62418127
6.76483435	8.94656675	4.57739116
1.80223435	8.94656675	4.57739116
9.24612251	27.76138426	3.25910494
4.28352251	27.76138426	3.25910494
9.86456216	20.12158333	3.21128671
4.90196216	20.12158333	3.21128671
9.30861026	2.26415712	3.18260004
4.34601026	2.26415712	3.18260004
9.20960370	22.65670644	3.17134211
4.24700371	22.65670644	3.17134211
4.96812105	9.89896532	3.16456211
0.00552105	9.89896532	3.16456211
8.52204736	25.09100083	3.13968419
3.55944736	25.09100083	3.13968419
5.00124143	4.79749282	3.10531621
0.03864143	4.79749282	3.10531621
5.69257026	7.22604701	3.04871129
0.72997026	7.22604701	3.04871129
6.71159581	23.18894458	2.93729548
1.74899581	23.18894458	2.93729548
4.99990924	35.39979044	2.92138045
0.03730924	35.39979044	2.92138045
9.21372593	17.56302896	2.91521417
4.25112593	17.56302896	2.91521417
6.74204497	28.47463470	2.90913909
1.77944497	28.47463470	2.90913909
7.50425460	5.32887441	2.86831169
2.54165460	5.32887441	2.86831169
7.39597179	20.71646460	2.85523456
2.43337179	20.71646460	2.85523456
5.68090947	32.74534134	2.84602191
0.71830947	32.74534134	2.84602191
6.81670303	2.86332060	2.83223207
1.85410303	2.86332060	2.83223207
7.47344171	10.61064888	2.81618637
2.51084171	10.61064888	2.81618637

4.96522166	30.17957856	2.81534406
0.00262166	30.17957856	2.81534406
8.52880696	14.89672144	2.79970311
3.56620696	14.89672144	2.79970311
6.03629228	25.72915613	2.76887183
1.07369228	25.72915613	2.76887183
9.24757282	12.31955036	2.73988200
4.28497282	12.31955036	2.73988200
7.49534593	0.23115104	2.69592866
2.53274593	0.23115104	2.69592866
6.71328750	18.08060457	2.69163520
1.75068750	18.08060457	2.69163520
8.17882182	7.86441356	2.67880713
3.21622182	7.86441356	2.67880713
8.17355319	33.40652885	2.56622865
3.21095319	33.40652885	2.56622865
6.03776926	15.55654963	2.51983408
1.07516926	15.55654963	2.51983408
7.49447047	30.85872780	2.49740260
2.53187047	30.85872780	2.49740260
6.72108247	12.99988577	2.42674709
1.75848247	12.99988577	2.42674709
9.91520623	24.02647141	1.12085827
4.95260623	24.02647141	1.12085827
9.18486310	26.61507501	1.11099576
4.22226310	26.61507501	1.11099576
8.46302203	29.06586399	1.05157884
3.50042203	29.06586399	1.05157884
9.26125082	6.15852872	1.03676506
4.29865082	6.15852872	1.03676506
8.48655503	19.00840676	1.02832298
3.52395503	19.00840676	1.02832298
5.03053336	8.75192622	1.01839912
0.06793336	8.75192622	1.01839912
5.72628028	1.14241981	1.01343597
0.76368028	1.14241981	1.01343597
9.15640808	21.52841037	0.98082174
4.19380808	21.52841037	0.98082174
5.75150579	11.21341412	0.96905873
0.78890579	11.21341412	0.96905873
5.05627707	3.65851226	0.92646483
0.09367707	3.65851226	0.92646483
6.00252709	19.76895149	0.90823467
1.03992709	19.76895149	0.90823467

8.20531329	1.90535789	0.89102977
3.24271329	1.90535789	0.89102977
7.41772911	24.77801068	0.88141165
2.45512911	24.77801068	0.88141165
6.69496438	27.23859892	0.86630283
1.73236438	27.23859892	0.86630283
6.79909621	6.90754397	0.79373447
1.83649621	6.90754397	0.79373447
9.25337364	31.68568046	0.79212444
4.29077364	31.68568046	0.79212444
4.98772202	34.24595881	0.77425502
0.02512202	34.24595881	0.77425502
7.52056862	9.37412534	0.77404343
2.55796862	9.37412534	0.77404343
9.22045720	16.41781149	0.76148585
4.25785720	16.41781149	0.76148585
9.92118156	13.84284058	0.74572871
4.95858156	13.84284058	0.74572871
6.74570336	22.16354408	0.72981889
1.78310336	22.16354408	0.72981889
7.46471165	4.29149954	0.67112838
2.50211165	4.29149954	0.67112838
6.01418540	29.83354399	0.65751782
1.05158540	29.83354399	0.65751782
8.19782662	11.98442810	0.58064855
3.23522662	11.98442810	0.58064855
6.78728120	32.35036763	0.57577869
1.82468120	32.35036763	0.57577869
7.50002418	34.86104532	0.52685124
2.53742418	34.86104532	0.52685124
7.42630252	14.50589511	0.52376553
2.46370252	14.50589511	0.52376553
6.71374497	17.03293803	0.51961822
1.75114497	17.03293803	0.51961822

# Fe<sub>5</sub>C<sub>2</sub>(510)

1.000000000000

9.97980000	0.00000000	0.00000000
-0.76395804	12.66177393	0.00000000
0.00000004	0.00000004	19.64040000

C	Fe
36	80

Cart

9.14727584	9.28801470	7.45666124
4.15737584	9.28801470	7.45666124
7.21803862	4.23686176	7.23123905
2.22813862	4.23686176	7.23123905
8.38448181	11.90871859	7.20680633
3.39458181	11.90871859	7.20680633
4.69062376	6.74122964	6.35755638
-0.29927624	6.74122964	6.35755638
6.68416213	1.58919618	6.17284615
1.69426213	1.58919618	6.17284615
7.16890187	8.28279426	5.62693824
2.17900187	8.28279426	5.62693824
9.19720083	3.12319649	5.29942408
4.20730083	3.12319649	5.29942408
4.67276826	10.79822941	4.25586957
-0.31713174	10.79822941	4.25586957
6.72418055	5.68025081	4.01882195
1.73428055	5.68025081	4.01882195
7.18376534	12.33997230	3.63601452
2.19386533	12.33997230	3.63601452
9.23116553	7.20425854	3.36082261
4.24126553	7.20425854	3.36082261
5.47292217	2.23055554	2.34193027
0.48302217	2.23055554	2.34193027
6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348
4.22357812	11.29064837	1.28800348
5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
8.21533226	7.73841306	7.13833245
3.22543226	7.73841306	7.13833245
7.49863634	10.21301439	7.07945162
2.50873634	10.21301439	7.07945162
7.48897156	0.06261249	7.04241447
2.49907156	0.06261249	7.04241447
8.88651243	5.12024068	6.97274926
3.89661243	5.12024068	6.97274926

4.98340989	10.89812518	6.91591333
-0.00649011	10.89812518	6.91591333
8.17060532	2.65533424	6.90961165
3.18070532	2.65533424	6.90961165
5.67854845	8.36980533	6.90196390
0.68864845	8.36980533	6.90196390
6.40834893	5.86477336	6.75357631
1.41844893	5.86477336	6.75357631
5.68653655	3.28130403	6.69114834
0.69663655	3.28130403	6.69114834
4.95879567	0.84138419	6.66590003
-0.03110433	0.84138419	6.66590003
8.22567818	11.73736681	5.18096541
3.23577818	11.73736681	5.18096541
8.88798741	9.20222016	5.06897254
3.89808741	9.20222016	5.06897254
7.50976442	4.20318010	5.05911156
2.51986442	4.20318010	5.05911156
8.18692726	6.72764271	4.94274967
3.19702726	6.72764271	4.94274967
5.66736900	12.41155385	4.89114397
0.67746900	12.41155385	4.89114397
8.20719200	1.46326591	4.83442296
3.21729200	1.46326591	4.83442296
6.38100766	9.87487060	4.80341903
1.39110766	9.87487060	4.80341903
5.71098065	7.27161609	4.72475739
0.72108065	7.27161609	4.72475739
5.01494479	4.84338766	4.71175888
0.02504479	4.84338766	4.71175888
5.74186255	2.18422383	4.51002444
0.75196255	2.18422383	4.51002444
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422

5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946
7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# Fe<sub>5</sub>C<sub>2</sub>(021)

1.000000000000

14.90600000	0.00000000	0.00000000
0.42323971	8.40334839	0.00000000
0.00000004	0.00000004	23.05140000

C	Fe
36	80

Cart

2.75646521	1.99626514	7.65560511
10.20946521	1.99626514	7.65560511
9.64700270	5.32959722	7.51000160
2.19400270	5.32959722	7.51000160
5.22986629	8.29276539	7.44564863
12.68286629	8.29276539	7.44564863

6.56138453	2.53673647	6.91688374
14.01438453	2.53673647	6.91688374
8.43273561	0.18709738	6.26556255
0.97973561	0.18709738	6.26556255
7.24885480	5.55160716	6.02103235
14.70185480	5.55160716	6.02103235
9.26233584	3.27987850	5.43731951
1.80933584	3.27987850	5.43731951
3.70732341	6.06579030	4.68927424
11.16032341	6.06579030	4.68927424
5.61106020	3.76776343	4.10395773
13.06406020	3.76776343	4.10395773
4.13102612	0.74511710	3.95206386
11.58402612	0.74511710	3.95206386
6.45910589	6.85157748	3.36946502
13.91210589	6.85157748	3.36946502
7.93326219	1.23396887	2.61950339
0.48026219	1.23396887	2.61950339
2.91558683	7.36299520	2.03468359
10.36858682	7.36299520	2.03468359
8.76163548	4.32674248	1.79040838
1.30863548	4.32674248	1.79040838
3.18085377	1.97663541	1.14063552
10.63385377	1.97663541	1.14063552
4.93311057	4.62204310	0.60898984
12.38611057	4.62204310	0.60898984
7.97210488	7.58761194	0.54751449
0.51910488	7.58761194	0.54751449
6.98546138	2.51763785	0.40115633
14.43846138	2.51763785	0.40115633
7.88178233	4.46920414	7.50119695
0.42878234	4.46920414	7.50119695
4.63486419	1.81891752	7.41730680
12.08786419	1.81891752	7.41730680
6.11543052	6.58807191	7.26021497
13.56843052	6.58807191	7.26021497
2.80096822	0.15230482	7.25002250
10.25396822	0.15230482	7.25002250
8.66825276	6.89952881	7.17834663
1.21525276	6.89952881	7.17834663
2.92251912	3.70772587	7.00846882
10.37551912	3.70772587	7.00846882
5.40389081	4.14171637	6.84938652
12.85689081	4.14171637	6.84938652

6.59133836	0.54671759	6.81963266
14.04433836	0.54671759	6.81963266
8.50960507	2.06343281	6.80839736
1.05660507	2.06343281	6.80839736
3.74410532	6.08189962	6.64940381
11.19710532	6.08189962	6.64940381
5.07039091	8.07346573	5.52693394
12.52339091	8.07346573	5.52693394
9.15923998	5.26831907	5.36941597
1.70623998	5.26831907	5.36941597
3.01603684	1.72679856	5.25191520
10.46903684	1.72679856	5.25191520
7.30423532	3.66739113	5.22668025
14.75723532	3.66739113	5.22668025
5.48194083	2.08152447	5.11808654
12.93494083	2.08152447	5.11808654
7.53235331	7.24923903	5.02331241
14.98535331	7.24923903	5.02331241
2.54947683	7.67295807	4.90352835
10.00247683	7.67295807	4.90352835
5.69399829	5.65366385	4.81242114
13.14699829	5.65366385	4.81242114
3.81125062	4.10779653	4.75386951
11.26425062	4.10779653	4.75386951
7.95020331	1.22586791	4.56230518
0.49720331	1.22586791	4.56230518
9.24510071	3.28775039	3.49441626
1.79210071	3.28775039	3.49441626
5.93108567	0.40572785	3.30346416
13.38408567	0.40572785	3.30346416
4.47159556	7.26234241	3.24290903
11.92459556	7.26234241	3.24290903
7.61672836	5.24388297	3.15383184
15.06972836	5.24388297	3.15383184
2.63376818	5.66717645	3.03582541
10.08676818	5.66717645	3.03582541
4.26076753	2.43179305	2.93866864
11.71376753	2.43179305	2.93866864
9.89125461	0.84577288	2.82996937
2.43825461	0.84577288	2.82996937
6.72640678	2.78669560	2.80400847
14.17940678	2.78669560	2.80400847
8.45943730	7.64924825	2.68994600
1.00643730	7.64924825	2.68994600



5.09631502	4.84222144	2.52809293
12.54931502	4.84222144	2.52809293
6.42297029	6.83616858	1.40942586
13.87597029	6.83616858	1.40942586
8.68565999	2.45029785	1.24810272
1.23265999	2.45029785	1.24810272
3.15018112	3.96655686	1.23820480
10.60318112	3.96655686	1.23820480
4.33920252	0.37170254	1.20792719
11.79220252	0.37170254	1.20792719
6.82007300	0.80580680	1.04853930
14.27307300	0.80580680	1.04853930
8.95301238	6.01934631	0.88174964
1.50001238	6.01934631	0.88174964
6.94090946	4.36216166	0.80574113
14.39390946	4.36216166	0.80574113
4.05270049	6.32821708	0.79609851
11.50570049	6.32821708	0.79609851
5.10706029	2.69428362	0.63864447
12.56006029	2.69428362	0.63864447
9.31387541	0.04532212	0.55626550
1.86087541	0.04532212	0.55626550

# Fe<sub>5</sub>C<sub>2</sub>(111)

1.000000000000

12.37300000	0.00000000	0.00000000
-2.07134726	13.30634571	0.00000000
0.00000004	0.00000005	22.12540000

C	Fe
64	136

Cart

-0.13578315	1.75836189	9.89400891
6.05071685	1.75836189	9.89400891
-1.17145679	8.41153474	9.89400891
5.01504321	8.41153474	9.89400891
3.01727758	3.87820615	9.82306628
9.20377758	3.87820615	9.82306628
1.98160394	10.53137900	9.82306628
8.16810394	10.53137900	9.82306628
-0.51487310	5.10367355	9.71998023
5.67162690	5.10367355	9.71998023
-1.55054674	11.75684640	9.71998023
4.63595326	11.75684640	9.71998023

3.06449542	0.19798554	9.35191432
9.25099542	0.19798554	9.35191432
2.02882178	6.85115839	9.35191432
8.21532178	6.85115839	9.35191432
0.58328012	5.76440303	6.94130397
6.76978012	5.76440303	6.94130397
-0.45239352	12.41757588	6.94130397
5.73410648	12.41757588	6.94130397
4.28060010	1.03828795	6.72359696
10.46710010	1.03828795	6.72359696
3.24492645	7.69146081	6.72359696
9.43142646	7.69146081	6.72359696
1.29617924	2.07658644	6.61351546
7.48267924	2.07658644	6.61351546
0.26050560	8.72975929	6.61351546
6.44700560	8.72975929	6.61351546
3.94034426	4.02802448	6.25968196
10.12684426	4.02802448	6.25968196
2.90467062	10.68119733	6.25968196
9.09117062	10.68119733	6.25968196
2.23426325	2.90143398	3.87051158
8.42076325	2.90143398	3.87051158
1.19858961	9.55460683	3.87051158
7.38508961	9.55460683	3.87051158
4.87882202	4.85300752	3.51646118
11.06532202	4.85300752	3.51646118
3.84314838	11.50618037	3.51646118
10.02964838	11.50618037	3.51646118
1.89422261	5.89129596	3.40647146
8.08072261	5.89129596	3.40647146
0.85854897	12.54446881	3.40647146
7.04504897	12.54446881	3.40647146
5.59163241	1.16514631	3.18918617
11.77813241	1.16514631	3.18918617
4.55595877	7.81831916	3.18918617
10.74245877	7.81831916	3.18918617
4.14716344	0.07805078	0.77799783
10.33366344	0.07805078	0.77799783
3.11148979	6.73122363	0.77799783
9.29798979	6.73122363	0.77799783
0.50349241	1.82555237	0.41000686
6.68999241	1.82555237	0.41000686
-0.53218123	8.47872522	0.41000686
5.65431877	8.47872522	0.41000686

3.15748166	3.05093246	0.30731283
9.34398166	3.05093246	0.30731283
2.12180802	9.70410531	0.30731283
8.30830802	9.70410531	0.30731283
0.12411259	5.17102453	0.23606260
6.31061259	5.17102453	0.23606260
-0.91156105	11.82419738	0.23606260
5.27493895	11.82419738	0.23606260
2.54354945	2.04107493	9.87759492
8.73004945	2.04107493	9.87759492
1.50787581	8.69424778	9.87759492
7.69437581	8.69424778	9.87759492
4.97311458	3.36040282	9.86635013
11.15961458	3.36040282	9.86635013
3.93744094	10.01357568	9.86635013
10.12394094	10.01357568	9.86635013
3.74450109	5.58053888	9.57944947
9.93100109	5.58053888	9.57944947
2.70882745	12.23371173	9.57944947
8.89532745	12.23371173	9.57944947
0.85516145	0.26007315	9.40128633
7.04166145	0.26007315	9.40128633
-0.18051219	6.91324600	9.40128633
6.00598781	6.91324600	9.40128633
1.44926387	4.98590244	9.00041041
7.63576387	4.98590244	9.00041041
0.41359023	11.63907530	9.00041041
6.6009023	11.63907530	9.00041041
4.65131801	1.17912878	8.67155996
10.83781801	1.17912878	8.67155996
3.61564437	7.83230163	8.67155996
9.80214437	7.83230163	8.67155996
0.68655618	2.60587114	8.39307442
6.87305618	2.60587114	8.39307442
-0.34911746	9.25904399	8.39307442
5.83738254	9.25904399	8.39307442
3.21661313	3.30777362	7.96096037
9.40311313	3.30777362	7.96096037
2.18093949	9.96094648	7.96096037
8.36743949	9.96094648	7.96096037
5.41769758	4.73125257	7.83073245
11.60419758	4.73125257	7.83073245
4.38202394	11.38442542	7.83073245
10.56852394	11.38442542	7.83073245

2.50003429	0.76105554	7.55254770
8.68653429	0.76105554	7.55254770
1.46436065	7.41422839	7.55254770
7.65086065	7.41422839	7.55254770
3.22677048	5.71337528	6.97885688
9.41327048	5.71337528	6.97885688
2.19109684	12.36654813	6.97885688
8.37759684	12.36654813	6.97885688
0.18780405	0.46711117	6.86282790
6.37430405	0.46711117	6.86282790
-0.84786959	7.12028403	6.86282790
5.33863041	7.12028403	6.86282790
5.33990828	2.65823955	6.45808026
11.52640828	2.65823955	6.45808026
4.30423464	9.31141240	6.45808026
10.49073464	9.31141240	6.45808026
1.32419325	4.06593715	6.34322142
7.51069325	4.06593715	6.34322142
0.28851960	10.71911001	6.34322142
6.47501960	10.71911001	6.34322142
3.05860575	2.30377879	5.60858490
9.24510575	2.30377879	5.60858490
2.02293211	8.95695164	5.60858490
8.20943211	8.95695164	5.60858490
5.37358463	5.05121233	5.39310502
11.56008463	5.05121233	5.39310502
4.33791099	11.70438518	5.39310502
10.52441099	11.70438518	5.39310502
1.34574291	6.42451242	5.24320976
7.53224291	6.42451242	5.24320976
0.31006927	13.07768527	5.24320976
6.49656927	13.07768527	5.24320976
4.82898434	0.50507162	4.88689076
11.01548434	0.50507162	4.88689076
3.79331070	7.15824447	4.88689076
9.97981070	7.15824447	4.88689076
0.80122125	1.87819923	4.73704658
6.98772125	1.87819923	4.73704658
-0.23445240	8.53137208	4.73704658
5.95204760	8.53137208	4.73704658
3.11612786	4.62592205	4.52159329
9.30262786	4.62592205	4.52159329
2.08045421	11.27909490	4.52159329
8.26695421	11.27909490	4.52159329

4.85071815	2.86369815	3.78704125
11.03721815	2.86369815	3.78704125
3.81504450	9.51687100	3.78704125
10.00154450	9.51687100	3.78704125
0.83500999	4.27133459	3.67187500
7.02150999	4.27133459	3.67187500
-0.20066365	10.92450745	3.67187500
5.98583635	10.92450745	3.67187500
-0.19919967	6.46236576	3.26705842
5.98730033	6.46236576	3.26705842
-1.23487332	13.11553862	3.26705842
4.95162668	13.11553862	3.26705842
2.94809040	1.21606319	3.15154011
9.13459040	1.21606319	3.15154011
1.91241676	7.86923604	3.15154011
8.09891676	7.86923604	3.15154011
3.67501746	6.16859693	2.57775972
9.86151746	6.16859693	2.57775972
2.63934382	12.82176978	2.57775972
8.82584382	12.82176978	2.57775972
0.75723333	2.19821796	2.29912548
6.94373333	2.19821796	2.29912548
-0.27844031	8.85139081	2.29912548
5.90805968	8.85139081	2.29912548
2.95838719	3.62169241	2.16933240
9.14488719	3.62169241	2.16933240
1.92271355	10.27486526	2.16933240
8.10921355	10.27486526	2.16933240
3.63175877	4.88769613	0.25251889
9.81825877	4.88769613	0.25251889
2.59608513	11.54086898	0.25251889
8.78258513	11.54086898	0.25251889
1.52397664	5.75025257	1.45817901
7.71047664	5.75025257	1.45817901
0.48830300	12.40342542	1.45817901
6.67480300	12.40342542	1.45817901
4.72550757	1.94347770	1.13008651
10.91200757	1.94347770	1.13008651
3.68983393	8.59665055	1.13008651
9.87633393	8.59665055	1.13008651
0.16853991	0.01628161	0.72841987
6.35503991	0.01628161	0.72841987
-0.86713374	6.66945447	0.72841987
5.31936626	6.66945447	0.72841987

2.43038744	1.34844888	0.55037775
8.61688744	1.34844888	0.55037775
1.39471380	8.00162173	0.55037775
7.58121380	8.00162173	0.55037775
5.48859604	4.32356104	1.73705692
11.67509604	4.32356104	1.73705692
4.45292240	10.97673389	1.73705692
10.63942240	10.97673389	1.73705692
1.20186109	3.56898680	0.26360171
7.38836109	3.56898680	0.26360171
0.16618745	10.22215965	0.26360171
6.35268745	10.22215965	0.26360171

# Fe<sub>3</sub>C(031)

1.000000000000

10.06780000	0.00000000	0.00000000
0.00000003	14.99310000	0.00000000
0.00000004	0.00000004	22.23570000

C	Fe
40	96

Cart

3.33581958	9.93901126	7.64939125
8.36972037	9.93901063	7.64939070
1.00723939	2.44462252	7.64296826
6.04113905	2.44462223	7.64296832
4.09987548	12.57827736	7.59312183
9.13377616	12.57827639	7.59312199
0.24223475	5.08232425	7.58627108
5.27613440	5.08232504	7.58627042
1.55427276	14.88784013	6.51050952
6.58817262	14.88784057	6.51050931
2.78834442	7.39325411	6.50878839
7.82224340	7.39325393	6.50878879
0.27700685	8.92490044	5.70293141
5.31090757	8.92490069	5.70293124
4.06478046	1.43171416	5.69941795
9.09868022	1.43171408	5.69941737
2.79551536	11.47365883	4.47116655
7.82941525	11.47365878	4.47116669
1.54419257	3.97942742	4.46364247
6.57809290	3.97942762	4.46364304
0.27751192	13.07533816	3.96566563
5.31141213	13.07533806	3.96566567

4.06180103	5.58181796	3.95859428
9.09569998	5.58181815	3.95859421
2.79130916	0.63184285	2.72906463
7.82520916	0.63184285	2.72906463
1.54535573	8.13231273	2.72313032
6.57925573	8.13231273	2.72313032
4.06785280	9.66406961	1.91907410
9.10175279	9.66406961	1.91907410
0.26797625	2.17058199	1.91625857
5.30187625	2.17058199	1.91625857
1.57854441	11.97409711	0.84189010
6.61244441	11.97409711	0.84189010
2.75741239	4.47900702	0.83368792
7.79131239	4.47900702	0.83368792
0.81482184	14.61165756	0.78635431
5.84872184	14.61165756	0.78635431
3.52061226	7.11864006	0.77661362
8.55451226	7.11864006	0.77661362
4.99272054	10.90808455	7.45929249
10.02661935	10.90808386	7.45929213
4.38344345	3.41245228	7.45227101
9.41734331	3.41245202	7.45227139
0.73919554	13.36828871	7.37315677
5.77309496	13.36828856	7.37315726
3.60246380	5.87152605	7.36719416
8.63636251	5.87152709	7.36719386
2.49549231	11.59067613	7.29625643
7.52939297	11.59067547	7.29625622
4.29175340	8.40794634	7.29762978
9.32565243	8.40794753	7.29762936
0.05078877	0.91302929	7.29553910
5.08468801	0.91302947	7.29553902
1.84678288	4.09584769	7.28888611
6.88068236	4.09584844	7.28888542
1.76916680	9.06501586	7.09663462
6.80306856	9.06501500	7.09663374
2.57377417	1.56934628	7.09320942
7.60767387	1.56934687	7.09320941
3.28092887	14.14715326	7.03007280
8.31482969	14.14715311	7.03007264
1.06120898	6.65106932	7.02509843
6.09511031	6.65106873	7.02509728
4.24111031	12.43045071	5.50781999
9.27501079	12.43045047	5.50782001

0.09967912	4.93627341	5.50026974
5.13357989	4.93627385	5.50027027
3.59702367	9.96990179	5.48542838
8.63092366	9.96990088	5.48542957
0.74429776	2.47557691	5.48067754
5.77819799	2.47557756	5.48067745
1.09206508	10.66750398	5.20539338
6.12596586	10.66750361	5.20539326
3.24819392	3.17384721	5.19977790
8.28209291	3.17384742	5.19977719
1.83325834	13.09087733	5.19546440
6.86715858	13.09087692	5.19546394
0.02955142	14.78429959	5.18800609
5.06345118	14.78429984	5.18800634
4.30992253	7.28889004	5.18494279
9.34382107	7.28889079	5.18494364
2.50684053	5.59547316	5.18838553
7.54074001	5.59547313	5.18838518
1.81344019	8.01474477	4.88585605
6.84734066	8.01474438	4.88585687
2.52677832	0.51859988	4.88620640
7.56067887	0.51860044	4.88620563
0.00918142	9.04103988	3.54266272
5.04308142	9.04103988	3.54266272
4.32987586	1.54505514	3.54207018
9.36377586	1.54505514	3.54207018
4.34845778	11.46142514	3.23901360
9.38235778	11.46142514	3.23901360
2.54830413	9.76696481	3.24620375
7.58220413	9.76696481	3.24620375
1.79143322	2.27329987	3.24228414
6.82533322	2.27329987	3.24228414
5.02409751	3.96758047	3.23083026
10.05799751	3.96758047	3.23083026
3.60822974	13.88251509	3.22705915
8.64212974	13.88251509	3.22705915
0.73003615	6.39000861	3.22002510
5.76393615	6.39000861	3.22002510
1.07754811	14.57939366	2.94978844
6.11144811	14.57939366	2.94978844
3.26006399	7.08647723	2.94436823
8.29396399	7.08647723	2.94436823
1.72237339	12.11856813	2.92840370
6.75627339	12.11856813	2.92840370



2.61565651	4.62633989	2.91964270
7.64955651	4.62633989	2.91964270
0.76246345	10.40605247	1.40558607
5.79636345	10.40605247	1.40558607
3.57397777	2.91102596	1.39963465
8.60787777	2.91102596	1.39963465
4.28322759	0.49661291	1.33552128
9.31712759	0.49661291	1.33552128
0.05220732	7.99454736	1.33009197
5.08610732	7.99454736	1.33009197
5.00888201	12.96122609	1.13939367
10.04278201	12.96122609	1.13939367
1.77243282	1.15037400	1.13561856
6.80633282	1.15037400	1.13561856
2.56385952	8.64926670	1.13208874
7.59775952	8.64926670	1.13208874
4.36085369	5.46748741	1.12869317
9.39475369	5.46748741	1.12869317
3.25199205	11.18562412	1.06188466
8.28589205	11.18562412	1.06188466
1.08420257	3.69017515	1.05508973
6.11810257	3.69017515	1.05508973
2.47195572	13.64442610	0.97683454
7.50585572	13.64442610	0.97683454
1.86463212	6.15024343	0.96754395
6.89853212	6.15024343	0.96754395

# Fe<sub>3</sub>C(102)

1.000000000000

11.01580000	0.00000000	0.00000000
0.00000002	13.40160000	0.00000000
0.00000004	0.00000004	22.47150000

C	Fe
40	96

Cart

1.37564716	5.80022161	8.41471010
1.37563651	12.50098697	8.41470400
9.36760871	4.01945311	8.23748215
9.36759180	10.72020255	8.23746658
9.36825265	7.60733221	8.23450124
9.36827215	0.90652815	8.23449547
4.28462302	5.67301387	8.22658995
4.28461931	12.37381983	8.22658823

3.33088310	9.16125800	7.61127661
3.33088579	2.46045397	7.61126931
6.33016399	9.18441580	6.91770692
6.33017864	2.48361892	6.91769269
7.67057147	5.81325179	6.82723255
7.67056789	12.51407372	6.82723025
10.72777154	5.81292686	6.26202819
10.72777553	12.51373203	6.26202770
9.78855866	9.16311855	5.35041846
9.78856854	2.46231909	5.35041718
3.10975807	5.80800754	4.78531914
3.10975462	12.50881198	4.78531704
1.76543348	9.15990695	4.79975795
1.76543696	2.45910416	4.79975471
6.09387890	5.81395018	4.26611105
6.09387890	12.51475018	4.26611105
5.16361487	9.16121344	3.32155531
5.16361487	2.46041344	3.32155531
8.21825661	9.16481899	2.76375622
8.21825661	2.46401899	2.76375622
9.56017274	5.83251587	2.68237725
9.56017274	12.53331587	2.68237725
1.54647672	5.81414400	1.97793262
1.54647672	12.51494400	1.97793262
0.58884206	9.02470272	1.35454480
0.58884206	2.32390272	1.35454480
6.51847017	4.25338048	1.35242224
6.51847017	10.95418048	1.35242224
6.52053362	7.37137265	1.35086732
6.52053362	0.67057265	1.35086732
3.50100755	9.15109508	1.15644596
3.50100755	2.45029508	1.15644596
8.79575018	5.81526301	8.42337478
8.79574436	12.51608033	8.42338340
2.77795541	7.04998593	8.15091685
2.77796846	0.34920023	8.15092239
2.72049347	4.49812420	8.14668871
2.72048387	11.19893433	8.14668669
6.17443279	5.82629268	8.13616750
6.17443259	12.52709244	8.13617297
7.50566076	3.72843210	7.85973994
7.50568282	10.42923475	7.85974278
7.50755231	7.91794239	7.84750483
7.50754124	1.21714944	7.84750859

0.10734122	7.04172073	7.80224786
0.10731408	0.34094238	7.80225726
0.10213552	4.56950324	7.79609260
0.10217619	11.27032360	7.79609496
4.90352008	3.72170682	7.52785357
4.90351595	10.42249566	7.52784874
4.92416866	7.94035330	7.49402541
4.92416572	1.23954838	7.49403145
1.37134810	9.13884852	7.49310384
1.37134936	2.43805126	7.49309944
9.80374388	9.16057405	7.32182944
9.80376414	2.45973279	7.32181799
4.32797284	5.82456049	6.32398876
4.32797584	12.52534107	6.32399468
1.67750366	5.80946162	6.15670560
1.67750114	12.51023798	6.15670494
9.13458188	7.03106837	6.15033815
9.13458093	0.33026675	6.15032679
9.13300630	4.59401203	6.14874246
9.13300671	11.29478414	6.14874888
2.97383089	7.94632810	5.84693672
2.97383484	1.24552505	5.84693530
2.97430699	3.67835786	5.83409573
2.97430151	10.37914820	5.83409253
6.51953095	7.03332918	5.78067673
6.51403495	4.58572114	5.78666134
6.51403287	11.28651200	5.78665838
6.51953190	0.33252473	5.78066613
7.80184787	9.16452367	5.51917302
7.80183483	2.46372610	5.51916701
0.34938760	7.93862650	5.49587250
0.35206056	3.68611592	5.49989709
0.34938228	1.23781758	5.49587034
0.35206378	10.38690228	5.49989664
5.19930282	9.16455165	5.24876448
5.19930100	2.46375488	5.24876578
10.69425130	5.81395018	4.34699416
10.69425130	12.51475018	4.34699416
4.52206473	7.03530500	4.07911354
4.52206473	4.59259537	4.07911354
4.52206473	11.29339537	4.07911354
4.52206473	0.33450500	4.07911354
8.06567304	5.81395018	4.06464897
8.06567304	12.51475018	4.06464897

9.37696287	7.94299537	3.78912746
9.37696287	3.68490500	3.78912746
9.37696287	1.24219537	3.78912746
9.37696287	10.38570500	3.78912746
1.91001427	7.02113783	3.74295779
1.91001427	0.32033783	3.74295779
1.90148330	4.59789475	3.73080103
1.90148330	11.29869475	3.73080103
6.75760949	7.94480470	3.43389642
6.75760949	1.24400470	3.43389642
6.75540514	3.67919854	3.43265677
6.75540514	10.37999854	3.43265677
3.20063016	9.15871133	3.42493280
3.20063016	2.45791133	3.42493280
0.55113074	9.17330823	3.25715287
0.55113074	2.47250823	3.25715287
6.07962203	5.81109571	2.26416255
6.07962203	12.51189571	2.26416255
10.96803149	4.59199304	2.08241646
10.96803149	11.29279304	2.08241646
3.50234206	5.78909201	2.07739244
3.50234206	12.48989201	2.07739244
10.98624651	7.07002148	2.05453286
10.98624651	0.36922148	2.05453286
4.76950123	7.92010060	1.78491966
4.76950123	1.21930060	1.78491966
4.76405426	3.68990979	1.78023999
4.76405426	10.39070979	1.78023999
8.38025972	4.57472405	1.73071469
8.38025972	11.27552405	1.73071469
8.38388660	7.07043256	1.72176306
8.38388660	0.36963256	1.72176306
9.71496361	9.17632898	1.45127758
9.71496361	2.47552898	1.45127758
2.15475452	7.85452439	1.43979469
2.15475452	1.15372439	1.43979469
2.09838193	3.69581854	1.43469210
2.09838193	10.39661854	1.43469210
7.10175299	9.16563392	1.17035198
7.10175299	2.46483392	1.17035198

# Fe<sub>3</sub>C(131)

1.000000000000

12.25530000	0.00000000	0.00000000
-2.38850589	13.25166596	0.00000000
0.00000004	0.00000005	21.25600000

C	Fe
44	96

Cart

3.36503574	3.83424369	8.00177389
2.17078396	10.46004855	8.00175233
10.23824610	1.73393696	7.51389319
9.04399979	8.35974993	7.51388395
9.63361249	5.11765372	7.37708129
8.43936217	11.74348327	7.37706679
6.15933762	6.11830451	7.16127228
4.96510978	12.74414918	7.16127040
7.56444532	2.36544630	7.06717591
6.37019664	8.99125538	7.06717162
0.40189381	4.40720962	6.72726223
-0.79228377	11.03304265	6.72727510
0.72431665	1.34286868	6.71874525
-0.46994442	7.96869588	6.71873464
4.43284161	4.54432237	5.45083847
3.23858857	11.17015081	5.45084914
4.69920826	1.46983596	5.28991512
3.50494896	8.09565525	5.28991296
10.65320815	0.21186723	5.01276769
9.45895527	6.83769533	5.01276555
9.61846119	3.80479526	4.77013542
8.42420410	10.43062477	4.77014350
2.31291199	0.37301423	3.71090216
1.11865903	6.99884720	3.71090216
1.32024334	3.98045099	3.48570282
0.12599038	10.60628397	3.48570282
7.25680802	2.63475377	3.27525191
6.06255506	9.26058675	3.27525191
6.27615511	6.19979709	3.10429905
5.08190215	12.82563007	3.10429905
11.15591252	2.80662531	1.85426262
9.96165956	9.43245829	1.85426262
10.26668183	6.36503691	1.84332589
9.07242887	12.99086989	1.84332589
4.11546359	4.99648765	1.50322899
2.92121063	11.62232062	1.50322899
4.31588449	1.85071793	1.48528657
3.12163153	8.47655091	1.48528657

1.00381878	5.67873004	1.17111504
-0.19043418	12.30456301	1.17111504
1.64606686	2.42555158	1.06123795
0.45181390	9.05138456	1.06123795
8.50365986	0.27873533	0.54604718
7.30940690	6.90456830	0.54604718
2.16190112	2.33734436	7.74615936
0.96765824	8.96316640	7.74615610
-0.42476597	2.69718585	7.48863817
-1.61901866	9.32300000	7.48864217
3.95234273	0.42995750	7.35118106
2.75809310	7.05578633	7.35116473
4.52413284	5.24714129	7.28558868
3.32986667	11.87294376	7.28560510
9.19448616	3.29192687	7.34088309
8.00023959	9.91777305	7.34087469
0.36394297	6.30914682	7.14437418
-0.83031625	12.93498676	7.14437875
11.20431999	0.24958486	6.92672377
10.01006184	6.87544066	6.92672594
6.61212664	3.96874573	6.91457972
5.41785483	10.59456252	6.91455907
2.23627848	4.65047283	6.81441761
1.04198287	11.27628836	6.81444134
8.65098378	0.81255322	6.84313452
7.45674464	7.43837999	6.84312787
4.25896632	2.86946856	6.65484819
3.06468811	9.49531722	6.65487343
6.23441947	1.12910738	6.52662671
5.04016441	7.75493100	6.52661356
10.93189035	4.64780484	6.02170638
9.73756748	11.27364484	6.02169801
8.48485738	5.20319997	5.78753085
7.29061122	11.82903018	5.78754055
0.80112390	2.96104006	5.48200484
-0.39312250	9.58686523	5.48200336
2.62809933	1.26469459	5.49607171
1.43383908	7.89052565	5.49606020
10.47862991	2.15622514	5.39675138
9.28437936	8.78205920	5.39674514
6.00890710	5.70364611	5.29925703
4.81465230	12.32947528	5.29926040
7.98953482	2.70450427	5.15620900
6.79528382	9.33032518	5.15619280

3.35182423	6.14719646	5.11424508
2.15757518	12.77302567	5.11426491
0.34298360	0.48706657	4.93275138
-0.85126403	7.11289765	4.93274488
0.92305550	5.36917480	4.81770441
-0.27119032	11.99500223	4.81770685
5.57365025	3.16513254	4.65288804
4.37940483	9.79096065	4.65287297
2.97787761	3.66058054	4.44366890
1.78361708	10.28641186	4.44367366
8.92109347	0.48566630	4.12896801
7.72684257	7.11149732	4.12895599
6.34998212	0.96901608	3.95198499
5.15572821	7.59485026	3.95197802
9.76671039	5.40936247	3.71097645
8.57245743	12.03519544	3.71097645
-0.65484260	3.68870680	3.62123843
-1.84909556	10.31453978	3.62123843
7.30014230	4.57573596	3.45908970
6.10588934	11.20156893	3.45908970
3.94268519	1.50069597	3.44737102
2.74843223	8.12652895	3.44737102
4.69885086	5.05109938	3.28788573
3.50459791	11.67693236	3.28788573
1.40509240	2.01450321	3.18216970
0.21083944	8.64033618	3.18216970
9.28441439	2.89875797	3.07764541
8.09016143	9.52459094	3.07764541
11.10470670	1.19581732	3.08856476
9.91045374	7.82165029	3.08856476
2.27633666	5.56089735	2.69547478
1.08208370	12.18673033	2.69547478
-0.23673893	6.12739290	2.55241003
-1.43099189	12.75322587	2.55241003
5.68936019	2.97972054	2.12121331
4.49510723	9.60555352	2.12121331
7.63962321	1.24280357	1.88798441
6.44537026	7.86863654	1.88798441
3.21765000	3.35256592	1.74998804
2.02339705	9.97839890	1.74998804
8.41606614	6.08661360	1.74018732
7.22181318	12.71244657	1.74018732
5.30755531	0.30048524	1.67762645
4.11330235	6.92631822	1.67762645

0.66523143	3.91109670	1.60902896
-0.52902153	10.53692967	1.60902896
10.31909699	4.46215435	1.41221317
9.12484403	11.08798732	1.41221317
2.69262559	0.87311534	1.25545245
1.49837263	7.49894831	1.25545245
6.08439118	5.48753317	1.23569618
4.89013822	12.11336615	1.23569618
7.91476177	3.69234291	1.22194364
6.72050881	10.31817589	1.22194364
0.06142718	1.44478720	1.08450753
-1.13282577	8.07062017	1.08450753
9.73022084	1.78445990	0.82899424
8.53596788	8.41029287	0.82899424

# Fe<sub>5</sub>C<sub>2</sub>(510) step

1.000000000000

9.97980000	0.00000000	0.00000000
-0.76395804	12.66177393	0.00000000
0.00000004	0.00000004	19.64040000

C	Fe
36	77

Cart

4.69256664	1.87006002	7.57905530
5.50640881	9.29920613	7.49868099
7.18747223	4.11863741	7.13240407
2.18313815	4.17890081	7.16702176
2.98250097	6.82887457	7.12053827
7.87917096	6.82579068	7.09071060
4.57851059	11.95829075	6.66404757
2.61474404	10.06564558	6.09253694
1.92046633	1.27293365	6.29481212
7.69016318	10.06840444	6.10406467
8.09741710	0.41968874	6.60520266
0.40706299	8.77525869	5.96296997
4.16146519	3.11775619	5.22313061
9.16608118	3.09579603	5.22233835
-0.31152314	10.88365217	4.25587159
4.70445978	10.62824800	4.15255738
6.70764085	5.63412921	4.03791096
1.70671187	5.66262167	4.02072069
2.22800749	12.34156604	3.67857502
7.19601255	12.33664160	3.64559526



4.22291572	7.22554656	3.47352448
9.20777785	7.20041201	3.40964648
5.47292217	2.23055554	2.34193027
0.48302217	2.23055554	2.34193027
6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348
4.22357812	11.29064837	1.28800348
5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
4.01084754	10.30322941	7.25002068
3.74453527	0.34432819	7.06542532
6.34126277	11.05079580	6.95975493
3.85033199	5.17127061	6.98018613
8.80515823	5.10651817	6.98961404
-0.39234560	7.48621558	6.97662614
4.63624703	7.71103152	6.93551634
8.18524624	2.53151605	6.90906710
3.15572832	2.66048368	6.87267185
1.36189713	5.81839917	6.80347871
6.32908613	5.80989267	6.76893045
6.98453919	8.44951662	6.72808780
5.57376140	3.31093633	6.73455804
0.62452769	3.25849329	6.66759483
2.09438309	8.35294560	6.60915661
0.03951291	0.82136134	6.62897036
6.24731227	0.90177425	6.94608666
8.17705976	11.69143213	5.27943562
3.28484671	11.54108048	5.18782607
2.48395874	4.17867786	5.04420109
7.46474522	4.10530032	5.07855566
3.13420185	6.66183185	5.03751974
8.11705522	6.68194634	5.02836166
5.64516117	12.29979529	4.89553037
8.88600194	9.21958836	4.96946201
0.73749003	12.38043584	4.98792496
3.85712411	9.06117408	4.88050473
3.25050144	1.40438602	4.82035485

8.18681994	1.40760357	4.86370036
1.32101196	9.86788724	4.72193418
-0.00547674	4.85260603	4.73463815
5.71366038	7.30885069	4.75267864
4.99189109	4.85314066	4.72226020
0.69337712	7.29041830	4.70695187
6.41253044	9.74667826	4.61159085
0.77864569	2.13929695	4.53170577
5.78199824	2.18342006	4.53146872
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422
5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946

1.41918241	7.83185195	0.60482946
7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

## 2. TS sampling for CO dissociation

# TS for CO dissociation on Fe<sub>2</sub>C(111) without a C<sub>v</sub>

1.000000000000

10.94560000	0.00000000	0.00000000
2.91646047	9.85136206	0.00000000
0.00000004	0.00000003	22.33820000

C	O	Fe
45	1	80

Cart

4.57273985	3.51389668	10.90406726
7.28158549	1.44625942	9.68203580
3.30941314	6.47033027	9.71393369
6.01426210	8.59001063	10.73877577
10.05194169	3.55104871	10.88002496
5.99843242	6.20861245	11.69178106
1.81459485	3.67142354	11.07398325
12.90226841	9.60907519	8.64258421
7.33428039	3.57522769	11.03649843
8.66736857	6.46711218	9.71698169
11.50934002	8.44434067	10.88907991
8.75059834	8.55486749	11.10804299
1.79038154	1.50839546	9.68123608
7.45017234	9.63589613	8.61834778
5.97032609	4.69691139	8.67531333
3.28790953	8.58296992	11.14564498
11.44778982	4.69805875	8.64158114
8.69967527	2.83791223	7.60522600
4.68485413	7.76517367	7.57814330
3.23627853	2.85392170	7.60569260
10.16823829	7.74805357	7.60604443
7.43816529	5.86362844	6.53201566
5.98788430	0.94549656	6.52298106
1.96854243	5.87439542	6.53687334
0.51022174	0.95057753	6.53188749
6.18124437	8.91008091	5.47339487
4.72301388	3.98440003	5.47339487
11.65404415	8.91008091	5.47339487

10.19581413	3.98440003	5.47339487
8.91616154	7.05424500	4.42384434
7.45793152	2.12856388	4.42384434
3.44336176	7.05424500	4.42384434
1.98513138	2.12856388	4.42384434
6.16477823	5.32385874	3.37705779
4.70654774	0.39817780	3.37705779
11.63757801	5.32385874	3.37705779
10.17934799	0.39817780	3.37705779
8.85213566	3.26925707	2.18423510
4.83756590	8.19493771	2.18423510
3.37933564	3.26925707	2.18423510
10.31036568	8.19493771	2.18423510
7.58465672	8.10247421	1.99986386
6.12642622	3.17679358	1.99986386
13.05745697	8.10247421	1.99986386
11.59922600	3.17679358	1.99986386
4.56289975	2.15194188	12.08192717
10.08365349	7.18938920	10.87010396
3.10052119	2.28539354	10.89586015
4.69917523	7.21924287	10.88860115
8.68354909	2.24799348	10.83076684
10.15471208	9.67092440	10.63210808
5.96365703	4.75802843	10.64013609
11.42992768	2.28240435	10.84572524
12.93333537	7.21332211	10.87285922
6.02529001	2.21954147	10.88088424
7.44483847	9.73218394	10.49775714
11.40941783	4.82684761	10.52219679
12.86914373	9.73183622	10.53190014
11.54598518	8.24740533	8.87775087
3.22057895	4.80837247	10.61083861
4.60650803	9.71198759	10.57075249
8.69418070	4.79368285	10.60909410
8.79653572	8.24179063	8.85077038
7.32422857	3.30644916	8.88278654
1.87237810	3.33037788	8.87957112
3.32233178	8.24264404	8.84033289
6.07924465	8.29943270	8.80200216
4.61887593	3.33015857	8.89539820
7.31988023	7.20846596	10.89283755
10.07706824	3.35285595	8.86519890
7.32480964	6.01818912	8.43906620
5.88945821	1.10175341	8.42763112

0.39897540	1.09560022	8.44315366
1.89084698	6.01741074	8.46164231
8.63413670	1.09775510	8.41701143
4.61476747	6.02614596	8.40939700
3.14857946	1.11793340	8.40643688
10.06111450	6.02580083	8.45754824
7.55431960	9.45497928	6.71111627
6.08738219	4.52029719	6.74210357
13.02631157	9.45152497	6.72356219
11.56505677	4.53552714	6.73227507
8.82468409	4.52319625	6.70712039
4.81433388	9.46103144	6.69864709
3.35762819	4.53287869	6.70676041
10.28468232	9.44368542	6.70783377
6.05616091	7.21082826	6.35022747
4.60165675	2.29686215	6.37094463
11.53053817	7.21689488	6.37172748
10.06964665	2.29381298	6.37018566
8.79437814	7.20824976	6.34838694
7.33727353	2.28939891	6.34478588
3.31501351	7.21400646	6.34198902
1.86134821	2.29783041	6.34572534
8.81910992	0.78674275	4.63805676
4.80454063	5.71242380	4.63805676
3.34631014	0.78674275	4.63805676
10.27734089	5.71242380	4.63805676
7.55727768	5.71838522	4.62066126
6.09904766	0.79270440	4.62066126
2.08447790	5.71838522	4.62066126
0.62624747	0.79270440	4.62066126
8.82021332	3.47978425	4.20587540
4.80564356	8.40546513	4.20587540
3.34741306	3.47978425	4.20587540
10.27844334	8.40546513	4.20587540
7.54940796	8.42789936	4.20249939
6.09117746	3.50221849	4.20249939
13.02220726	8.42789936	4.20249939
11.56397724	3.50221849	4.20249939
8.93827438	6.93054914	2.54134583
7.48004389	2.00486803	2.54134583
3.46547413	6.93054914	2.54134583
2.00724387	2.00486803	2.54134583
6.19786596	6.96187782	2.44749212
4.73963594	2.03619671	2.44749212

11.67066574	6.96187782	2.44749212
10.21243572	2.03619671	2.44749212
6.23309374	9.47346973	2.22578788
4.77486372	4.54778910	2.22578788
11.70589352	9.47346973	2.22578788
10.24766350	4.54778910	2.22578788
8.92396069	9.46470928	2.21652770
7.46573067	4.53902865	2.21652770
3.45116115	9.46470928	2.21652770
1.99293077	4.53902865	2.21652770

# TS for CO dissociation on Fe<sub>2</sub>C(111) with a C<sub>v</sub>

1.000000000000

10.94560000	0.00000000	0.00000000
2.91646047	9.85136206	0.00000000
0.00000004	0.00000003	22.33820000

C	O	Fe
44	1	80

Cart

7.30390540	3.71084583	11.15345096
11.51915944	8.47893203	10.88801154
6.05515167	8.40822600	10.87694503
1.84230643	3.62917343	11.06820409
8.77800228	8.52172255	11.07726504
4.58043448	3.52166462	10.88520662
3.29551488	8.57862694	11.06825898
10.07417679	3.53848166	10.88473026
8.74257555	6.40955432	9.65347504
7.27948244	1.50009124	9.70479365
3.24863670	6.40969173	9.68223719
1.81063820	1.47242098	9.68918589
7.44314163	9.59350079	8.65226972
5.97637845	4.68805798	8.63384977
12.90926091	9.61144564	8.63467465
11.45580490	4.67280918	8.63677018
8.71167690	2.83937405	7.60825406
4.69702263	7.75394038	7.60050058
3.24515941	2.82591237	7.60299757
10.16906773	7.76315508	7.59603607
7.44431077	5.86785965	6.52630980
5.98747834	0.94204342	6.53672864
1.97513782	5.86946138	6.53213741
0.51845798	0.94374265	6.53154641
6.18124437	8.91008091	5.47339487

4.72301388	3.98440003	5.47339487
11.65404415	8.91008091	5.47339487
10.19581413	3.98440003	5.47339487
8.91616154	7.05424500	4.42384434
7.45793152	2.12856388	4.42384434
3.44336176	7.05424500	4.42384434
1.98513138	2.12856388	4.42384434
6.16477823	5.32385874	3.37705779
4.70654774	0.39817780	3.37705779
11.63757801	5.32385874	3.37705779
10.17934799	0.39817780	3.37705779
8.85213566	3.26925707	2.18423510
4.83756590	8.19493771	2.18423510
3.37933564	3.26925707	2.18423510
10.31036568	8.19493771	2.18423510
7.58465672	8.10247421	1.99986386
6.12642622	3.17679358	1.99986386
13.05745697	8.10247421	1.99986386
11.59922600	3.17679358	1.99986386
7.24948518	5.24067046	11.93280849
10.14856533	7.18904703	10.82552525
5.99763977	2.28495129	10.87026319
4.61254604	7.19842905	10.84350500
11.45380878	2.26490974	10.84119058
8.66505601	2.27935952	10.84665815
7.44558125	7.09753407	10.95460188
3.18635918	2.25532954	10.85046327
12.90190379	7.20693580	10.83800772
8.75425039	4.82282859	10.67611019
7.41467748	9.66659631	10.53826072
3.22296608	4.77304063	10.61578078
12.88805717	9.74870711	10.51963063
10.14822401	9.69460078	10.62753851
5.88227113	4.83042433	10.51473392
4.70887297	9.68620775	10.62226416
11.44303802	4.80996027	10.52040851
8.80164458	8.21689940	8.87469077
7.34276678	3.31801567	8.85981641
1.86002767	6.01538718	8.44221743
0.41178469	1.09146343	8.44429131
6.08302210	8.23830996	8.87254274
4.62083075	3.33031943	8.86420313
11.54372055	8.27123513	8.86318499
10.09168799	3.33564276	8.87349349

7.34124846	6.02418177	8.43046058
5.88688095	1.08281635	8.45706422
1.87260300	3.29665211	8.86358922
3.32481783	8.23659302	8.85897512
8.63154408	1.10344073	8.43048932
4.60933064	6.02172757	8.42355902
3.17123673	1.08793030	8.43224638
10.10048474	6.02294575	8.40939897
7.55708689	9.44617473	6.72939219
6.09663429	4.52504736	6.72068910
13.03019066	9.45450768	6.71760662
11.57578616	4.51983497	6.71789854
8.82967336	4.52223734	6.70287008
4.81649467	9.44729477	6.70800598
3.35440443	4.51846007	6.70202435
10.28680059	9.44996687	6.70356959
6.06223661	7.21600098	6.36441778
4.60955066	2.28866934	6.36771144
11.53659087	7.21666964	6.36581770
10.07927486	2.29074733	6.37024084
8.79600183	7.21364031	6.34416714
7.33962134	2.28679198	6.34787004
3.32628251	7.21167474	6.34380481
1.87073966	2.28483654	6.34546424
8.81910992	0.78674275	4.63805676
4.80454063	5.71242380	4.63805676
3.34631014	0.78674275	4.63805676
10.27734089	5.71242380	4.63805676
7.55727768	5.71838522	4.62066126
6.09904766	0.79270440	4.62066126
2.08447790	5.71838522	4.62066126
0.62624747	0.79270440	4.62066126
8.82021332	3.47978425	4.20587540
4.80564356	8.40546513	4.20587540
3.34741306	3.47978425	4.20587540
10.27844334	8.40546513	4.20587540
7.54940796	8.42789936	4.20249939
6.09117746	3.50221849	4.20249939
13.02220726	8.42789936	4.20249939
11.56397724	3.50221849	4.20249939
8.93827438	6.93054914	2.54134583
7.48004389	2.00486803	2.54134583
3.46547413	6.93054914	2.54134583
2.00724387	2.00486803	2.54134583



6.19786596	6.96187782	2.44749212
4.73963594	2.03619671	2.44749212
11.67066574	6.96187782	2.44749212
10.21243572	2.03619671	2.44749212
6.23309374	9.47346973	2.22578788
4.77486372	4.54778910	2.22578788
11.70589352	9.47346973	2.22578788
10.24766350	4.54778910	2.22578788
8.92396069	9.46470928	2.21652770
7.46573067	4.53902865	2.21652770
3.45116115	9.46470928	2.21652770
1.99293077	4.53902865	2.21652770

# TS for CO dissociation on Fe<sub>2</sub>C(111) with a C<sub>v</sub>

1.000000000000

10.94560000	0.00000000	0.00000000
2.91646047	9.85136206	0.00000000
0.00000004	0.00000003	22.33820000

C	O	Fe
44	1	80

Cart

7.33256235	3.67285722	11.07527726
11.52983131	8.46370972	10.88127284
6.04322341	8.44656522	10.87561914
1.82958578	3.66213136	11.06717534
8.79139211	8.55596571	11.05652783
4.60183921	3.58253317	10.90564285
3.30193478	8.56863193	11.06771630
10.06700302	3.55224341	10.88103140
8.74773805	6.41260019	9.67362392
7.28227283	1.49010571	9.70162199
3.26919118	6.42196811	9.66632136
1.81114173	1.49008369	9.69896613
7.44465311	9.61506332	8.64125923
5.97871076	4.67863792	8.63695982
12.91658394	9.61325907	8.63400533
11.46689460	4.67845724	8.63137583
8.71300731	2.83507383	7.60207042
4.70242544	7.76279224	7.59022537
3.24637649	2.83880559	7.60806760
10.17573626	7.75847933	7.59370511
7.44920152	5.86957686	6.52982492
5.99256546	0.94835427	6.53428037

1.97939738	5.86975832	6.52931460
0.52129101	0.95010570	6.53246776
6.18124437	8.91008091	5.47339487
4.72301388	3.98440003	5.47339487
11.65404415	8.91008091	5.47339487
10.19581413	3.98440003	5.47339487
8.91616154	7.05424500	4.42384434
7.45793152	2.12856388	4.42384434
3.44336176	7.05424500	4.42384434
1.98513138	2.12856388	4.42384434
6.16477823	5.32385874	3.37705779
4.70654774	0.39817780	3.37705779
11.63757801	5.32385874	3.37705779
10.17934799	0.39817780	3.37705779
8.85213566	3.26925707	2.18423510
4.83756590	8.19493771	2.18423510
3.37933564	3.26925707	2.18423510
10.31036568	8.19493771	2.18423510
7.58465672	8.10247421	1.99986386
6.12642622	3.17679358	1.99986386
13.05745697	8.10247421	1.99986386
11.59922600	3.17679358	1.99986386
4.59383778	2.23698594	12.09931442
10.13485224	7.18310496	10.83877774
6.05285832	2.30345808	10.89984954
4.64418785	7.18712750	10.84025270
11.44031446	2.27495174	10.84035423
8.68190836	2.26891751	10.84260487
7.44832775	7.19847601	10.83287350
3.13874391	2.27686975	10.90297934
12.91995415	7.20575822	10.83124549
8.71814580	4.78753917	10.61208069
7.41413035	9.71287251	10.52925114
3.22589321	4.79782403	10.60004299
12.89599789	9.74482672	10.51747077
10.17657569	9.68653749	10.59770684
5.97290909	4.85053884	10.51579552
4.68814592	9.68780264	10.60031096
11.42944550	4.82786656	10.51584258
8.80635649	8.23462924	8.85841416
7.34067510	3.30260916	8.86279991
1.87254874	6.01718569	8.43734504
0.42108946	1.09073712	8.44616720
6.08560245	8.25788995	8.85896180

4.62377945	3.31787673	8.89221126
11.55694359	8.26174505	8.85771817
10.09887431	3.33760964	8.85948877
7.34738303	6.01270666	8.43939711
5.89534772	1.08662245	8.44608122
1.88157612	3.30685122	8.88266812
3.33615701	8.24039858	8.85281895
8.63654896	1.09882009	8.42737386
4.62224564	6.02387659	8.40357929
3.16192440	1.09859629	8.42440920
10.10240398	6.02160783	8.41238489
7.55991360	9.45437050	6.71967591
6.10107467	4.52278092	6.72025871
13.03173673	9.45890454	6.71681080
11.57982638	4.52014309	6.71631516
8.83193157	4.52350232	6.70335940
4.81914137	9.45468034	6.70220085
3.36354005	4.52302663	6.70628445
10.29114151	9.45107754	6.70351483
6.06852690	7.21717764	6.36225832
4.60614437	2.29091000	6.36685664
11.54189992	7.21684870	6.36348896
10.07989202	2.29160515	6.36896292
8.79971656	7.21459043	6.34340807
7.34427952	2.28845785	6.34431542
3.32494665	7.21709703	6.34242856
1.87392698	2.28984476	6.34634666
8.81910992	0.78674275	4.63805676
4.80454063	5.71242380	4.63805676
3.34631014	0.78674275	4.63805676
10.27734089	5.71242380	4.63805676
7.55727768	5.71838522	4.62066126
6.09904766	0.79270440	4.62066126
2.08447790	5.71838522	4.62066126
0.62624747	0.79270440	4.62066126
8.82021332	3.47978425	4.20587540
4.80564356	8.40546513	4.20587540
3.34741306	3.47978425	4.20587540
10.27844334	8.40546513	4.20587540
7.54940796	8.42789936	4.20249939
6.09117746	3.50221849	4.20249939
13.02220726	8.42789936	4.20249939
11.56397724	3.50221849	4.20249939
8.93827438	6.93054914	2.54134583

7.48004389	2.00486803	2.54134583
3.46547413	6.93054914	2.54134583
2.00724387	2.00486803	2.54134583
6.19786596	6.96187782	2.44749212
4.73963594	2.03619671	2.44749212
11.67066574	6.96187782	2.44749212
10.21243572	2.03619671	2.44749212
6.23309374	9.47346973	2.22578788
4.77486372	4.54778910	2.22578788
11.70589352	9.47346973	2.22578788
10.24766350	4.54778910	2.22578788
8.92396069	9.46470928	2.21652770
7.46573067	4.53902865	2.21652770
3.45116115	9.46470928	2.21652770
1.99293077	4.53902865	2.21652770

# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(510) with a C<sub>v</sub>

1.000000000000

9.97980000	0.00000000	0.00000000
-0.76395804	12.66177393	0.00000000
0.00000004	0.00000004	19.64040000

C	O	Fe
36	1	80

Cart

4.22894339	9.34246877	7.53042485
9.12906483	9.31432311	7.47472943
7.23342538	4.27054869	7.23638707
2.23500035	4.28608505	7.22986778
3.38259569	11.95845136	7.20059018
8.37208010	11.95284413	7.23791789
4.70523615	6.77497085	6.33617041
-0.28447956	6.77315740	6.34826501
6.68400133	1.64159167	6.17344242
1.69345557	1.62814543	6.19905249
7.17771161	8.25735516	5.56733696
2.19920171	8.31983738	5.66053024
4.21146365	3.13584923	5.30399978
9.20867402	3.14714886	5.30283336
-0.33210958	10.81234643	4.26807742
4.67288000	10.83193113	4.27292149
1.74477879	5.71382340	4.01855213
6.72818573	5.69065197	4.01047710
2.18380751	12.34504378	3.63915708

7.18348370	12.34428276	3.64572262
4.24497222	7.20709130	3.35008470
9.23800491	7.20098379	3.34132926
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
5.70954227	9.76071192	8.24773410
3.26437348	7.78017997	7.15943400
8.22978766	7.75670001	7.11395487
2.52319639	10.23140302	7.08733019
-0.03690638	10.92866430	6.95141728
5.74265879	2.20417744	4.50862175
-0.03142283	0.87136633	6.66599411
8.90240009	5.15230063	6.96391370
3.90975555	5.16186447	6.97251602
8.18484704	2.69648017	6.91339126
3.18703923	2.70062742	6.91515928
4.97456328	11.00384917	6.88549703
5.72913879	8.34306529	6.88607720
0.66322793	12.42003465	4.89815823
0.69086111	8.40934611	6.91265988
1.44442682	5.91873363	6.74673977
6.42616085	5.88524638	6.72759908
2.48172391	0.08514746	7.04342653
0.70849793	3.32047062	6.69122084
5.69641805	3.31999837	6.69331051
7.49083643	0.14088454	7.04593572
8.20204506	11.73202075	5.21302204
5.66644447	12.43821821	4.88302945
2.52899853	4.23203442	5.05240824
3.91154145	9.22946253	5.05891222
7.52104376	4.21949492	5.04779095
8.87253754	9.24445433	5.12674186

3.20363589	6.76759832	4.94741586
8.21105421	6.74213940	4.92507792
3.22590278	11.76279869	5.17875690
7.45825337	10.26583759	7.27575521
8.21125297	1.48433236	4.83849955
3.20320389	1.48576244	4.84191768
1.38854391	9.89645921	4.80879389
6.38903159	9.89986995	4.81649573
0.03869025	4.86382367	4.70663550
5.71821489	7.26984929	4.70290519
0.73558782	7.31178722	4.71945367
5.01672572	4.85278104	4.70804061
0.75583291	2.19761487	4.51628927
4.95192135	0.88727541	6.64515096
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367

6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(510) with a C<sub>v</sub>

1.000000000000

9.97980000	0.00000000	0.00000000
-0.76395804	12.66177393	0.00000000
0.00000004	0.00000004	19.64040000

C	O	Fe
36	1	80

Cart

4.15668973	9.31269523	7.48575892
9.15602651	9.32237250	7.46783181
7.20169698	4.27349351	7.29018045
2.27395494	4.28187903	7.21211953
3.38568094	11.92141792	7.20857695
8.38448010	11.94065539	7.20420419
4.66938641	6.79346275	6.30380578
-0.28410251	6.76138295	6.36890930
6.68527563	1.61304509	6.16728693
1.69145611	1.61223999	6.18925790
7.17360271	8.29277750	5.62792592
2.18318572	8.30228107	5.62716483
4.21567772	3.10752381	5.28883033
9.20354819	3.14967696	5.32206176
-0.32236214	10.81646292	4.26572851
4.66969084	10.81348426	4.26391479
1.74236112	5.69101711	4.01819565
6.72613819	5.70277262	4.01448962
2.18898139	12.34043550	3.63979562
7.18104366	12.34493039	3.63858236
4.24335620	7.20477847	3.34737253
9.23803091	7.20538785	3.36006428
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015

6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
5.72774594	4.64553756	8.07736540
3.22879178	7.76551361	7.14364610
8.23187217	7.77339356	7.13484769
2.50878416	10.22624004	7.08189650
7.50018588	10.24044500	7.08558147
3.21047942	1.46955807	4.83605671
3.22966428	11.74327252	5.18093611
8.88388073	5.14606916	6.95592063
3.98823656	5.16056445	7.10791275
8.17465784	2.68707995	6.92663110
3.17526408	2.67122897	6.90076957
4.98208413	10.92166311	6.92891463
5.67794726	8.41512021	6.89600487
-0.00823196	10.92958216	6.91839362
0.69090685	8.39928920	6.89676413
1.44756978	5.89541049	6.75412810
6.42409778	5.97046640	6.76177023
5.74583054	2.18303062	4.50074932
0.71328597	3.32305618	6.69823832
5.67352766	3.22889028	6.69205167
4.95500894	0.84152372	6.64273303
0.67161373	12.42428218	4.89540143
7.48423051	0.08745822	7.04267450
2.55257767	4.23380667	5.07316552
3.89747125	9.21838926	5.06461576
7.49590986	4.22075170	5.05534952
8.88739466	9.21766100	5.06388903
3.20596913	6.74907630	4.93994543
8.19768492	6.74511910	4.93842958
8.22210136	11.75683906	5.18054396
2.49262653	0.07933933	7.04561184
-0.04122890	0.87851990	6.66174659



0.75321199	2.20254091	4.51757993
1.39219299	9.88861823	4.79734900
6.38566958	9.88802898	4.80348056
0.03568681	4.85471762	4.70889096
5.71708412	7.28152324	4.72036427
0.73000095	7.28367580	4.72513937
5.01590900	4.85669593	4.71797183
5.66813990	12.41867671	4.89245627
8.20615218	1.48977777	4.84466776
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943

1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(510) without a C<sub>v</sub>

1.000000000000

9.97980000	0.00000000	0.00000000
-0.76395804	12.66177393	0.00000000
0.00000004	0.00000004	19.64040000

C	O	Fe
37	1	80

Cart

8.53740553	12.05605193	7.41394617
4.14963676	9.28354586	7.53845259
9.25653596	9.32134903	7.58823792
7.23662990	4.28711670	7.23551708
2.25568104	4.27482370	7.23785665
3.36378038	11.95320462	7.25773045
6.49567552	11.22654303	6.16481893
4.71080559	6.77280276	6.35255876
-0.28344302	6.78169350	6.33690013
6.70434860	1.63389092	6.21482960
1.71664878	1.65407348	6.16426257
7.18548782	8.24637117	5.64082395
2.19098894	8.25357531	5.59488485
4.22697920	3.13615759	5.30608665
9.21146580	3.13529947	5.30506231
-0.32215342	10.81667368	4.27472758
4.63557142	10.75666615	4.20497737
1.73919146	5.69228070	4.01363861
6.73240037	5.69699063	4.01456037
2.19566492	12.34210410	3.64591290
7.18836725	12.36422669	3.60720805
4.24770379	7.20320773	3.34619116
9.23619403	7.20494511	3.34733001
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899

9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
0.78673389	9.74555961	8.27771564
3.25011307	7.73968933	7.13521081
8.25324038	7.79672506	7.15782070
2.47059307	10.24297631	7.28115373
7.64017826	10.30981681	7.34136252
0.66901510	12.42221342	4.88453374
7.58174262	0.17061754	7.11299787
8.90834226	5.16442693	6.96814971
3.92274286	5.14676958	6.96175134
8.19742802	2.71036111	6.92389975
3.20865779	2.69620728	6.91266696
4.86585787	10.90087131	7.04036162
5.69505306	8.38324593	6.92606533
0.03252937	11.01442571	6.93914036
0.74818320	8.33364092	6.90793021
1.44140469	5.88756271	6.72602907
6.44168950	5.91388652	6.74552915
0.71932169	3.33150573	6.69478889
0.76295482	2.20387223	4.50404151
5.71159509	3.31829743	6.69708575
4.97332664	0.87070181	6.67019810
8.19468131	11.73963861	5.21393451
3.21567369	11.71000949	5.22103385
2.53552877	4.21466888	5.04696140
3.87408649	9.22921126	5.12671653
7.52533664	4.22234238	5.05583324
8.89103856	9.22784097	5.09537264
3.21748183	6.73844875	4.92866321
8.20750510	6.75013970	4.94326842
-0.00319173	0.91548393	6.64800613
5.64966753	12.37647241	4.89782200
8.20582236	1.47799159	4.85299090
3.23139968	1.46988545	4.83768302
1.38292449	9.88632847	4.82111333
6.37150264	9.83697597	4.83997216
0.03433482	4.84811835	4.70430718

5.72179789	7.27694708	4.72039818
0.73070824	7.27477120	4.70808940
5.03142484	4.84883095	4.70723430
2.50680471	0.14545589	7.04433813
5.75820124	2.19662536	4.52315947
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002

0.69460732      10.28863907      0.50651002

# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(021) without a C<sub>v</sub>

1.000000000000

14.90600000	0.00000000	0.00000000
0.42323971	8.40334839	0.00000000
0.00000004	0.00000004	23.05139900

C	O	Fe
37	1	80

Cart

9.60627360	5.27497748	7.53396297
2.74437388	2.03559761	7.68094536
10.18904981	1.91704687	7.61835986
14.77382592	5.55356884	5.88704617
2.20212875	5.35425901	7.50036032
5.20956062	8.33446973	7.45108387
12.75340221	8.22065249	7.41967755
6.56126914	2.56125457	6.95486934
13.98235130	2.46261514	6.82427644
8.36524960	0.14786392	6.22857508
1.02359293	0.23837863	6.24750727
7.22423950	5.56072736	6.05081204
11.15853333	6.05776815	4.68306465
9.25671866	3.26375364	5.43805503
1.79308462	3.29603039	5.43950443
3.71299392	6.07006750	4.68175344
13.66673046	5.08097054	8.28207637
5.60633565	3.77425845	4.10090610
13.05639917	3.75303228	4.10358442
4.13073833	0.74735852	3.95331516
11.58099601	0.73944829	3.95404889
6.45910597	6.85157728	3.36946511
13.91210556	6.85157728	3.36946511
7.93326235	1.23396885	2.61950350
0.48026219	1.23396885	2.61950350
2.91558671	7.36299515	2.03468370
10.36858654	7.36299515	2.03468370
8.76163578	4.32674265	1.79040837
1.30863547	4.32674265	1.79040837
3.18085384	1.97663546	1.14063549
10.63385391	1.97663546	1.14063549
4.93311071	4.62204313	0.60898984
12.38611031	4.62204313	0.60898984

7.97210503	7.58761215	0.54751450
0.51910490	7.58761215	0.54751450
6.98546123	2.51763773	0.40115634
14.43846130	2.51763773	0.40115634
10.21822342	6.74780589	8.28237671
11.22723932	6.03075622	6.64587704
13.67285896	6.55979504	7.24146873
4.62994083	1.86911995	7.44992436
12.05049738	1.72028583	7.39434425
6.06049840	6.60776561	7.27363664
14.98791027	7.26003196	5.00069397
2.81607762	0.19805766	7.26828190
10.20148819	0.03699565	7.31862389
8.55001986	6.86795593	7.21919296
1.29245950	6.97439408	7.18511726
2.90490992	3.72970300	7.00481874
10.37265262	3.65624344	7.02766441
5.39463118	4.15807910	6.82686655
12.87469378	4.04398009	7.00812975
6.55425035	0.56947996	6.82206004
14.06824283	0.51791435	6.77059275
8.48860824	2.03107271	6.79838838
1.04815002	2.09317325	6.80609311
3.74660926	6.09186147	6.63718161
0.38876947	4.61033343	7.51579560
5.05583508	8.07980582	5.52650389
7.83544745	4.41462153	7.49766766
9.15617204	5.26765732	5.39939574
14.73299831	3.66926667	5.25679191
3.00635981	1.73795464	5.24725080
10.45951371	1.70674105	5.27740981
7.30881685	3.66559907	5.20725378
0.49234227	1.23819836	4.55698103
5.47408159	2.08927897	5.12203499
12.90602058	2.07075351	5.10783362
7.52120153	7.25325334	5.03164082
12.49688883	8.05580213	5.52639094
1.72476011	5.27555508	5.37980063
9.98828272	7.65790753	4.90006194
5.69791576	5.65843964	4.80855537
13.14398582	5.63717251	4.82116814
3.81134721	4.11323414	4.74452431
11.25571526	4.09278730	4.77394757
7.94524070	1.22619084	4.55654892

2.55361031	7.68735284	4.89201376
9.24510097	3.28775048	3.49441624
1.79210067	3.28775048	3.49441624
5.93108559	0.40572783	3.30346417
13.38408565	0.40572783	3.30346417
4.47159576	7.26234245	3.24290895
11.92459583	7.26234245	3.24290895
7.61672831	5.24388313	3.15383196
15.06972790	5.24388313	3.15383196
2.63376808	5.66717625	3.03582549
10.08676815	5.66717625	3.03582549
4.26076746	2.43179297	2.93866873
11.71376801	2.43179297	2.93866873
9.89125442	0.84577286	2.82996941
2.43825460	0.84577286	2.82996941
6.72640657	2.78669548	2.80400848
14.17940712	2.78669548	2.80400848
8.45943737	7.64924812	2.68994594
1.00643730	7.64924812	2.68994594
5.09631491	4.84222126	2.52809286
12.54931545	4.84222126	2.52809286
6.42297029	6.83616877	1.40942586
13.87596989	6.83616877	1.40942586
8.68566036	2.45029783	1.24810267
1.23265994	2.45029783	1.24810267
3.15018106	3.96655679	1.23820484
10.60318089	3.96655679	1.23820484
4.33920240	0.37170255	1.20792723
11.79220295	0.37170255	1.20792723
6.82007313	0.80580682	1.04853928
14.27307320	0.80580682	1.04853928
8.95301247	6.01934624	0.88174963
1.50001240	6.01934624	0.88174963
6.94090939	4.36216164	0.80574113
14.39390945	4.36216164	0.80574113
4.05270052	6.32821703	0.79609853
11.50570011	6.32821703	0.79609853
5.10706043	2.69428372	0.63864446
12.56006050	2.69428372	0.63864446
9.31387520	0.04532212	0.55626547
1.86087537	0.04532212	0.55626547

# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(021) with a C<sub>v</sub>

1.000000000000

14.90600000	0.00000000	0.00000000
0.42323971	8.40334839	0.00000000
0.00000004	0.00000004	23.05139900

C	O	Fe
36	1	80

Cart

2.15241619	5.29087621	7.54473519
2.73222517	1.95934037	7.62885600
10.18961034	2.01008234	7.66530477
9.62677056	5.32517772	7.50546433
5.27505042	8.30871482	7.44908065
12.64633864	8.29849934	7.44340526
6.56202345	2.54532089	6.92448334
14.00154497	2.54328745	6.94351127
8.42848109	0.18626884	6.26940549
0.92244489	0.16279741	6.23397783
7.24595158	5.54462256	6.01850306
14.67991775	5.55724825	6.04009036
9.25974475	3.28007078	5.43321140
1.80025488	3.27237418	5.43735169
3.70952078	6.06539778	4.68161776
11.16041970	6.07247704	4.69085351
5.59691125	3.76217054	4.10251256
13.05091868	3.76730638	4.10292848
4.12741978	0.74342964	3.96026698
11.58574558	0.74505288	3.94924362
6.45910597	6.85157728	3.36946511
13.91210556	6.85157728	3.36946511
7.93326235	1.23396885	2.61950350
0.48026219	1.23396885	2.61950350
2.91558671	7.36299515	2.03468370
10.36858654	7.36299515	2.03468370
8.76163578	4.32674265	1.79040837
1.30863547	4.32674265	1.79040837
3.18085384	1.97663546	1.14063549
10.63385391	1.97663546	1.14063549
4.93311071	4.62204313	0.60898984
12.38611031	4.62204313	0.60898984
7.97210503	7.58761215	0.54751450
0.51910490	7.58761215	0.54751450
6.98546123	2.51763773	0.40115634
14.43846130	2.51763773	0.40115634
2.79235766	6.75700655	8.28448108



7.85702378	4.45382194	7.49939191
0.38110435	4.42702188	7.50193560
4.61201004	1.80276267	7.40801131
12.06891006	1.82995513	7.43474173
6.13490901	6.60073262	7.25561785
13.51902442	6.58736239	7.26567476
2.77625414	0.07625821	7.34254259
10.23066062	0.16376248	7.25943564
8.65480850	6.89409516	7.17570193
1.11464230	6.88349112	7.21812891
2.89961421	3.68424637	7.01816760
10.36329016	3.71111179	7.00114246
5.38794909	4.12701545	6.83128466
12.83764615	4.13849609	6.82789725
6.59206070	0.55988375	6.80052788
14.00452619	0.55025670	6.81634373
8.50339818	2.06671536	6.80038434
1.02939784	2.03777728	6.79847167
3.75991447	6.03893148	6.64574914
11.17609941	6.07906788	6.64619596
5.04268052	8.06607978	5.54098168
12.49473676	8.06520194	5.52576801
9.14799683	5.26546796	5.36974519
1.69216796	5.27724829	5.38346148
3.00686329	1.71961418	5.27823140
10.46345846	1.72736011	5.24837873
7.29822827	3.66149899	5.21301388
14.75453170	3.66445062	5.21086253
5.46699903	2.07503709	5.11482923
12.92254273	2.08026827	5.12019576
7.52661633	7.24499943	5.01752741
14.97078848	7.25112272	5.02682727
2.53716446	7.67042733	4.90863887
9.99012611	7.67332287	4.90153787
5.68882177	5.65138974	4.81377776
13.14489817	5.65310240	4.80964019
3.79630238	4.10363400	4.75618676
11.25533346	4.11452838	4.74664142
7.94397403	1.22468475	4.55970205
0.49011810	1.22639848	4.55585235
9.24510097	3.28775048	3.49441624
1.79210067	3.28775048	3.49441624
5.93108559	0.40572783	3.30346417
13.38408565	0.40572783	3.30346417

4.47159576	7.26234245	3.24290895
11.92459583	7.26234245	3.24290895
7.61672831	5.24388313	3.15383196
15.06972790	5.24388313	3.15383196
2.63376808	5.66717625	3.03582549
10.08676815	5.66717625	3.03582549
4.26076746	2.43179297	2.93866873
11.71376801	2.43179297	2.93866873
9.89125442	0.84577286	2.82996941
2.43825460	0.84577286	2.82996941
6.72640657	2.78669548	2.80400848
14.17940712	2.78669548	2.80400848
8.45943737	7.64924812	2.68994594
1.00643730	7.64924812	2.68994594
5.09631491	4.84222126	2.52809286
12.54931545	4.84222126	2.52809286
6.42297029	6.83616877	1.40942586
13.87596989	6.83616877	1.40942586
8.68566036	2.45029783	1.24810267
1.23265994	2.45029783	1.24810267
3.15018106	3.96655679	1.23820484
10.60318089	3.96655679	1.23820484
4.33920240	0.37170255	1.20792723
11.79220295	0.37170255	1.20792723
6.82007313	0.80580682	1.04853928
14.27307320	0.80580682	1.04853928
8.95301247	6.01934624	0.88174963
1.50001240	6.01934624	0.88174963
6.94090939	4.36216164	0.80574113
14.39390945	4.36216164	0.80574113
4.05270052	6.32821703	0.79609853
11.50570011	6.32821703	0.79609853
5.10706043	2.69428372	0.63864446
12.56006050	2.69428372	0.63864446
9.31387520	0.04532212	0.55626547
1.86087537	0.04532212	0.55626547

# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(021) with a C<sub>v</sub>

1.000000000000

14.90600000	0.00000000	0.00000000
0.42323971	8.40334839	0.00000000
0.00000004	0.00000004	23.05139900
C	O	Fe

	36	1	80
Cart			
	3.69364612	6.05393068	4.69179117
	2.74552901	1.97487704	7.63382001
	10.20532542	2.01776877	7.66825355
	9.61815645	5.33742917	7.50821107
	4.90456639	0.01658196	7.38910808
	12.65990573	8.30122829	7.44397491
	6.58805617	2.57464317	6.93814147
	14.01169548	2.54194856	6.95222466
	8.44238074	0.19022975	6.27074959
	0.95512264	0.15140859	6.29988850
	7.21423905	5.57789453	6.06594689
	13.03874022	3.75681470	4.09903773
	9.27879699	3.29367991	5.43131508
	1.78467277	3.24275421	5.42606073
	2.09491244	5.27073295	7.47747657
	11.15651168	6.07633148	4.68717287
	5.60849371	3.77977092	4.10410867
	14.67279121	5.54201827	6.02747143
	4.13096370	0.74617308	3.94679163
	11.58579395	0.74528064	3.94207573
	6.45910597	6.85157728	3.36946511
	13.91210556	6.85157728	3.36946511
	7.93326235	1.23396885	2.61950350
	0.48026219	1.23396885	2.61950350
	2.91558671	7.36299515	2.03468370
	10.36858654	7.36299515	2.03468370
	8.76163578	4.32674265	1.79040837
	1.30863547	4.32674265	1.79040837
	3.18085384	1.97663546	1.14063549
	10.63385391	1.97663546	1.14063549
	4.93311071	4.62204313	0.60898984
	12.38611031	4.62204313	0.60898984
	7.97210503	7.58761215	0.54751450
	0.51910490	7.58761215	0.54751450
	6.98546123	2.51763773	0.40115634
	14.43846130	2.51763773	0.40115634
	4.32782936	7.05618260	8.18839797
	7.85558014	4.45059779	7.50081494
	0.34569097	4.40036919	7.49387943
	4.63190794	1.87774481	7.39960793
	12.08120127	1.83102655	7.44181527
	6.05907017	6.60380467	7.28625751

13.52011491	6.58250499	7.27025984
2.78748880	0.10680269	7.29661777
10.24110375	0.16785987	7.25875349
8.62598470	6.89577568	7.17649989
1.12018916	6.84883764	7.16265171
2.88757014	3.67968500	6.98159636
10.36772179	3.72416154	7.01230954
5.39409623	4.14128997	6.80734238
12.82340186	4.13727570	6.81616551
6.62904078	0.60238561	6.80202494
14.01640337	0.54305373	6.82358705
8.52618083	2.08112887	6.79798169
1.04110744	2.01936319	6.80624249
3.68115126	6.04769239	6.70222042
11.16891220	6.08889569	6.64312102
5.07646639	8.08520288	5.51702428
12.50322308	8.06753098	5.52464428
9.13853880	5.27721584	5.37246878
1.68604287	5.23747466	5.37511437
3.01682276	1.71229356	5.26415403
10.46889722	1.72733822	5.24929694
7.30825599	3.67793719	5.21170604
14.74278328	3.65094869	5.20692258
5.48726399	2.09210525	5.10249622
12.92696006	2.07039783	5.12477048
7.51546989	7.25403707	5.02858348
14.97513260	7.24507152	5.01966969
2.54040916	7.65481939	4.92890279
9.98740656	7.67296595	4.90437242
5.68185308	5.66527423	4.81246911
13.14039949	5.65112201	4.80611539
3.80407176	4.10783756	4.74567484
11.24895404	4.11962401	4.74957248
7.94719437	1.22830506	4.55964555
0.49599476	1.21163813	4.56511301
9.24510097	3.28775048	3.49441624
1.79210067	3.28775048	3.49441624
5.93108559	0.40572783	3.30346417
13.38408565	0.40572783	3.30346417
4.47159576	7.26234245	3.24290895
11.92459583	7.26234245	3.24290895
7.61672831	5.24388313	3.15383196
15.06972790	5.24388313	3.15383196
2.63376808	5.66717625	3.03582549

10.08676815	5.66717625	3.03582549
4.26076746	2.43179297	2.93866873
11.71376801	2.43179297	2.93866873
9.89125442	0.84577286	2.82996941
2.43825460	0.84577286	2.82996941
6.72640657	2.78669548	2.80400848
14.17940712	2.78669548	2.80400848
8.45943737	7.64924812	2.68994594
1.00643730	7.64924812	2.68994594
5.09631491	4.84222126	2.52809286
12.54931545	4.84222126	2.52809286
6.42297029	6.83616877	1.40942586
13.87596989	6.83616877	1.40942586
8.68566036	2.45029783	1.24810267
1.23265994	2.45029783	1.24810267
3.15018106	3.96655679	1.23820484
10.60318089	3.96655679	1.23820484
4.33920240	0.37170255	1.20792723
11.79220295	0.37170255	1.20792723
6.82007313	0.80580682	1.04853928
14.27307320	0.80580682	1.04853928
8.95301247	6.01934624	0.88174963
1.50001240	6.01934624	0.88174963
6.94090939	4.36216164	0.80574113
14.39390945	4.36216164	0.80574113
4.05270052	6.32821703	0.79609853
11.50570011	6.32821703	0.79609853
5.10706043	2.69428372	0.63864446
12.56006050	2.69428372	0.63864446
9.31387520	0.04532212	0.55626547
1.86087537	0.04532212	0.55626547

# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(021) with a C<sub>v</sub>

1.000000000000

14.90600000	0.00000000	0.00000000
0.42323971	8.40334839	0.00000000
0.00000004	0.00000004	23.05140000

C	O	Fe
36	1	80

Cart

2.16906253	5.31411016	7.50916312
2.71217309	1.98310741	7.64249565
10.19794211	2.00518232	7.66140113

9.65841274	5.33111170	7.51501148
5.15411377	8.23750633	7.43924410
12.64071250	8.28624247	7.44547186
6.56937620	2.43769624	6.88314549
13.99848520	2.54211198	6.93785561
8.41735925	0.19068015	6.24738097
0.93101055	0.15675522	6.26343468
7.27877065	5.55337003	6.00424937
13.05383712	3.76861504	4.10285899
9.23907523	3.28347675	5.44521937
1.78636274	3.26549153	5.43150632
3.70735144	6.06849325	4.69762836
11.15781609	6.06602398	4.68182967
5.61383373	3.76618651	4.10992705
14.69235591	5.54915799	6.03302963
4.13156597	0.74532485	3.95021989
11.58533001	0.74088400	3.95150515
6.45910597	6.85157728	3.36946511
13.91210556	6.85157728	3.36946511
7.93326235	1.23396885	2.61950350
0.48026219	1.23396885	2.61950350
2.91558671	7.36299515	2.03468370
10.36858654	7.36299515	2.03468370
8.76163578	4.32674265	1.79040837
1.30863547	4.32674265	1.79040837
3.18085384	1.97663546	1.14063549
10.63385391	1.97663546	1.14063549
4.93311071	4.62204313	0.60898984
12.38611031	4.62204313	0.60898984
7.97210503	7.58761215	0.54751450
0.51910490	7.58761215	0.54751450
6.98546123	2.51763773	0.40115634
14.43846130	2.51763773	0.40115634
6.51786106	3.53604782	8.31004269
7.87865074	4.57603769	7.53258945
0.40198333	4.43434676	7.50230320
4.57950978	1.76155168	7.40478488
12.07698778	1.82905396	7.43117731
6.11836189	6.59253112	7.24144017
13.54496185	6.57985895	7.27044038
2.73020685	0.13780871	7.23699437
10.25354714	0.16294995	7.24798719
8.72286269	6.93629797	7.18961592
1.16946260	6.86001107	7.17516379

2.88799193	3.69536104	6.99816262
10.36363786	3.69978418	7.00161282
5.35475464	4.17642002	6.98099373
12.83380571	4.13588523	6.82834745
6.56024937	0.50187140	6.82762290
14.00766179	0.54049197	6.82966964
8.50408221	2.03351642	6.79126259
1.02343959	2.04623379	6.79473066
3.72302362	6.09109094	6.65847872
11.20011623	6.08147009	6.64712627
5.05025861	8.05054218	5.51868689
12.51992228	8.06498323	5.52268014
9.14840751	5.26152738	5.37463620
1.69526994	5.26190466	5.36053829
2.99238964	1.71701395	5.24543016
10.46067563	1.72973366	5.23493090
7.27634162	3.62043042	5.27500742
14.74699386	3.66430929	5.21606304
5.43788612	2.06684911	5.11531270
12.92435054	2.07820939	5.11881253
7.52754505	7.25391239	5.01870789
14.97726516	7.24868789	5.02500714
2.53441057	7.66495608	4.89698541
10.00302500	7.67507798	4.89552057
5.69305708	5.64129795	4.82626247
13.14895041	5.65219716	4.81096421
3.81397527	4.10990704	4.76933493
11.26229632	4.11328915	4.74903933
7.94282828	1.22439283	4.55547811
0.48871478	1.22055615	4.55814856
9.24510097	3.28775048	3.49441624
1.79210067	3.28775048	3.49441624
5.93108559	0.40572783	3.30346417
13.38408565	0.40572783	3.30346417
4.47159576	7.26234245	3.24290895
11.92459583	7.26234245	3.24290895
7.61672831	5.24388313	3.15383196
15.06972790	5.24388313	3.15383196
2.63376808	5.66717625	3.03582549
10.08676815	5.66717625	3.03582549
4.26076746	2.43179297	2.93866873
11.71376801	2.43179297	2.93866873
9.89125442	0.84577286	2.82996941
2.43825460	0.84577286	2.82996941

6.72640657	2.78669548	2.80400848
14.17940712	2.78669548	2.80400848
8.45943737	7.64924812	2.68994594
1.00643730	7.64924812	2.68994594
5.09631491	4.84222126	2.52809286
12.54931545	4.84222126	2.52809286
6.42297029	6.83616877	1.40942586
13.87596989	6.83616877	1.40942586
8.68566036	2.45029783	1.24810267
1.23265994	2.45029783	1.24810267
3.15018106	3.96655679	1.23820484
10.60318089	3.96655679	1.23820484
4.33920240	0.37170255	1.20792723
11.79220295	0.37170255	1.20792723
6.82007313	0.80580682	1.04853928
14.27307320	0.80580682	1.04853928
8.95301247	6.01934624	0.88174963
1.50001240	6.01934624	0.88174963
6.94090939	4.36216164	0.80574113
14.39390945	4.36216164	0.80574113
4.05270052	6.32821703	0.79609853
11.50570011	6.32821703	0.79609853
5.10706043	2.69428372	0.63864446
12.56006050	2.69428372	0.63864446
9.31387520	0.04532212	0.55626547
1.86087537	0.04532212	0.55626547

# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(111) without a C<sub>v</sub>

1.000000000000

12.37300000	0.00000000	0.00000000
-2.07134726	13.30634571	0.00000000
0.00000004	0.00000005	22.12540000

C	O	Fe
65	1	136

Cart

5.06690461	8.35549373	9.90467888
6.77813595	1.86205009	10.15418027
5.77426700	5.10709050	9.93121465
-1.19020086	8.41138299	9.91336006
-0.17574838	1.74221328	9.91829322
9.30371619	3.83741602	9.95997671
8.23812546	10.51975441	9.86094363
2.40780391	3.73468889	9.48821676



2.03874727	10.50866389	9.89065863
6.73189437	5.75813415	6.87182434
4.68394636	11.71005320	9.73583372
-1.51019745	11.77627077	9.77230493
-0.47094256	5.06166644	9.67424015
9.25984373	0.20611544	9.37256648
8.18477149	6.75382681	9.33115864
3.11369329	0.09116220	9.32916850
1.93157946	6.89241867	9.39836731
5.03386062	2.95343610	8.38071984
5.77606106	12.40647705	6.94251386
0.57971481	5.74881573	6.94429937
-0.50832098	12.42569511	6.86245041
9.42200104	7.69370125	6.73753746
4.21877672	0.95279141	6.61939835
3.25140625	7.68197728	6.78011233
10.50549726	1.03361422	6.74428892
7.54125775	2.04401376	6.58261846
6.42461824	8.71433905	6.60765098
1.28063351	2.10561897	6.68530055
0.26709221	8.70588579	6.60758133
9.08413218	10.67398359	6.25769199
3.82310412	3.99228400	6.12324256
2.90759674	10.64793884	6.25543823
10.12947285	4.02910274	6.29172786
8.44706331	2.90720534	3.88563091
7.38506834	9.55264092	3.87101528
2.18910083	2.88656005	3.83471877
1.20437810	9.55180436	3.87877817
4.87882185	4.85300732	3.51646113
3.84314847	11.50618076	3.51646113
11.06532192	4.85300732	3.51646113
10.02964878	11.50618076	3.51646113
8.08072281	5.89129591	3.40647149
7.04504919	12.54446888	3.40647149
1.89422262	5.89129591	3.40647149
0.85854894	12.54446888	3.40647149
5.59163237	1.16514635	3.18918610
4.55595875	7.81831932	3.18918610
11.77813244	1.16514635	3.18918610
10.74245834	7.81831932	3.18918610
9.29798985	6.73122358	0.77799785
4.14716339	0.07805078	0.77799785
3.11148977	6.73122358	0.77799785

10.33366299	0.07805078	0.77799785
6.68999243	1.82555234	0.41000685
5.65431881	8.47872543	0.41000685
-0.53218126	8.47872543	0.41000685
0.50349241	1.82555234	0.41000685
9.34398174	3.05093241	0.30731282
8.30830765	9.70410538	0.30731282
3.15748167	3.05093241	0.30731282
2.12180805	9.70410538	0.30731282
6.31061268	5.17102432	0.23606260
5.27493906	11.82419777	0.23606260
-0.91156107	11.82419777	0.23606260
0.12411259	5.17102432	0.23606260
3.52874300	3.53983996	10.82680223
6.93148491	2.54527526	8.34446521
7.71202418	8.68956452	9.88219518
2.90270425	1.90942880	9.96118948
1.46173300	8.72237063	9.90908040
5.43860576	3.25222545	10.18603404
3.97836078	9.96013725	9.87981644
11.16586793	3.34306276	9.89268690
10.16584281	10.02392079	9.89393970
9.96213564	5.56340860	9.57135309
8.94881733	12.24552030	9.62061222
3.75455283	5.37189674	9.62001844
2.76710059	12.18275401	9.53775086
7.13107556	0.19392911	9.40579358
6.07334862	6.85541102	9.44925080
0.93203112	0.29138631	9.47877429
-0.19385277	6.91849600	9.44691372
7.65107300	4.80933046	9.44976654
6.65832959	11.56799701	9.08015266
1.39591723	5.15110598	8.81933476
0.41149211	11.52733508	9.21601367
9.77139137	7.81752291	8.70417998
4.72784745	1.10271539	8.56209411
3.61871226	7.70456968	8.77433065
10.85360194	1.17709991	8.69775022
8.68360821	2.03981606	9.97361982
5.86209719	9.22395804	8.41182247
0.85299819	2.64675133	8.55953298
-0.35608052	9.24123812	8.38785719
9.39037667	3.31648763	8.02146153
8.41939631	9.95193754	7.97991375

3.23891670	3.29068601	7.85024728
2.22439905	9.94178714	7.99592289
5.52164384	4.75667432	8.00456217
4.45075869	11.36704025	7.85256360
11.56840916	4.70602411	7.80961596
-1.76006622	11.39842425	7.87087617
8.73126908	0.75230994	7.54783818
7.63387262	7.42205684	7.53350352
2.50909547	0.73868904	7.55194239
1.46869576	7.41611675	7.55910898
9.38573678	5.70667109	7.01528441
8.39699514	12.35319882	6.99939539
3.25177330	5.69006280	6.95873167
2.23657390	12.31828515	7.00468928
6.42782621	0.43123118	6.81487771
5.31445187	7.09838537	6.90925352
-0.86885691	7.11099579	6.88174611
0.19158335	0.48886048	6.90614733
5.28276624	2.64658054	6.44304276
4.31350364	9.28836939	6.48921755
11.55441774	2.66178507	6.50854437
10.49125071	9.30910133	6.45801806
7.50901271	4.04975072	6.34863616
6.49883157	10.70423320	6.36113772
1.34123831	4.05761941	6.31251326
0.30521788	10.71780376	6.38332873
9.27840001	2.32033774	5.62856332
8.20822274	8.95173530	5.61015700
3.03093484	2.24876469	5.55075146
2.02583489	8.95342660	5.62765869
5.35014260	5.02621024	5.43536026
4.35266030	11.66097732	5.39476191
11.55567193	5.05041301	5.39203220
10.52572130	11.70315113	5.40637471
7.53298866	6.42226241	5.23679985
6.50822789	13.07487293	5.23887577
1.34065786	6.41709527	5.24277766
0.34612841	13.06532427	5.24440157
9.97652008	7.15757916	4.89509172
4.87256115	0.46892725	4.87259285
3.78812843	7.16227112	4.89865684
11.02366552	0.49881242	4.89957894
7.01241752	1.87787497	4.73482359
5.94561905	8.52898906	4.73895302

0.77549532	1.87149395	4.75770545
-0.23154217	8.52712830	4.73976955
9.30100298	4.63003661	4.53707143
8.27143233	11.27388932	4.52039092
3.11230784	4.60876420	4.45460038
2.08494254	11.26645811	4.52224129
4.86458023	2.86012994	3.79297429
3.81171706	9.51258211	3.78890497
11.03018436	2.86274632	3.78306301
10.00154495	9.51687145	3.78704119
7.02151012	4.27133465	3.67187500
5.98583651	10.92450714	3.67187500
0.83500999	4.27133465	3.67187500
-0.20066364	10.92450714	3.67187500
5.98730040	6.46236563	3.26705837
4.95162678	13.11553860	3.26705837
-1.23487330	13.11553860	3.26705837
-0.19919968	6.46236563	3.26705837
9.13459015	1.21606314	3.15154004
8.09891701	7.86923599	3.15154004
2.94809031	1.21606314	3.15154004
1.91241682	7.86923599	3.15154004
9.86151791	6.16859675	2.57775974
8.82584381	12.82176971	2.57775974
3.67501736	6.16859675	2.57775974
2.63934374	12.82176971	2.57775974
6.94373321	2.19821787	2.29912543
5.90805960	8.85139084	2.29912543
0.75723332	2.19821787	2.29912543
-0.27844033	8.85139084	2.29912543
9.14488697	3.62169242	2.16933250
8.10921383	10.27486515	2.16933250
2.95838714	3.62169242	2.16933250
1.92271352	10.27486515	2.16933250
5.48859596	4.32356119	1.73705697
4.45292234	10.97673416	1.73705697
11.67509651	4.32356119	1.73705697
10.63942242	10.97673416	1.73705697
7.71047688	5.75025272	1.45817900
6.67480278	12.40342522	1.45817900
1.52397668	5.75025272	1.45817900
0.48830301	12.40342522	1.45817900
9.87633419	8.59665012	1.13008654
4.72550774	1.94347775	1.13008654

3.68983388	8.59665012	1.13008654
10.91200733	1.94347775	1.13008654
6.35504007	0.01628161	0.72841984
5.31936645	6.66945457	0.72841984
-0.86713374	6.66945457	0.72841984
0.16853991	0.01628161	0.72841984
8.61688709	1.34844887	0.55037773
7.58121395	8.00162220	0.55037773
2.43038750	1.34844887	0.55037773
1.39471376	8.00162220	0.55037773
7.38836098	3.56898689	0.26360172
6.35268736	10.22215939	0.26360172
1.20186114	3.56898689	0.26360172
0.16618745	10.22215939	0.26360172
9.81825924	4.88769627	0.25251889
8.78258514	11.54086876	0.25251889
3.63175869	4.88769627	0.25251889
2.59608507	11.54086876	0.25251889

# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(111) with a C<sub>v</sub>

1.000000000000

12.37300000	0.00000000	0.00000000
-2.07134726	13.30634571	0.00000000
0.00000004	0.00000005	22.12540100
C	O	Fe
64	1	136

Cart

2.33690376	3.77682780	9.42831009
6.34352568	1.75366777	9.88731698
5.03086904	8.37347395	9.90100754
-1.23249439	8.46245085	9.93019275
-0.22490981	1.78447699	9.90214670
9.17400301	3.87079964	9.82406366
8.19706097	10.53325386	9.84524645
1.98067978	10.51954899	9.82581952
5.69982844	5.03302827	9.69641514
4.66185065	11.68562647	9.71673811
-1.53507655	11.79016441	9.73665469
-0.53681699	5.09772978	9.67965771
9.21717063	0.19735524	9.34928922
8.18648599	6.84477380	9.36233162
3.17067392	0.14415431	9.35834535
1.97052950	6.87298269	9.38789957

6.78166339	5.74512443	6.93771070
5.73990924	12.39831100	6.92824512
0.57167667	5.74568493	6.96467126
-0.43587897	12.42041344	6.95671038
9.42761809	7.69546355	6.73918935
4.29549097	1.04095061	6.72781828
3.23707228	7.67033769	6.75538537
10.50123506	1.03002118	6.73760408
7.51821455	2.04765805	6.57640180
6.43740112	8.70471214	6.60446167
1.29498361	2.09538850	6.69133053
0.25730962	8.71955738	6.62140263
9.08882256	10.67615207	6.26187511
3.94466995	4.00812610	6.25160048
2.90865501	10.66164502	6.26054747
10.13655907	4.02107831	6.26565848
8.43259705	2.90522354	3.87415236
7.38535899	9.55260583	3.87167821
2.22946549	2.89775889	3.87269491
1.20058125	9.55175654	3.87522293
4.87882185	4.85300732	3.51646113
3.84314847	11.50618076	3.51646113
11.06532192	4.85300732	3.51646113
10.02964878	11.50618076	3.51646113
8.08072281	5.89129591	3.40647149
7.04504919	12.54446888	3.40647149
1.89422262	5.89129591	3.40647149
0.85854894	12.54446888	3.40647149
5.59163237	1.16514635	3.18918610
4.55595875	7.81831932	3.18918610
11.77813244	1.16514635	3.18918610
10.74245834	7.81831932	3.18918610
9.29798985	6.73122358	0.77799785
4.14716339	0.07805078	0.77799785
3.11148977	6.73122358	0.77799785
10.33366299	0.07805078	0.77799785
6.68999243	1.82555234	0.41000685
5.65431881	8.47872543	0.41000685
-0.53218126	8.47872543	0.41000685
0.50349241	1.82555234	0.41000685
9.34398174	3.05093241	0.30731282
8.30830765	9.70410538	0.30731282
3.15748167	3.05093241	0.30731282
2.12180805	9.70410538	0.30731282

6.31061268	5.17102432	0.23606260
5.27493906	11.82419777	0.23606260
-0.91156107	11.82419777	0.23606260
0.12411259	5.17102432	0.23606260
3.39489046	3.57344631	10.86596046
8.59470652	2.05461173	9.88283631
7.65594307	8.70570332	9.88413292
2.85445378	1.93772353	9.98540346
1.50070419	8.69712516	9.89763152
5.13247331	3.24695985	10.00752184
3.93808598	9.95529716	9.85221792
11.08784253	3.36449659	9.85235264
10.11856326	10.05285890	9.88306063
9.89923018	5.59035111	9.59065137
8.91195069	12.25950637	9.60532691
3.68861457	5.36683574	9.55827371
2.74203068	12.18993579	9.57219990
7.12140468	0.15282173	9.36242895
5.98697318	6.85329399	9.41532137
0.86494284	0.32151764	9.46100807
-0.25110549	6.96367761	9.45932078
7.63091844	4.97139568	8.99482370
6.64302289	11.57351194	9.01144738
1.30319778	5.19311125	8.83074080
0.41230962	11.64547179	9.02123740
9.76992855	7.84808370	8.69510878
4.80018956	1.16568581	8.67712272
3.61902983	7.71978101	8.73003376
10.81020998	1.18333905	8.69327554
6.89016203	2.61303932	8.30722746
5.83247404	9.22399425	8.39238977
0.84682164	2.66328606	8.55039983
-0.36578745	9.26135468	8.40677865
9.37341279	3.29324261	7.95323690
8.38739695	9.95305796	7.97145263
3.36203638	3.22114341	7.95473109
2.18809754	9.93764057	7.96749565
5.43046292	4.69429990	7.83779406
4.40281921	11.35711078	7.82954598
11.52002238	4.71654610	7.80509909
10.57648649	11.39809191	7.85071132
8.70888219	0.74585913	7.52324367
7.63633166	7.40474805	7.55685317
2.54808128	0.75269356	7.59949570

1.45407043	7.42289530	7.56723407
9.38105718	5.71233284	6.96891601
8.39528004	12.36039782	6.98514400
3.23099826	5.68689027	6.97592365
2.20856069	12.35152496	6.98889140
6.39834521	0.44291083	6.83192962
5.32801515	7.08897911	6.86922185
-0.86736806	7.11841816	6.87233195
0.22049652	0.48172499	6.90976406
5.35423407	2.64127461	6.41452655
4.30105480	9.28301112	6.47019894
11.54982874	2.65101162	6.50283467
10.49005008	9.31285836	6.46347792
7.51211177	4.05613159	6.31028872
6.48392622	10.70013958	6.34739672
1.33413623	4.05328549	6.34538593
0.29385784	10.71603886	6.35731700
9.27368594	2.29961135	5.60248123
8.20714331	8.95049935	5.61365363
3.05344908	2.28536580	5.60833383
2.01978709	8.94980621	5.61883000
5.37491434	5.04156028	5.39151759
4.34331870	11.67643101	5.38879314
11.56565772	5.04667419	5.38959844
10.52753809	11.70974481	5.40243143
7.52601522	6.42416998	5.23791782
6.50590846	13.06672248	5.23574184
1.34078753	6.41241133	5.25257954
0.31347870	13.07594198	5.25686603
9.97454283	7.16030044	4.89161535
4.82755904	0.49576723	4.88940096
3.78261184	7.15677077	4.89365522
11.03687316	0.50078780	4.90011257
7.00540804	1.86722668	4.71990042
5.94729594	8.52769890	4.73579900
0.80205726	1.87808201	4.76610924
-0.23448084	8.52754616	4.74291799
9.30812731	4.62625316	4.52324121
8.27114430	11.27427847	4.52351736
3.11873893	4.61677945	4.51864325
2.07947746	11.27260568	4.52486916
4.85254870	2.86020762	3.78663891
3.81029260	9.51354550	3.78786587
11.04088509	2.86110899	3.78395749



10.00154495	9.51687145	3.78704119
7.02151012	4.27133465	3.67187500
5.98583651	10.92450714	3.67187500
0.83500999	4.27133465	3.67187500
-0.20066364	10.92450714	3.67187500
5.98730040	6.46236563	3.26705837
4.95162678	13.11553860	3.26705837
-1.23487330	13.11553860	3.26705837
-0.19919968	6.46236563	3.26705837
9.13459015	1.21606314	3.15154004
8.09891701	7.86923599	3.15154004
2.94809031	1.21606314	3.15154004
1.91241682	7.86923599	3.15154004
9.86151791	6.16859675	2.57775974
8.82584381	12.82176971	2.57775974
3.67501736	6.16859675	2.57775974
2.63934374	12.82176971	2.57775974
6.94373321	2.19821787	2.29912543
5.90805960	8.85139084	2.29912543
0.75723332	2.19821787	2.29912543
-0.27844033	8.85139084	2.29912543
9.14488697	3.62169242	2.16933250
8.10921383	10.27486515	2.16933250
2.95838714	3.62169242	2.16933250
1.92271352	10.27486515	2.16933250
5.48859596	4.32356119	1.73705697
4.45292234	10.97673416	1.73705697
11.67509651	4.32356119	1.73705697
10.63942242	10.97673416	1.73705697
7.71047688	5.75025272	1.45817900
6.67480278	12.40342522	1.45817900
1.52397668	5.75025272	1.45817900
0.48830301	12.40342522	1.45817900
9.87633419	8.59665012	1.13008654
4.72550774	1.94347775	1.13008654
3.68983388	8.59665012	1.13008654
10.91200733	1.94347775	1.13008654
6.35504007	0.01628161	0.72841984
5.31936645	6.66945457	0.72841984
-0.86713374	6.66945457	0.72841984
0.16853991	0.01628161	0.72841984
8.61688709	1.34844887	0.55037773
7.58121395	8.00162220	0.55037773
2.43038750	1.34844887	0.55037773

1.39471376	8.00162220	0.55037773
7.38836098	3.56898689	0.26360172
6.35268736	10.22215939	0.26360172
1.20186114	3.56898689	0.26360172
0.16618745	10.22215939	0.26360172
9.81825924	4.88769627	0.25251889
8.78258514	11.54086876	0.25251889
3.63175869	4.88769627	0.25251889
2.59608507	11.54086876	0.25251889

# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(111) with a C<sub>v</sub>

1.000000000000

12.37300000	0.00000000	0.00000000
-2.07134726	13.30634571	0.00000000
0.00000004	0.00000005	22.12540100

C	O	Fe
64	1	136

Cart

2.28433068	3.79162773	9.43111638
6.37170777	1.64385671	9.89958205
5.35415402	8.29664825	9.88295442
10.99299888	8.51851228	9.91770963
1.27714273	2.09037112	6.68850760
9.21834354	3.79845530	9.95796686
8.15456615	10.47704835	9.91981320
-0.45507443	12.40666041	6.98080794
5.56712474	4.98100800	9.80723451
4.55944057	11.65164812	9.77647787
-1.58933081	11.79531673	9.66512639
-0.59697535	5.18225483	9.63385236
9.16197197	0.09111637	9.30849316
8.10073155	6.69034524	9.30245151
3.07594569	0.20637990	9.39656126
2.29227225	6.69616125	9.32146304
6.75042733	5.75905518	6.87619738
5.70500460	12.41288179	6.87836770
0.54696402	5.75156739	6.98537481
1.27568787	10.48551730	9.44480489
9.43226691	7.69613834	6.73563268
4.28194463	1.03790041	6.74490438
3.21641633	7.69022519	6.73789164
10.48299679	1.03804233	6.73693530
7.50012486	2.04602551	6.53889145

6.46193149	8.69575695	6.52596226
-0.26259483	1.85434423	9.91867827
0.22515446	8.73897907	6.69904605
9.08881207	10.67759489	6.27342381
3.92923366	4.01332878	6.24468142
2.89217984	10.65732806	6.24148807
10.11444823	4.01987692	6.27683896
8.43478435	2.90730841	3.87261168
7.39697707	9.56080444	3.86927186
2.23082112	2.89781107	3.87462167
1.19375787	9.54875015	3.87732343
4.87882185	4.85300732	3.51646113
3.84314847	11.50618076	3.51646113
11.06532192	4.85300732	3.51646113
10.02964878	11.50618076	3.51646113
8.08072281	5.89129591	3.40647149
7.04504919	12.54446888	3.40647149
1.89422262	5.89129591	3.40647149
0.85854894	12.54446888	3.40647149
5.59163237	1.16514635	3.18918610
4.55595875	7.81831932	3.18918610
11.77813244	1.16514635	3.18918610
10.74245834	7.81831932	3.18918610
9.29798985	6.73122358	0.77799785
4.14716339	0.07805078	0.77799785
3.11148977	6.73122358	0.77799785
10.33366299	0.07805078	0.77799785
6.68999243	1.82555234	0.41000685
5.65431881	8.47872543	0.41000685
-0.53218126	8.47872543	0.41000685
0.50349241	1.82555234	0.41000685
9.34398174	3.05093241	0.30731282
8.30830765	9.70410538	0.30731282
3.15748167	3.05093241	0.30731282
2.12180805	9.70410538	0.30731282
6.31061268	5.17102432	0.23606260
5.27493906	11.82419777	0.23606260
-0.91156107	11.82419777	0.23606260
0.12411259	5.17102432	0.23606260
1.30985887	7.27253402	10.87321249
10.77532675	1.19404464	8.71643148
7.52375533	8.65121449	9.88285174
2.90652886	2.06102503	9.96825202
3.78171599	7.72179059	8.70548150

5.24810054	3.14443470	9.89844135
2.60998006	11.96296192	9.52775797
11.09307709	3.41203216	9.86397204
4.22476359	9.81763789	9.89200490
9.84496575	5.56105385	9.54301652
10.01669123	10.08139080	9.86321195
3.62144917	5.21714440	9.53618909
4.45715130	11.33802418	7.85766480
8.56506194	1.99364461	9.90976212
6.08930826	6.70422878	9.32868074
10.47439100	11.36780311	7.80086761
-0.21588895	7.07453850	9.78238796
7.54360971	4.69403559	9.48958019
7.11807733	0.07227783	9.32179221
1.22804343	5.20010258	8.81134082
0.23070602	11.88469964	8.83507093
9.72853977	7.80710905	8.71831340
4.78583542	1.04353783	8.71659358
2.35454923	9.91343426	7.96382734
8.82712499	12.23767822	9.55484729
6.92368422	2.55285504	8.28957914
5.88331021	9.20129214	8.27334594
0.83778374	2.68769164	8.54657111
-0.23044164	9.33884428	8.55781079
9.36904176	3.29440516	8.00382082
8.34761563	9.94856667	7.98337746
3.40227366	3.23486767	7.96369843
1.87412681	8.81611623	10.03234091
5.51306364	4.68117824	7.87253514
6.53653805	11.39519624	9.32513048
11.48881148	4.68824703	7.78623903
0.81749303	0.39247862	9.52249588
8.69178268	0.76841980	7.49824026
7.65064453	7.43247301	7.49493898
2.52668697	0.78969867	7.59628218
1.47859730	7.44921761	7.66991355
9.36753606	5.70572037	6.99554735
8.34638967	12.36334591	6.99246102
3.24909004	5.69134700	7.00958091
2.21227925	12.34544989	6.97314945
6.37191737	0.44061476	6.83029099
5.33835264	7.08356018	6.81775417
-0.85920444	7.13062279	6.92901590
0.18569057	0.48023581	6.92764076

5.35399862	2.63912026	6.41135681
4.30716394	9.28304894	6.41715178
11.54313587	2.64950270	6.49470276
10.50896948	9.30207589	6.50484244
7.51417051	4.05872800	6.32080221
6.47830775	10.71542915	6.32984848
1.34058622	4.06271068	6.35720167
0.30134986	10.70591063	6.36069023
9.26865216	2.31666056	5.60352396
8.22994045	8.97610047	5.59835134
3.05188337	2.29069418	5.61622377
2.00061127	8.93179772	5.63474366
5.37011356	5.02160522	5.39545124
4.33477050	11.67556090	5.39156594
11.56369580	5.05676102	5.39412281
10.53244912	11.70882951	5.39592782
7.53719085	6.43564491	5.22095934
6.50108795	13.08321535	5.22392859
1.34080333	6.41898447	5.28493369
0.30491237	13.06808003	5.26388569
9.99521829	7.15715381	4.90396782
4.81455937	0.49777441	4.88763386
3.77452901	7.14941690	4.89157976
11.02892406	0.50313203	4.89982671
6.99839669	1.86702907	4.70294020
5.95529176	8.52446326	4.69960196
0.80120570	1.87857664	4.76536863
-0.23824044	8.52746996	4.76680376
9.30778300	4.63132589	4.52604761
8.27261360	11.28652750	4.52595393
3.11275524	4.61653459	4.51666195
2.07717889	11.26408579	4.51265014
4.84754821	2.86161917	3.78175267
3.80833867	9.51237148	3.78658289
11.03897990	2.86286138	3.78405325
10.00154495	9.51687145	3.78704119
7.02151012	4.27133465	3.67187500
5.98583651	10.92450714	3.67187500
0.83500999	4.27133465	3.67187500
-0.20066364	10.92450714	3.67187500
5.98730040	6.46236563	3.26705837
4.95162678	13.11553860	3.26705837
-1.23487330	13.11553860	3.26705837
-0.19919968	6.46236563	3.26705837

9.13459015	1.21606314	3.15154004
8.09891701	7.86923599	3.15154004
2.94809031	1.21606314	3.15154004
1.91241682	7.86923599	3.15154004
9.86151791	6.16859675	2.57775974
8.82584381	12.82176971	2.57775974
3.67501736	6.16859675	2.57775974
2.63934374	12.82176971	2.57775974
6.94373321	2.19821787	2.29912543
5.90805960	8.85139084	2.29912543
0.75723332	2.19821787	2.29912543
-0.27844033	8.85139084	2.29912543
9.14488697	3.62169242	2.16933250
8.10921383	10.27486515	2.16933250
2.95838714	3.62169242	2.16933250
1.92271352	10.27486515	2.16933250
5.48859596	4.32356119	1.73705697
4.45292234	10.97673416	1.73705697
11.67509651	4.32356119	1.73705697
10.63942242	10.97673416	1.73705697
7.71047688	5.75025272	1.45817900
6.67480278	12.40342522	1.45817900
1.52397668	5.75025272	1.45817900
0.48830301	12.40342522	1.45817900
9.87633419	8.59665012	1.13008654
4.72550774	1.94347775	1.13008654
3.68983388	8.59665012	1.13008654
10.91200733	1.94347775	1.13008654
6.35504007	0.01628161	0.72841984
5.31936645	6.66945457	0.72841984
-0.86713374	6.66945457	0.72841984
0.16853991	0.01628161	0.72841984
8.61688709	1.34844887	0.55037773
7.58121395	8.00162220	0.55037773
2.43038750	1.34844887	0.55037773
1.39471376	8.00162220	0.55037773
7.38836098	3.56898689	0.26360172
6.35268736	10.22215939	0.26360172
1.20186114	3.56898689	0.26360172
0.16618745	10.22215939	0.26360172
9.81825924	4.88769627	0.25251889
8.78258514	11.54086876	0.25251889
3.63175869	4.88769627	0.25251889
2.59608507	11.54086876	0.25251889

# TS for CO dissociation on Fe<sub>3</sub>C(031) without a C<sub>v</sub>

1.000000000000

10.06780000	0.00000000	0.00000000
0.00000003	14.99310000	0.00000000
0.00000004	0.00000004	22.23570000

C	O	Fe
41	1	96

Cart

2.80576365	7.44925591	6.51882491
3.29337795	10.00216602	7.75650065
8.40630244	9.97050417	7.66903384
0.99305307	2.45695064	7.69586686
6.08382250	2.48101039	7.65151688
4.12754302	12.63898832	7.55800371
9.15962723	12.60846602	7.58566557
0.21308943	5.11806245	7.59679117
5.42819971	5.21079475	7.80869071
1.55602481	14.94017738	6.51048250
6.59604501	14.92447458	6.52531956
3.38758434	4.45439608	6.48271512
7.82882850	7.43562034	6.50555930
0.28653699	8.91036058	5.69075945
5.31682807	8.96373558	5.73512107
4.06628804	1.39809795	5.70235475
9.09572113	1.44997162	5.70087890
2.79815375	11.50868240	4.47264330
7.84523053	11.49314361	4.47407244
1.52465380	3.98774937	4.43049734
6.57151598	3.99751798	4.46668492
0.28578107	13.07211575	3.95883359
5.32649363	13.07160937	3.95501344
4.06583893	5.60701061	3.90763191
9.08339347	5.57410052	3.94722186
2.79130912	0.63184285	2.72906470
7.82520914	0.63184285	2.72906470
1.54535568	8.13231278	2.72313023
6.57925558	8.13231278	2.72313023
4.06785297	9.66406918	1.91907406
9.10175324	9.66406918	1.91907406
0.26797625	2.17058206	1.91625857
5.30187607	2.17058206	1.91625857
1.57854438	11.97409725	0.84189010

6.61244440	11.97409725	0.84189010
2.75741243	4.47900724	0.83368790
7.79131222	4.47900724	0.83368790
0.81482184	14.61165714	0.78635430
5.84872198	14.61165714	0.78635430
3.52061224	7.11863995	0.77661365
8.55451202	7.11863995	0.77661365
1.83548884	10.35771410	8.52756743
5.00351278	10.94036398	7.46067781
7.57654580	11.61407354	7.30264903
6.91318664	4.15051829	7.30752340
9.39883209	3.42941205	7.46430199
5.08859375	14.79900167	5.18390774
8.32643080	14.16801362	7.01258241
3.71109359	6.01525584	7.44980722
8.63076837	5.91003109	7.35609130
4.25092225	12.45618729	5.49370153
9.29587415	12.43572772	5.51863319
4.29643033	8.48997258	7.32665423
9.32330969	8.42746202	7.28588913
5.08622168	0.96479428	7.29746216
0.03300258	14.80191224	5.18216917
1.75689444	4.10558902	7.35894943
8.26737516	3.18880295	5.19329713
1.75731945	9.03139896	7.08349840
6.82481137	9.10966615	7.11449101
7.61472178	1.58694957	7.09249455
2.55742808	1.57429751	7.11130161
2.52784073	11.71151324	7.27743565
5.80482525	13.39512036	7.36178327
1.06235032	6.67045570	6.99190769
6.10200540	6.71712266	7.01534580
0.74403065	13.43129870	7.36247321
0.02351989	10.93496402	7.59853196
0.08890064	4.94529303	5.50320701
5.09426345	4.95274608	5.50827522
3.58913573	10.00077792	5.47617901
8.65961483	10.00319682	5.50054529
0.73103704	2.49875103	5.47983835
4.51094253	3.52933470	7.66437927
1.09464025	10.68042228	5.20394148
6.13985981	10.68502057	5.20465223
3.22575493	3.10476402	5.17812961
5.76818994	2.51075175	5.49990368



1.83467484	13.10572957	5.18710684
6.88311246	13.10119981	5.19455205
7.55820345	0.53583305	4.88482430
3.30000794	14.19921661	6.98330516
4.31511106	7.32887364	5.20613963
9.33685842	7.29354882	5.17203980
2.51107717	5.57855578	5.19039647
7.52217347	5.60879642	5.18630412
1.82817716	8.02405737	4.87386442
6.85149378	8.04642650	4.88809052
2.51946738	0.52984358	4.87827823
0.03612908	0.94035609	7.29886795
0.00918142	9.04103947	3.54266262
5.04308128	9.04103947	3.54266262
4.32987595	1.54505515	3.54207015
9.36377621	1.54505515	3.54207015
4.34845781	11.46142483	3.23901367
9.38235760	11.46142483	3.23901367
2.54830408	9.76696491	3.24620366
7.58220434	9.76696491	3.24620366
1.79143322	2.27329993	3.24228406
6.82533312	2.27329993	3.24228406
5.02409744	3.96758056	3.23083019
10.05799770	3.96758056	3.23083019
3.60822964	13.88251495	3.22705913
8.64212990	13.88251495	3.22705913
0.73003614	6.39000845	3.22002506
5.76393604	6.39000845	3.22002506
1.07754815	14.57939339	2.94978833
6.11144829	14.57939339	2.94978833
3.26006389	7.08647728	2.94436812
8.29396439	7.08647728	2.94436812
1.72237337	12.11856842	2.92840362
6.75627327	12.11856842	2.92840362
2.61565661	4.62633991	2.91964269
7.64955664	4.62633991	2.91964269
0.76246345	10.40605259	1.40558612
5.79636335	10.40605259	1.40558612
3.57397771	2.91102600	1.39963460
8.60787773	2.91102600	1.39963460
4.28322744	0.49661291	1.33552134
9.31712723	0.49661291	1.33552134
0.05220732	7.99454737	1.33009195
5.08610725	7.99454737	1.33009195

5.00888205	12.96122646	1.13939369
10.04278183	12.96122646	1.13939369
1.77243280	1.15037405	1.13561857
6.80633259	1.15037405	1.13561857
2.56385946	8.64926624	1.13208878
7.59775972	8.64926624	1.13208878
4.36085367	5.46748734	1.12869322
9.39475346	5.46748734	1.12869322
3.25199199	11.18562412	1.06188464
8.28589249	11.18562412	1.06188464
1.08420253	3.69017506	1.05508971
6.11810255	3.69017506	1.05508971
2.47195578	13.64442635	0.97683454
7.50585556	13.64442635	0.97683454
1.86463213	6.15024328	0.96754396
6.89853191	6.15024328	0.96754396

# TS for CO dissociation on Fe<sub>3</sub>C(031) with a C<sub>v</sub>

1.000000000000

10.06780000	0.00000000	0.00000000
0.00000003	14.99310000	0.00000000
0.00000004	0.00000004	22.23570100

C	O	Fe
40	1	96

Cart

3.27922881	9.97064209	7.75342061
8.38875291	9.94488438	7.66779630
1.00763401	2.45777566	7.65579673
6.04387373	2.46245908	7.65385713
4.12422293	12.61449171	7.55929754
9.15219003	12.58780374	7.58771226
0.23563298	5.08216515	7.57071025
5.27395689	5.09818475	7.56650702
1.56039467	14.91945732	6.51029863
6.59762444	14.90751263	6.52407559
2.78244308	7.41278946	6.50817548
7.80866537	7.39646216	6.51501496
0.27530253	8.90010051	5.69176252
5.30399619	8.94164950	5.73513254
4.06348351	1.43354481	5.71054667
9.09663800	1.43947345	5.70727525
2.79566449	11.49738238	4.47580595
7.84017011	11.48449786	4.47650900

1.54182747	3.99261692	4.46572397
6.57255366	3.99330843	4.46643053
0.28402712	13.07139480	3.96066743
5.32284931	13.07208866	3.95645546
4.05577590	5.58090442	3.95291002
9.08593788	5.57345438	3.94979850
2.79130912	0.63184285	2.72906470
7.82520914	0.63184285	2.72906470
1.54535568	8.13231278	2.72313023
6.57925558	8.13231278	2.72313023
4.06785297	9.66406918	1.91907406
9.10175324	9.66406918	1.91907406
0.26797625	2.17058206	1.91625857
5.30187607	2.17058206	1.91625857
1.57854438	11.97409725	0.84189010
6.61244440	11.97409725	0.84189010
2.75741243	4.47900724	0.83368790
7.79131222	4.47900724	0.83368790
0.81482184	14.61165714	0.78635430
5.84872198	14.61165714	0.78635430
3.52061224	7.11863995	0.77661365
8.55451202	7.11863995	0.77661365
1.82925632	10.33482772	8.52373593
4.98868890	10.90853231	7.45888155
7.56989877	11.59138839	7.30034061
4.38341069	3.42394848	7.45246954
9.41620063	3.41384431	7.45131091
0.73848342	13.41420887	7.36132212
5.79957485	13.37346579	7.35908672
3.59824754	5.88736991	7.35709392
8.63095207	5.87443851	7.36046265
2.52111657	11.68754622	7.27203719
9.29520385	12.42435477	5.52093578
4.27094395	8.44209598	7.32006290
9.30716957	8.39967015	7.28572173
7.60345584	1.57700477	7.09930599
2.57059550	1.58196647	7.09977063
1.84491280	4.10431335	7.28414093
6.87402607	4.10946099	7.28120242
1.74185878	9.00564144	7.08576783
6.81000987	9.07673696	7.10952823
0.04661479	0.93323340	7.29518968
5.08707534	0.93149933	7.29872083
3.29811082	14.17969622	6.99375109

8.32684928	14.15515844	7.01634542
1.04937196	6.63916956	6.98942111
6.07148858	6.67798107	7.01049800
4.24966841	12.44358682	5.49522956
0.01120448	10.91170424	7.60112083
0.09145862	4.93703238	5.49145187
5.12730030	4.94877069	5.49337395
3.58144945	9.98375051	5.47698654
8.65391154	9.99190488	5.50126386
0.74351192	2.48511443	5.47334007
5.77548772	2.48716378	5.47495334
1.08892109	10.67310802	5.20647411
6.13394919	10.67161212	5.20670101
3.24696421	3.17618917	5.19927569
8.27785961	3.17825589	5.19773419
1.83522866	13.10078696	5.18711455
6.87993763	13.09495341	5.19512304
5.07876153	14.79641832	5.18390046
0.03260370	14.79333808	5.18286294
4.30338079	7.30924649	5.19456067
9.33156487	7.28713523	5.17502579
2.50672073	5.59770299	5.18566959
7.53240502	5.60175712	5.19091823
1.81667603	8.01087731	4.86877716
6.84356641	8.03085882	4.89066356
7.56001928	0.52837278	4.88800762
2.52593550	0.53345673	4.88267414
0.00918142	9.04103947	3.54266262
5.04308128	9.04103947	3.54266262
4.32987595	1.54505515	3.54207015
9.36377621	1.54505515	3.54207015
4.34845781	11.46142483	3.23901367
9.38235760	11.46142483	3.23901367
2.54830408	9.76696491	3.24620366
7.58220434	9.76696491	3.24620366
1.79143322	2.27329993	3.24228406
6.82533312	2.27329993	3.24228406
5.02409744	3.96758056	3.23083019
10.05799770	3.96758056	3.23083019
3.60822964	13.88251495	3.22705913
8.64212990	13.88251495	3.22705913
0.73003614	6.39000845	3.22002506
5.76393604	6.39000845	3.22002506
1.07754815	14.57939339	2.94978833

6.11144829	14.57939339	2.94978833
3.26006389	7.08647728	2.94436812
8.29396439	7.08647728	2.94436812
1.72237337	12.11856842	2.92840362
6.75627327	12.11856842	2.92840362
2.61565661	4.62633991	2.91964269
7.64955664	4.62633991	2.91964269
0.76246345	10.40605259	1.40558612
5.79636335	10.40605259	1.40558612
3.57397771	2.91102600	1.39963460
8.60787773	2.91102600	1.39963460
4.28322744	0.49661291	1.33552134
9.31712723	0.49661291	1.33552134
0.05220732	7.99454737	1.33009195
5.08610725	7.99454737	1.33009195
5.00888205	12.96122646	1.13939369
10.04278183	12.96122646	1.13939369
1.77243280	1.15037405	1.13561857
6.80633259	1.15037405	1.13561857
2.56385946	8.64926624	1.13208878
7.59775972	8.64926624	1.13208878
4.36085367	5.46748734	1.12869322
9.39475346	5.46748734	1.12869322
3.25199199	11.18562412	1.06188464
8.28589249	11.18562412	1.06188464
1.08420253	3.69017506	1.05508971
6.11810255	3.69017506	1.05508971
2.47195578	13.64442635	0.97683454
7.50585556	13.64442635	0.97683454
1.86463213	6.15024328	0.96754396
6.89853191	6.15024328	0.96754396

# TS for CO dissociation on Fe<sub>3</sub>C(102) without a C<sub>v</sub>

1.000000000000

11.01580000	0.00000000	0.00000000
0.00000002	13.40160000	0.00000000
0.00000004	0.00000004	22.47150000

C	O	Fe
41	1	96

Cart

4.24905847	5.40069156	8.26510359
1.34490739	5.81001942	8.40856548
1.33738216	12.60128310	8.47344568

9.32971809	4.07977509	8.23628818
9.40850645	10.78832066	8.27668932
9.35563930	7.66164727	8.23477127
9.36298229	0.98711580	8.26472338
4.70826832	7.55096796	5.95183663
4.28041442	12.62993116	8.23270907
3.31745757	9.44119555	7.69086249
3.28873021	2.45400908	7.62273518
6.33315947	9.41948022	6.99358256
6.30704894	2.49383622	6.92131016
7.61904485	5.80253487	6.87254099
7.68589712	12.54593711	6.85373923
10.70322061	5.86487518	6.26318311
10.72149903	12.57924546	6.26821636
9.77480003	9.18222672	5.37653280
9.76089641	2.46462758	5.36093451
3.07409861	5.69537645	4.76388538
3.10730960	12.50243685	4.77571608
1.76415014	9.22609609	4.79069545
1.74703062	2.46962757	4.79270915
6.09387875	5.81395006	4.26611090
6.09387875	12.51475048	4.26611090
5.16361475	9.16121387	3.32155538
5.16361475	2.46041346	3.32155538
8.21825695	9.16481876	2.76375627
8.21825695	2.46401906	2.76375627
9.56017304	5.83251572	2.68237734
9.56017304	12.53331566	2.68237734
1.54647672	5.81414414	1.97793257
1.54647672	12.51494408	1.97793257
0.58884203	9.02470303	1.35454476
0.58884203	2.32390261	1.35454476
6.51847029	4.25338030	1.35242224
6.51847029	10.95418072	1.35242224
6.52053356	7.37137270	1.35086727
6.52053356	0.67057264	1.35086727
3.50100756	9.15109539	1.15644598
3.50100756	2.45029497	1.15644598
4.63406237	6.91058701	9.08537671
8.75630838	5.88166058	8.42986240
9.11368019	0.37650418	6.15806044
2.79184537	7.00043927	8.24338957
2.71134438	0.47235633	8.17366005
2.63349238	4.43634211	8.13905154

2.72220892	11.36051315	8.18895828
6.12070866	5.94259181	8.14811286
6.21718252	12.62990680	8.18009665
7.46741313	3.79104740	7.85640054
7.55215067	10.55668488	7.91935283
7.52860404	8.07350201	7.84398086
0.07929382	0.40513556	7.80505071
0.10721509	7.09620332	7.81968220
1.66941245	12.55911521	6.15211327
0.05673239	4.61682982	7.77997681
8.83310911	12.59660878	8.46363570
4.87271085	3.66585936	7.56732758
4.90125851	10.64132161	7.58416259
4.90044296	8.23170338	7.65178469
4.89339161	1.21636176	7.53042296
1.37941367	9.23044832	7.59009227
1.30797339	2.46730913	7.46216078
9.82237023	9.22347179	7.34450155
9.76744050	2.52244228	7.32003130
4.22015262	5.78223050	6.36716401
4.32971605	12.58493969	6.30364971
1.65246903	5.83728378	6.15417818
0.11255325	11.34686052	7.81185067
9.10504298	7.08557920	6.16452527
7.50629931	1.28992544	7.87470071
9.10761916	4.64556081	6.14496418
9.14609216	11.33869411	6.15910510
2.88195751	8.05319208	5.96510131
2.95266788	1.27293167	5.83890175
2.94696618	3.67871796	5.82603472
2.95961357	10.46287003	5.85422165
6.52254143	6.99585796	5.78044249
6.46846208	4.57738621	5.79828874
6.53545031	11.32367212	5.80944424
6.52625614	0.36260671	5.78713144
7.78583310	9.19519743	5.54777809
7.77833896	2.49405168	5.52332943
0.34930477	7.96044449	5.51182430
0.32373543	3.69796085	5.48711033
0.32896517	1.24921863	5.48220831
0.34943565	10.40288300	5.51533322
5.23140819	9.23540958	5.28116587
5.17650314	2.46270191	5.25726326
10.69425106	5.81395006	4.34699440

10.69425106	12.51475048	4.34699440
4.52206469	7.03530502	4.07911348
4.52206469	4.59259558	4.07911348
4.52206469	11.29339504	4.07911348
4.52206469	0.33450499	4.07911348
8.06567287	5.81395006	4.06464910
8.06567287	12.51475048	4.06464910
9.37696266	7.94299555	3.78912735
9.37696266	3.68490505	3.78912735
9.37696266	1.24219537	3.78912735
9.37696266	10.38570499	3.78912735
1.91001427	7.02113771	3.74295783
1.91001427	0.32033783	3.74295783
1.90148330	4.59789467	3.73080110
1.90148330	11.29869461	3.73080110
6.75760937	7.94480467	3.43389630
6.75760937	1.24400473	3.43389630
6.75540495	3.67919850	3.43265676
6.75540495	10.37999821	3.43265676
3.20063019	9.15871143	3.42493272
3.20063019	2.45791125	3.42493272
0.55113077	9.17330837	3.25715280
0.55113077	2.47250819	3.25715280
6.07962179	5.81109572	2.26416254
6.07962179	12.51189613	2.26416254
10.96803188	4.59199285	2.08241653
10.96803188	11.29279327	2.08241653
3.50234199	5.78909206	2.07739234
3.50234199	12.48989201	2.07739234
10.98624611	7.07002163	2.05453277
10.98624611	0.36922148	2.05453277
4.76950121	7.92010069	1.78491962
4.76950121	1.21930063	1.78491962
4.76405430	3.68990970	1.78023994
4.76405430	10.39070988	1.78023994
8.38025951	4.57472420	1.73071468
8.38025951	11.27552414	1.73071468
8.38388634	7.07043266	1.72176302
8.38388634	0.36963257	1.72176302
9.71496391	9.17632866	1.45127761
9.71496391	2.47552896	1.45127761
2.15475440	7.85452461	1.43979466
2.15475440	1.15372443	1.43979466
2.09838200	3.69581842	1.43469214



2.09838200	10.39661884	1.43469214
7.10175276	9.16563415	1.17035198
7.10175276	2.46483397	1.17035198

# TS for CO dissociation on Fe<sub>3</sub>C(102) with a C<sub>v</sub>

1.000000000000

11.01580000	0.00000000	0.00000000
0.00000002	13.40160000	0.00000000
0.00000004	0.00000004	22.47150000

C	O	Fe
40	1	96

Cart

4.27244856	5.33598732	8.23031916
1.36368801	5.78503569	8.38505069
1.34733305	12.51741876	8.43793690
9.32822035	4.02822486	8.23448303
9.37401677	10.72700744	8.24272207
9.35566375	7.61116532	8.23010171
9.36458249	0.91361843	8.25145038
4.28049435	12.52073754	8.21502972
3.32686867	9.29988789	7.57193048
3.29556583	2.40119076	7.61794572
6.31574358	9.23616817	6.90582862
6.30978565	2.41413047	6.91938502
7.62224946	5.80773948	6.8566253
7.68069724	12.50631995	6.81190513
10.70809859	5.81987733	6.26274064
10.71800888	12.52623551	6.26343451
9.77750183	9.16544973	5.36696406
9.76284943	2.46090922	5.36908338
3.10692751	5.80723472	4.80253299
3.10606087	12.50517440	4.76632106
1.76412239	9.14653202	4.80482393
1.75227320	2.45906744	4.79921869
6.09387875	5.81395006	4.26611090
6.09387875	12.51475048	4.26611090
5.16361475	9.16121387	3.32155538
5.16361475	2.46041346	3.32155538
8.21825695	9.16481876	2.76375627
8.21825695	2.46401906	2.76375627
9.56017304	5.83251572	2.68237734
9.56017304	12.53331566	2.68237734
1.54647672	5.81414414	1.97793257

1.54647672	12.51494408	1.97793257
0.58884203	9.02470303	1.35454476
0.58884203	2.32390261	1.35454476
6.51847029	4.25338030	1.35242224
6.51847029	10.95418072	1.35242224
6.52053356	7.37137270	1.35086727
6.52053356	0.67057264	1.35086727
3.50100756	9.15109539	1.15644598
3.50100756	2.45029497	1.15644598
4.63953454	6.88742363	9.06480390
8.76386007	5.82546579	8.42077662
0.08609460	0.34132551	7.79786546
2.79816813	7.00929754	8.19652421
2.71892607	0.38847399	8.15841753
2.64589063	4.40555999	8.12658974
2.72587028	11.25967796	8.14155998
6.11947502	5.88362325	8.13204699
6.20494568	12.53671369	8.14160604
7.46627136	3.72775988	7.83773705
7.51521503	10.44283437	7.86426591
7.52389740	7.97115384	7.83139489
7.50677204	1.22424197	7.88213774
0.10775146	7.05297789	7.81005750
0.33176901	1.23988289	5.48338987
0.06516704	4.57577472	7.78934651
0.10461094	11.27615053	7.79689287
4.88043616	3.60805225	7.52986462
4.90426683	10.51639581	7.51585639
4.90978859	8.06913110	7.57761504
4.89067896	1.15449055	7.53198134
1.38371387	9.15281074	7.50080237
1.32138690	2.41782092	7.47298379
9.81534543	9.16680203	7.32756761
9.77770382	2.46904115	7.33125971
4.29810298	5.81850627	6.37465318
4.32159473	12.52955591	6.29615811
1.65888927	5.81143629	6.16537851
1.66758037	12.51912009	6.14463989
9.10969189	7.03352533	6.15235491
8.80405947	12.52061723	8.42619943
9.10823462	4.60035589	6.14942523
9.13835516	11.29346395	6.14777449
2.98027900	7.94083425	5.87075115
2.95907064	1.25032816	5.84198580

2.95460861	3.67666683	5.81925563
2.95631100	10.39214336	5.82467919
6.47400151	7.04062870	5.79881189
6.48090586	4.59438268	5.79091111
6.52081730	11.28834340	5.78079723
6.51822080	0.34273101	5.78954079
7.79066300	9.16846163	5.51188150
7.78007438	2.46993458	5.52439134
0.34035979	7.93532894	5.49803388
0.33008226	3.68813954	5.49536411
9.12072951	0.33862370	6.15309827
0.35294630	10.38347626	5.49593398
5.18631074	9.16811105	5.25578966
5.18643630	2.45978810	5.25308315
10.69425106	5.81395006	4.34699440
10.69425106	12.51475048	4.34699440
4.52206469	7.03530502	4.07911348
4.52206469	4.59259558	4.07911348
4.52206469	11.29339504	4.07911348
4.52206469	0.33450499	4.07911348
8.06567287	5.81395006	4.06464910
8.06567287	12.51475048	4.06464910
9.37696266	7.94299555	3.78912735
9.37696266	3.68490505	3.78912735
9.37696266	1.24219537	3.78912735
9.37696266	10.38570499	3.78912735
1.91001427	7.02113771	3.74295783
1.91001427	0.32033783	3.74295783
1.90148330	4.59789467	3.73080110
1.90148330	11.29869461	3.73080110
6.75760937	7.94480467	3.43389630
6.75760937	1.24400473	3.43389630
6.75540495	3.67919850	3.43265676
6.75540495	10.37999821	3.43265676
3.20063019	9.15871143	3.42493272
3.20063019	2.45791125	3.42493272
0.55113077	9.17330837	3.25715280
0.55113077	2.47250819	3.25715280
6.07962179	5.81109572	2.26416254
6.07962179	12.51189613	2.26416254
10.96803188	4.59199285	2.08241653
10.96803188	11.29279327	2.08241653
3.50234199	5.78909206	2.07739234
3.50234199	12.48989201	2.07739234

10.98624611	7.07002163	2.05453277
10.98624611	0.36922148	2.05453277
4.76950121	7.92010069	1.78491962
4.76950121	1.21930063	1.78491962
4.76405430	3.68990970	1.78023994
4.76405430	10.39070988	1.78023994
8.38025951	4.57472420	1.73071468
8.38025951	11.27552414	1.73071468
8.38388634	7.07043266	1.72176302
8.38388634	0.36963257	1.72176302
9.71496391	9.17632866	1.45127761
9.71496391	2.47552896	1.45127761
2.15475440	7.85452461	1.43979466
2.15475440	1.15372443	1.43979466
2.09838200	3.69581842	1.43469214
2.09838200	10.39661884	1.43469214
7.10175276	9.16563415	1.17035198
7.10175276	2.46483397	1.17035198

# TS for CO dissociation on Fe<sub>3</sub>C(131) without a C<sub>v</sub>

1.000000000000

12.25530000	0.00000000	0.00000000
-2.38850589	13.25166596	0.00000000
0.00000004	0.00000005	21.25600100
C	O	Fe
45	1	96

Cart

2.25283085	6.50809331	6.74770278
3.38202521	3.84914996	8.00249531
1.43438635	12.32104235	7.89109136
10.25440587	1.66290386	7.52327762
9.04593900	8.30289213	7.50996332
9.72370532	5.09947995	7.44062741
8.46354309	10.43240961	4.76127381
6.33330259	5.97558209	7.24987213
5.07495947	12.65917475	7.27596811
7.58138349	2.35122788	7.06159644
6.35172144	8.97777428	7.05118458
0.41347613	4.27249179	6.86819464
-0.71102036	10.96862145	6.61299395
0.81800889	1.20388502	6.77373780
-0.45037969	7.90733040	6.57624985
4.47608110	4.59137434	5.36231622

3.13651228	11.06057860	5.71598200
4.69873365	1.49117113	5.32010716
3.56616281	8.14045706	5.17415664
10.70168174	0.20499279	4.99871701
9.48005095	6.83669201	4.98458038
9.68289661	3.78831825	4.75189750
8.51207505	11.69939214	7.44426573
2.31291199	0.37301424	3.71090221
1.11865902	6.99884701	3.71090221
1.32024336	3.98045111	3.48570275
0.12599038	10.60628414	3.48570275
7.25680780	2.63475370	3.27525186
6.06255484	9.26058674	3.27525186
6.27615499	6.19979715	3.10429907
5.08190203	12.82563019	3.10429907
11.15591240	2.80662537	1.85426259
9.96165943	9.43245792	1.85426259
10.26668167	6.36503696	1.84332585
9.07242870	12.99086952	1.84332585
4.11546373	4.99648762	1.50322902
2.92121053	11.62232018	1.50322902
4.31588459	1.85071790	1.48528659
3.12163162	8.47655106	1.48528659
1.00381875	5.67873001	1.17111504
-0.19043419	12.30456257	1.17111504
1.64606690	2.42555165	1.06123793
0.45181391	9.05138493	1.06123793
8.50366020	0.27873534	0.54604721
7.30940676	6.90456820	0.54604721
3.42620038	7.74615123	7.78968714
1.17579659	10.89563510	6.78459682
4.11124432	0.78101335	7.41242021
2.18958085	2.33703468	7.72482612
-0.23638911	11.96324191	4.83043729
2.65636700	1.24348550	5.49876013
3.07182163	9.30288621	6.82760815
4.51576107	5.32504096	7.33029128
8.03920303	5.56808579	8.12400030
9.20686050	3.24142366	7.39543808
7.98716556	9.86151572	7.38663898
0.35054553	6.25044273	7.07403374
-0.41472095	9.50278392	5.40512272
10.50777384	2.12852659	5.41033722
10.05459289	6.87449068	6.89374520

6.60449744	3.93481270	6.96145393
6.81565804	12.18473928	8.11355953
2.22076086	4.63312016	6.83155006
3.28048625	12.04290961	7.34037762
8.68818466	0.83960102	6.76696071
7.45256507	7.47714082	6.76590899
4.23682604	3.02744843	6.56968460
5.36766080	10.56916826	6.97665278
6.26655017	1.16111923	6.47217521
4.95793774	7.76892895	6.59212977
-0.38377617	2.59168248	7.50633021
9.77985038	11.24806429	6.05493269
8.50382188	5.18667625	5.75202930
7.31017514	11.81292778	5.75646216
11.29249132	0.22744910	6.93702062
-0.46618883	12.82689647	7.21570988
0.81201006	2.92853789	5.48347689
1.48876449	7.82524768	5.56518967
10.97284760	4.58652354	6.07181837
9.27611826	8.76797333	5.40016912
6.02529150	5.73826259	5.33305752
4.79742107	12.30311333	5.34992782
8.02264151	2.73760085	5.15177892
6.78909903	9.37523092	5.15610465
3.36809667	6.18015602	5.19037566
2.18529180	12.74980784	5.12587035
0.39801416	0.45980230	4.94091932
-0.82740876	7.05898510	4.87254228
0.94873401	5.36061163	4.79695796
-1.57849156	9.28048710	7.42199830
5.61464835	3.16100700	4.62178848
4.34213973	9.84169225	4.71047274
2.97331079	3.66679784	4.44797140
1.81638501	10.26121003	4.42124790
8.91923550	0.46496729	4.15201493
7.72590621	7.10952912	4.12777664
6.35152880	0.95552196	3.95820542
5.16760858	7.62272408	3.95749693
9.76671028	5.40936232	3.71097636
8.57245731	12.03519535	3.71097636
-0.65484261	3.68870687	3.62123847
-1.84909558	10.31453991	3.62123847
7.30014229	4.57573605	3.45908976
6.10588932	11.20156860	3.45908976

3.94268513	1.50069594	3.44737101
2.74843216	8.12652874	3.44737101
4.69885063	5.05109930	3.28788567
3.50459790	11.67693234	3.28788567
1.40509236	2.01450324	3.18216968
0.21083943	8.64033604	3.18216968
9.28441429	2.89875793	3.07764530
8.09016132	9.52459049	3.07764530
11.10470676	1.19581735	3.08856487
9.91045380	7.82165051	3.08856487
2.27633667	5.56089735	2.69547486
1.08208370	12.18673039	2.69547486
-0.23673894	6.12739277	2.55241013
-1.43099189	12.75322628	2.55241013
5.68936014	2.97972059	2.12121320
4.49510717	9.60555363	2.12121320
7.63962316	1.24280357	1.88798439
6.44537020	7.86863661	1.88798439
3.21764994	3.35256600	1.74998808
2.02339697	9.97839928	1.74998808
8.41606617	6.08661365	1.74018729
7.22181320	12.71244621	1.74018729
5.30755520	0.30048525	1.67762649
4.11330223	6.92631817	1.67762649
0.66523141	3.91109681	1.60902893
-0.52902150	10.53693008	1.60902893
10.31909657	4.46215439	1.41221321
9.12484360	11.08798695	1.41221321
2.69262552	0.87311536	1.25545239
1.49837267	7.49894810	1.25545239
6.08439112	5.48753309	1.23569620
4.89013815	12.11336613	1.23569620
7.91476154	3.69234300	1.22194362
6.72050858	10.31817627	1.22194362
0.06142718	1.44478715	1.08450759
-1.13282573	8.07062054	1.08450759
9.73022079	1.78445995	0.82899422
8.53596783	8.41029263	0.82899422

# TS for CO dissociation on Fe<sub>3</sub>C(131) with a C<sub>v</sub>

1.000000000000

12.25530000	0.00000000	0.00000000
-2.38850589	13.25166596	0.00000000

	0.00000004	0.00000005	21.25600100
	C	O	Fe
	44	1	96
Cart			
	3.30232401	3.63360673	8.08234714
	2.18900547	10.44043019	7.99906056
	10.27076452	1.73588523	7.50520496
	9.06845427	8.36387241	7.49681823
	9.72571508	5.11745239	7.38667369
	8.45291684	11.75227168	7.37093845
	6.68737324	5.75610284	7.00368406
	4.97841494	12.72569391	7.16983544
	7.61068017	2.32517270	7.08919535
	6.38767035	8.97713239	7.09842907
	0.43142129	4.41657579	6.65662650
	-0.77941744	11.02438128	6.70957637
	0.72618558	1.32500443	6.69274103
	-0.44295778	7.96973092	6.70760907
	4.46260435	4.54054705	5.43567422
	3.24262503	11.16097529	5.44312022
	4.71075066	1.46637873	5.31361208
	3.48664437	8.11346235	5.24460429
	10.67522004	0.21929935	4.99526850
	9.48490856	6.83678459	5.00914460
	9.62365181	3.80594359	4.76131182
	8.45036284	10.42619934	4.75823510
	2.31291199	0.37301424	3.71090221
	1.11865902	6.99884701	3.71090221
	1.32024336	3.98045111	3.48570275
	0.12599038	10.60628414	3.48570275
	7.25680780	2.63475370	3.27525186
	6.06255484	9.26058674	3.27525186
	6.27615499	6.19979715	3.10429907
	5.08190203	12.82563019	3.10429907
	11.15591240	2.80662537	1.85426259
	9.96165943	9.43245792	1.85426259
	10.26668167	6.36503696	1.84332585
	9.07242870	12.99086952	1.84332585
	4.11546373	4.99648762	1.50322902
	2.92121053	11.62232018	1.50322902
	4.31588459	1.85071790	1.48528659
	3.12163162	8.47655106	1.48528659
	1.00381875	5.67873001	1.17111504
	-0.19043419	12.30456257	1.17111504



1.64606690	2.42555165	1.06123793
0.45181391	9.05138493	1.06123793
8.50366020	0.27873534	0.54604721
7.30940676	6.90456820	0.54604721
3.28327843	5.40027760	8.48167394
2.14159564	2.20368553	7.76084113
1.01243043	8.93005884	7.73683971
-0.40309066	2.71425365	7.45884667
-1.59085406	9.32413079	7.48147363
3.97405037	0.42547229	7.33382337
2.76280744	7.03341135	7.48845111
4.75839893	5.37733474	7.27319723
3.33804255	11.85022171	7.28557001
9.22823851	3.29500315	7.35307109
8.01611136	9.92319281	7.35539128
0.37417640	6.30306761	7.12445488
-0.81964244	12.91824589	7.13186377
11.22668185	0.25196955	6.90920365
10.05790655	6.88262018	6.92175085
6.60944037	3.83915614	6.85673752
5.44107721	10.59384657	6.93160952
2.26324003	4.61935709	6.87246360
1.05831900	11.25761712	6.80755227
8.67922372	0.78969282	6.86157063
7.48374148	7.45841222	6.82240789
4.27488118	2.94281901	6.67680768
3.07548196	9.47905215	6.64041670
6.25369885	1.10939661	6.53615138
5.02046648	7.84520423	6.44418616
10.93231481	4.65429431	5.98826757
9.74833984	11.26745481	6.01824888
8.43303213	5.24443565	5.88036285
7.30168814	11.82489440	5.78563168
0.82597055	2.95051321	5.45881899
-0.37150161	9.57721365	5.47144619
2.65042543	1.26047045	5.49150234
1.46599730	7.86902973	5.50545101
10.48927428	2.15386616	5.38895189
9.30093552	8.78117494	5.39883923
6.00974053	5.72412720	5.23670350
4.82392616	12.31423784	5.30605519
8.01532246	2.70305290	5.15881410
6.81036309	9.33647804	5.16468605
3.36846440	6.14474005	5.15587531

2.16548794	12.76297758	5.11458635
0.36478226	0.47764159	4.91541949
-0.82549876	7.10992667	4.91408367
0.95155161	5.36333189	4.82013892
-0.26005074	11.98907497	4.81377718
5.58247610	3.14092948	4.63189716
4.39438176	9.79837893	4.63509600
2.98919574	3.66246446	4.44322700
1.79542374	10.27776058	4.42171378
8.92368164	0.47764384	4.14143339
7.74446458	7.11389095	4.12431324
6.35539339	0.96013587	3.96644092
5.15323623	7.60557206	3.93955174
9.76671028	5.40936232	3.71097636
8.57245731	12.03519535	3.71097636
-0.65484261	3.68870687	3.62123847
-1.84909558	10.31453991	3.62123847
7.30014229	4.57573605	3.45908976
6.10588932	11.20156860	3.45908976
3.94268513	1.50069594	3.44737101
2.74843216	8.12652874	3.44737101
4.69885063	5.05109930	3.28788567
3.50459790	11.67693234	3.28788567
1.40509236	2.01450324	3.18216968
0.21083943	8.64033604	3.18216968
9.28441429	2.89875793	3.07764530
8.09016132	9.52459049	3.07764530
11.10470676	1.19581735	3.08856487
9.91045380	7.82165051	3.08856487
2.27633667	5.56089735	2.69547486
1.08208370	12.18673039	2.69547486
-0.23673894	6.12739277	2.55241013
-1.43099189	12.75322628	2.55241013
5.68936014	2.97972059	2.12121320
4.49510717	9.60555363	2.12121320
7.63962316	1.24280357	1.88798439
6.44537020	7.86863661	1.88798439
3.21764994	3.35256600	1.74998808
2.02339697	9.97839928	1.74998808
8.41606617	6.08661365	1.74018729
7.22181320	12.71244621	1.74018729
5.30755520	0.30048525	1.67762649
4.11330223	6.92631817	1.67762649
0.66523141	3.91109681	1.60902893

-0.52902150	10.53693008	1.60902893
10.31909657	4.46215439	1.41221321
9.12484360	11.08798695	1.41221321
2.69262552	0.87311536	1.25545239
1.49837267	7.49894810	1.25545239
6.08439112	5.48753309	1.23569620
4.89013815	12.11336613	1.23569620
7.91476154	3.69234300	1.22194362
6.72050858	10.31817627	1.22194362
0.06142718	1.44478715	1.08450759
-1.13282573	8.07062054	1.08450759
9.73022079	1.78445995	0.82899422
8.53596783	8.41029263	0.82899422

# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(510) step without a Cv

1.000000000000

9.97980022	0.00000000	0.00000000
-0.76395801	12.66177369	0.00000000
0.00000004	0.00000004	19.64039993

C	O	Fe
37	1	77

Cart

7.98500981	0.24311057	6.50403060
4.16108332	3.09734108	5.21220520
5.44920097	9.32178136	7.51579372
1.92923198	1.27531672	6.26532453
4.81729353	6.24790580	6.01287849
2.81200966	6.93744617	7.44188576
7.87675246	6.87224723	7.13408705
4.69461734	10.64657533	4.16023984
7.19952985	12.34307220	3.64282859
2.15195274	4.20623431	7.16341879
7.66991977	10.04777252	6.10300379
2.57785477	10.09189240	6.11234606
0.39259000	8.80563456	5.95543876
9.15914801	3.11784614	5.21483155
4.65981955	1.89373950	7.58882159
-0.31678094	10.89276153	4.25144680
4.21869124	7.23803489	3.38804628
6.72914204	5.59803959	4.00612288
1.70825732	5.68505978	4.02180814
2.22496053	12.34875417	3.66518450
4.54135191	11.97933704	6.64272822

7.19774284	4.13219427	7.17679536
9.21181863	7.19559625	3.41261540
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
8.81405025	1.08134787	8.03343483
3.96554752	10.35110526	7.27206126
0.12183735	0.87953082	6.72116092
-0.41264127	7.54609581	6.99088311
8.11750728	6.68355266	5.03992099
6.30525834	11.05170753	6.92323747
3.72969807	5.26215029	7.19814535
5.78831364	2.18624568	4.52942417
4.48768762	7.77747438	7.05910129
8.20194953	1.41992433	4.94941046
3.14288046	2.68947033	6.86020128
0.00798523	4.86903216	4.72649218
6.41715714	5.80131999	6.86374612
5.57663358	3.30460729	6.75691838
6.92515519	8.46809133	6.71951303
0.77850979	2.14380434	4.52342540
2.06062532	8.37380364	6.61878015
0.74207378	12.37906292	4.98398824
5.64352339	12.31723348	4.87799654
6.21566412	0.92428697	6.89791682
7.47538542	4.11600054	5.11844021
2.50047167	4.22376992	5.06681562
0.69867638	7.30119912	4.71363428
5.72423749	7.32356347	4.71871897
6.40621696	9.77194343	4.59436856
8.24659145	2.59093839	7.06225327
3.26611826	11.55105518	5.18548326
1.31255242	9.88274165	4.71163002

0.61632354	3.31069032	6.63484577
3.72704354	0.37236651	7.06097859
1.32074495	5.87346490	6.85717857
3.16370159	6.69116816	5.02623050
8.87080629	9.21705599	4.95684184
5.01202266	4.81523471	4.74992697
8.83079033	5.15190000	7.01286888
3.84782344	9.09093253	4.91533702
8.16720172	11.67757896	5.30238950
3.25349971	1.41393197	4.81086906
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453

6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(510) step with a Cv

1.000000000000

9.97980022	0.00000000	0.00000000
-0.76395801	12.66177369	0.00000000
0.00000004	0.00000004	19.64039993

C	O	Fe
36	1	77

Cart

2.48635936	10.25799228	6.23266095
4.67975845	1.84157453	7.58996655
5.48808262	9.34201311	7.47815593
7.18424392	4.13430745	7.13717024
2.20364204	4.17389035	7.17067272
2.98206342	6.84779849	7.09626547
7.88359853	6.84044420	7.07985898
4.63290537	11.98693637	6.57163815
1.84157245	1.37536127	6.22342712
7.69004354	10.07632318	6.09641836
8.10012162	0.44285547	6.61999343
0.41389007	8.79068544	5.95921619
4.17354090	3.11097189	5.23461128
9.17481130	3.12323118	5.23118191
-0.32192491	10.89610380	4.25065617
4.70569158	10.64608662	4.16562862
6.70808815	5.65445731	4.04104957
1.71696352	5.67997494	4.02669849
2.22648122	12.34779982	3.67810211
7.20231671	12.34089014	3.63364955
4.22848771	7.22140868	3.46996472
9.21694650	7.20195949	3.41083034
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899

9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
2.24347991	11.23942663	7.78225794
3.96909621	10.40387311	7.34613742
3.73822784	0.20698388	7.19303956
6.34341599	11.05848668	6.94970429
3.85374887	5.18013210	6.98755873
8.80796767	5.11259879	6.98185202
-0.38689900	7.48987407	6.96181913
4.63777099	7.74590836	6.93761490
8.19120849	2.55224225	6.91060170
3.16916269	2.62076829	6.88431014
1.37771547	5.82262414	6.79332148
6.32804904	5.82446383	6.77002742
6.97596031	8.46260035	6.73407236
5.57904224	3.30321137	6.75121492
0.65907818	3.24557213	6.66053920
2.11431888	8.40196908	6.59439514
0.01954634	0.82828536	6.62914425
6.25254998	0.91784243	6.94200565
8.17735802	11.70175640	5.27628245
3.30797480	11.56749963	5.16388546
2.49789491	4.18344684	5.04732921
7.46353069	4.12219909	5.07589821
3.14573432	6.67677894	5.03501498
8.12143519	6.69783628	5.02485235
5.66948332	12.32758554	4.88136211
8.89016669	9.22833076	4.96947972
0.70883928	12.41563364	4.97072098
3.83588209	9.09847880	4.91496108
3.23810260	1.40756031	4.82300197
8.19295358	1.43205413	4.86585214
1.32301269	9.94550976	4.77535397
0.00350536	4.86883471	4.73383751
5.70907910	7.32957893	4.75745186
4.99431243	4.85554010	4.72668103
0.70645737	7.31199054	4.70642101
6.41605488	9.76075381	4.60388321

0.76722750	2.16356979	4.50960446
5.78066301	2.19633585	4.52966121
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002



# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(510) step with a Cv

1.000000000000

9.97980022	0.00000000	0.00000000
-0.76395801	12.66177369	0.00000000
0.00000004	0.00000004	19.64039993

C	O	Fe
36	1	77

Cart

2.59877784	10.09229951	6.10819542
4.70030758	1.90194043	7.57516097
5.49642778	9.30456461	7.50623271
7.19634560	4.17531709	7.13590926
2.20982142	4.21802342	7.16547903
2.99315450	6.85404262	7.12912482
7.88860073	6.86370189	7.08659821
4.56670144	11.97305789	6.65565092
1.94585008	1.27954627	6.27419341
7.69647281	10.05922078	6.10712693
8.01441089	0.25469972	6.50867404
0.41341470	8.80683272	5.96238007
4.17806101	3.12622652	5.21922936
9.16959316	3.12733800	5.22477362
2.22985908	12.35074668	3.67315431
4.70407922	10.64513249	4.15992184
6.71501016	5.64274899	4.04513134
1.71464859	5.68766328	4.02019805
-0.30716775	10.89943423	4.25138618
7.20365134	12.34534453	3.64564584
4.23144014	7.22160416	3.46872599
9.21749768	7.19969686	3.40777104
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304

8.80298600	1.13253745	8.02769775
4.01574031	10.32055447	7.24210806
3.75969412	0.37873032	7.06062450
6.33747782	11.05910304	6.93432404
3.86924256	5.19816870	6.98055455
8.81972409	5.16906066	6.97825203
-0.38249256	7.52698123	6.98180962
4.64251284	7.72300801	6.93378166
8.25940816	2.63590919	7.04106566
3.16898812	2.69173024	6.86446465
1.37566122	5.85366841	6.80025275
6.33668115	5.84880947	6.75315423
6.97718172	8.46496674	6.72715050
5.58779402	3.34089051	6.73776593
0.64518380	3.33264452	6.64144272
2.10074965	8.36778003	6.60186356
0.13088658	0.90244682	6.72918265
6.24206510	0.92207081	6.90497590
8.18374055	11.68808189	5.29978966
3.28294136	11.55037445	5.18782205
2.49879664	4.20202513	5.03555039
7.47966183	4.12443997	5.09449400
3.14648645	6.68200982	5.03554694
8.12510009	6.70686350	5.02070204
5.65570888	12.31562204	4.88368105
8.89147106	9.22578584	4.96133973
0.74975716	12.39078933	4.98925155
3.85728510	9.08356005	4.88848084
3.26529392	1.42167049	4.81662528
8.20492012	1.42824678	4.94971660
1.32321051	9.89271670	4.72169781
0.00343917	4.87687836	4.72165514
5.71725763	7.32811635	4.75062306
4.99646665	4.86369148	4.71983440
0.70405809	7.31044911	4.70775493
6.42000429	9.76564596	4.60489200
0.77909970	2.14936979	4.52729054
5.79213221	2.19491054	4.52692607
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337

7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(510) step with a Cv

1.000000000000

9.97980022	0.00000000	0.00000000
-0.76395801	12.66177369	0.00000000
0.00000004	0.00000004	19.64039993
C	O	Fe
36	1	77

Cart

2.61616958	10.07390057	6.08231749
4.71906680	1.87123720	7.58750303
5.51518192	9.30212397	7.50746254
7.20893627	4.12558035	7.13726903
2.19705373	4.20677288	7.20901309
2.99344600	6.84357861	7.11999372
7.89423742	6.82990679	7.08652290
4.56354297	11.96909322	6.67944092
1.81876015	1.59734377	6.18856030
7.69364337	10.07177863	6.10511378
8.08896745	0.45198503	6.61904644
0.41343233	8.79307807	5.97111361
4.18704224	3.12294149	5.23032798
9.18285042	3.12199584	5.23116787
-0.31651914	10.87988902	4.24786686
4.70706527	10.65062847	4.16319832
6.71154274	5.64947289	4.03977587
1.71566104	5.68156061	4.02134331
2.22928813	12.35103292	3.68818847
7.19392129	12.34203527	3.64131037
4.23088418	7.22402149	3.47450292
9.21658813	7.19995309	3.41103611
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.77123974	0.02037981	7.08202666
4.01950896	10.29932128	7.23621294
3.73162825	0.34622238	7.12073938
6.33890503	11.04741428	6.96183881
3.86873240	5.19313143	6.98545936
8.82467446	5.10838493	6.98118032
-0.38226321	7.49607508	6.97501721
4.65120898	7.71760352	6.93568246

8.21753477	2.54217363	6.91074522
3.21111081	2.71631045	6.89366204
1.37389663	5.82902558	6.80602236
6.34241925	5.81582015	6.77004352
6.99131884	8.45074543	6.72712688
5.60720730	3.31356479	6.73708003
0.68649374	3.22473063	6.65253737
2.10184467	8.36363654	6.60648893
0.01080437	0.72194006	6.72875278
6.23650286	0.89622456	6.95602725
8.16016467	11.69171854	5.26026623
3.29729843	11.55602307	5.19226732
2.49956739	4.18999281	5.03654464
7.46860480	4.11471809	5.07503664
3.14468900	6.67370225	5.03886471
8.12762840	6.69020285	5.02689973
5.65506486	12.31915122	4.90208063
8.88931322	9.21680727	4.97236844
0.75435908	12.32745570	5.01816203
3.86252087	9.07617550	4.87745172
3.21868201	1.43602529	4.82827681
8.19810224	1.42645611	4.87239527
1.32974711	9.86758660	4.71431880
0.00952488	4.86223912	4.73804506
5.71967174	7.32190301	4.75617355
4.99918032	4.85982563	4.72571899
0.70363995	7.30007514	4.70989740
6.41791785	9.76017754	4.60807341
0.74979435	2.12158331	4.51424437
5.78300860	2.19011410	4.52649486
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899

5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(510) step with a Cv

1.000000000000

9.97980022	0.00000000	0.00000000
-0.76395801	12.66177369	0.00000000
0.00000004	0.00000004	19.64039993

C	O	Fe
36	1	77

Cart

2.59865290	10.09878693	6.09551256
4.64855487	1.89418596	7.57645155
5.49851454	9.30929227	7.50546803
7.19628176	4.13289154	7.11985543
2.09966284	4.21609970	7.25641351
2.99336007	6.86768158	7.10859361
7.88367393	6.83508111	7.09154187
4.55177732	11.97866980	6.67955531

1.86597812	1.33536253	6.26797482
7.68313609	10.06958781	6.10694030
8.05476808	0.41442091	6.59592953
0.41018818	8.82161750	5.95320887
4.14360463	3.14359001	5.24659313
9.15683985	3.08115763	5.18576186
-0.31725770	10.89782579	4.25148799
4.70555450	10.64844842	4.16181986
6.70972578	5.65115111	4.04004726
1.70445098	5.69611823	4.02068597
2.22724003	12.35651924	3.67779213
7.19269038	12.33308914	3.63730966
4.23002574	7.22133142	3.46979407
9.21272263	7.19849609	3.41147868
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
0.66074935	4.56356892	8.03449008
4.00781847	10.31802583	7.24257691
8.18329673	1.40489503	4.85432842
6.33039632	11.06391240	6.96201606
3.83155310	5.17735354	6.99158078
8.85124614	5.11140417	7.11215218
-0.42238954	7.56409994	6.96784277
4.64685354	7.71895130	6.93966175
8.14464217	2.51868096	6.88387371
3.11436490	2.70443666	6.89949082
1.36487788	5.92360858	6.78561907
6.34335439	5.82110736	6.76775086
6.97719902	8.45755922	6.73069001
5.55790007	3.34055556	6.75145314
0.59082175	3.15994240	6.63518833
2.09060899	8.38692173	6.59535370

3.24242909	1.43454425	4.83023451
6.21023052	0.91760580	6.97012085
8.17055033	11.68424633	5.27437646
3.28027860	11.55981514	5.18458079
2.46170889	4.20776911	5.04055541
7.48326736	4.13860735	5.09468889
3.13559659	6.68119543	5.03638357
8.12660315	6.67851252	5.04171881
5.65223387	12.31060850	4.90902433
8.87808708	9.22624114	4.95980546
0.73515797	12.38916302	4.98975448
3.85789004	9.08248520	4.88626929
0.77682614	2.13179985	4.50614753
5.77003723	2.20477663	4.54354183
1.32208204	9.89985433	4.71353627
-0.01097823	4.86110974	4.72567204
5.71555127	7.32514948	4.75759472
4.98925892	4.86508975	4.72401968
0.69151256	7.31502595	4.70853722
6.41377956	9.76072981	4.60621183
3.71271381	0.37756335	7.04177712
0.00049679	0.79349584	6.61542882
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425



8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CO dissociation on Fe<sub>5</sub>C<sub>2</sub>(510) step with a Cv

1.000000000000

9.97980022	0.00000000	0.00000000
-0.76395801	12.66177369	0.00000000
0.00000004	0.00000004	19.64039993
C	O	Fe
36	1	77

Cart

1.88501176	11.16113905	6.25668299
4.61155373	1.79655301	7.55472782
5.48782218	9.31519321	7.45688387
7.16399070	4.10312486	7.13876712
2.16774845	4.17637836	7.19335481
2.97075797	6.81260670	7.06687321
7.88466570	6.81479427	7.07881442
4.56061625	11.90657776	6.60190227
1.80751170	1.41582313	6.21055648
7.70616874	10.05599899	6.10768963
8.03671897	0.42128904	6.58950283
0.48700126	8.77145484	5.96414468
4.15814892	3.11970803	5.24368576
9.16601214	3.11000847	5.23322493
-0.28982357	10.89112848	4.25666143
4.71097830	10.58450571	4.15783307

6.70636163	5.64656111	4.04120057
1.71292755	5.68128918	4.02869935
2.20677068	12.36380240	3.64295502
7.20820221	12.33175824	3.63955075
4.22753590	7.21781868	3.46741927
9.22212923	7.20414834	3.42749447
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
2.22126816	9.94391115	7.78756430
3.93697425	10.24617788	7.18131956
3.58766335	0.22288385	6.98784052
6.30142095	11.00313516	6.92485125
3.84397821	5.15386020	6.98799517
8.79326398	5.08276037	6.99299538
-0.38915878	7.48655243	6.95077608
4.64310715	7.69137780	6.92844972
8.14785687	2.51188302	6.89694019
3.13144820	2.64140268	6.88799672
1.36347380	5.81616712	6.78681150
6.32505839	5.79877804	6.77232104
6.98642518	8.43818669	6.72316047
5.55432245	3.27180473	6.75723153
0.63473413	3.23749987	6.66184933
2.12259153	8.42596858	6.78683131
-0.01810388	0.80524008	6.61176825
6.16668506	0.85038905	6.97918454
8.17936892	11.67866206	5.28206115
3.32221307	11.57206276	5.11492712
2.48087339	4.18015397	5.03973731
7.45279732	4.10511040	5.07486097
3.14325447	6.66326932	5.03784657
8.12449219	6.68428282	5.02898448

5.67016900	12.31376947	4.89752761
8.92049034	9.22215154	4.97910449
0.82266283	12.28577429	5.16196466
3.81310778	9.04872322	4.90234151
3.20819272	1.44947488	4.78357795
8.18780935	1.41615690	4.84893656
1.37791906	9.95061801	4.85353195
-0.00382616	4.86112358	4.73362884
5.71297471	7.31374495	4.75531440
4.98660886	4.84971985	4.72635477
0.72446402	7.32118457	4.70135795
6.42934294	9.74105795	4.59919739
0.76344046	2.12856167	4.52085138
5.76931361	2.18775310	4.53449760
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367

6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

### 3. Overall reaction on Fe<sub>5</sub>C<sub>2</sub>(510)

# initial surface

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
1	40	4	80

Cart

6.23581648	11.29929823	7.98149737
4.18402567	9.28404395	7.39198609
4.61332398	2.61459424	8.23477451
9.61375556	2.58847831	8.22430880
1.76529787	7.56834535	8.41856012
6.76980137	7.56733894	8.42109808
9.18514733	9.29866646	7.38420566
2.19714686	4.25653243	7.20570056
7.18386037	4.24824034	7.20290182
3.39820142	11.91939810	7.21345754
8.44134990	11.94988251	7.17326582
-0.33921456	6.76553499	6.31033185
4.65310395	6.76493419	6.31078535
1.73848201	1.63316525	6.15918681
6.72629099	1.59948976	6.18356596
2.16829749	8.28863940	5.59900280
7.15779497	8.28096927	5.59436730
9.19439451	3.12966576	5.30384615
4.20751175	3.13172729	5.30732542
4.66889265	10.80422112	4.26160246
-0.31999390	10.80744823	4.26620420
6.72108418	5.68829989	4.01312451
1.73080471	5.69080495	4.01362675

7.17656074	12.34635592	3.64064963
2.19298306	12.34735744	3.63971322
9.22785870	7.20079090	3.34058915
4.23741461	7.20213005	3.34033314
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.59031470	7.33076881	9.57563206
4.74866807	2.45343336	9.41070087
9.76501884	2.41139664	9.39580214
1.59902275	7.32093222	9.57379847
2.51618224	10.23465133	7.11162346
0.02080486	10.91622962	6.85594722
3.17375016	7.77635171	7.13420743
8.16326911	7.79044147	7.13425611
0.68108432	12.42312823	4.88790136
7.50898239	0.06916714	7.07175689
3.86885519	5.15888083	6.98924869
8.85173415	5.16326629	6.99362039
3.21426300	2.72251373	6.92575149
8.19868839	2.71219198	6.92715227
0.70738833	8.32291023	6.95013195
5.69447264	8.31302644	6.95052580
4.97337580	10.91538622	6.93457971
7.52781401	10.28017104	7.19163431
1.37231834	5.88814328	6.79074136
6.36731069	5.88533869	6.78558044
0.69695899	3.27530121	6.73941934
5.68966396	3.25716975	6.74210586
0.01602308	0.88680686	6.69198122
4.99133995	0.86265993	6.71163248
3.24115544	11.75874324	5.18768513
8.22813416	11.76376084	5.17661396

8.87344097	9.23042709	5.09010797
3.89413180	9.22766598	5.08714145
7.50456064	4.21843951	5.04041005
2.51438309	4.22184758	5.03882501
8.19337780	6.74999671	4.92164703
3.20236614	6.75199129	4.91923472
5.66675401	12.41046644	4.90580039
2.51285314	0.08668885	7.02832621
3.23174038	1.47525429	4.84038903
8.21636223	1.46565068	4.84605967
1.39873464	9.88847819	4.80894164
6.39129681	9.89467078	4.84000954
5.01487350	4.84412015	4.73872418
0.02230192	4.84602481	4.73910395
0.72132859	7.28455396	4.70843742
5.71128964	7.28180970	4.70654873
5.74829465	2.18169740	4.51827188
0.75529832	2.18927466	4.51307417
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071

8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for  $C_{cv}+H \rightarrow CH_{cv}$

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
1	40	4	80

Cart

5.06922392	10.28275967	8.32986370
4.26271919	9.31394253	7.51129659
4.61092351	2.60035863	8.22733035
9.60452338	2.61099120	8.22727092
1.81045056	7.54945049	8.43592691
6.78677610	7.63363969	8.44136498
9.19112328	9.29486909	7.40229122
2.19452721	4.26084452	7.20373251
7.18869882	4.24821459	7.20872987
3.41612117	11.91381286	7.19008283
8.39738018	11.92946683	7.20409843
-0.32200302	6.76644307	6.31598722
4.66035613	6.77615076	6.31631023
1.73066062	1.62682420	6.17313465
6.72649848	1.61904361	6.16711010
2.19298011	8.31545475	5.63918302
7.16900384	8.28950287	5.60214588
9.19762873	3.14087555	5.30271512
4.20462897	3.13847212	5.30373982
4.67672384	10.82890639	4.27574562

-0.31889031	10.81401548	4.26623124
6.72515041	5.69501281	4.01392943
1.73812703	5.70675197	4.01681055
7.18272916	12.34880376	3.64375051
2.18661244	12.34953767	3.63785057
9.23140964	7.20150067	3.34538816
4.23941220	7.20401263	3.34689688
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.63751856	7.43745144	9.60706859
4.74887991	2.42708132	9.40104421
9.73994427	2.44528948	9.40324492
1.61269646	7.30485335	9.58480962
2.49367281	10.22562399	7.05929498
0.00899488	10.92093831	6.88791435
3.21414618	7.81576637	7.17231551
8.18024611	7.78753239	7.13708695
0.67740658	12.42323958	4.89609332
7.48345318	0.06402608	7.04080677
3.87384380	5.16629802	6.99049382
8.85815667	5.16676278	6.99241216
3.20887365	2.72672427	6.92413664
8.20079486	2.71952844	6.92219567
0.72096641	8.32711228	6.97098664
5.71316241	8.28808778	6.94808266
4.96122212	10.89096345	6.88646794
7.51817780	10.24506872	7.13621658
1.39732404	5.90651609	6.79223951
6.37424779	5.87716423	6.78069391
0.69823432	3.27003730	6.73817874
5.68649573	3.26396620	6.73993866
0.00592349	0.86678950	6.71301112



4.99620092	0.86451794	6.70852491
3.24329165	11.77754695	5.17652340
8.23182339	11.76561087	5.18792145
8.88677975	9.22847299	5.07833626
3.90748049	9.22836862	5.05204713
7.50535464	4.22399327	5.03926567
2.51505685	4.23225586	5.03968972
8.19992573	6.75339427	4.92414009
3.20493560	6.76852070	4.93570910
5.67709246	12.42929366	4.89987000
2.52053609	0.07858143	7.03036708
3.22204341	1.48225519	4.84069796
8.22090832	1.47873878	4.83821310
1.40309255	9.88802135	4.79882623
6.39371683	9.89496932	4.82906153
5.01440469	4.85066964	4.73475241
0.02957991	4.85771469	4.74124157
0.73269544	7.30508432	4.71412923
5.71714696	7.28642991	4.70164289
5.74298656	2.18641822	4.51463147
0.75410502	2.18827373	4.51670817
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233

3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>v</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
1	40	4	80

Cart

4.26760081	9.47085157	9.03246855
4.24370067	9.27096600	7.94522819
4.61315163	2.58784339	8.22648845
9.61005636	2.64526630	8.23192414
1.84557766	7.46888504	8.42360104
6.71163708	7.75905319	8.46142713
9.19656405	9.29234551	7.39296645
2.20367641	4.26398451	7.19054161
7.18278319	4.25912815	7.19732562
3.41507675	11.87387090	7.16443683
8.40042922	11.91871764	7.19530769
-0.32856796	6.77284141	6.32362767
4.65307110	6.81988165	6.31852018
1.73679618	1.61952222	6.17847915
6.72405995	1.62003638	6.16854660
2.20381969	8.34683058	5.67399986
7.15845454	8.29340890	5.61153518

9.19720835	3.13993186	5.30321651
4.20385276	3.13996645	5.30266302
4.67810468	10.82262329	4.27346587
-0.31932600	10.81815921	4.26867571
6.72398381	5.69752372	4.01757542
1.73352733	5.70897960	4.01653097
7.17916199	12.34932281	3.64084325
2.18819125	12.34927762	3.63833071
9.23267851	7.20034519	3.35087729
4.24025810	7.21190782	3.35908539
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.64903099	7.53241315	9.62971600
4.76025605	2.41762234	9.39983837
9.73678660	2.49349698	9.40970852
1.62944268	7.16922304	9.55856139
2.55868327	10.17405279	7.03951925
0.01571770	10.91880924	6.87746689
3.22967562	7.81806103	7.17094982
8.15866412	7.79573682	7.14232429
0.67888467	12.42795139	4.89445021
7.49618394	0.06740903	7.02696984
3.88479547	5.17239534	6.97188051
8.85555447	5.16924422	6.98861506
3.21434092	2.72578985	6.92381307
8.19999074	2.72575191	6.92385964
0.72385354	8.31809750	6.97933212
5.66905131	8.36100012	6.97126056
4.98291128	10.82729506	6.86489656
7.52670943	10.22948086	7.11104263
1.39155891	5.90700771	6.79543328
6.36278541	5.88993461	6.76448966

0.70078376	3.27331658	6.73715430
5.68615410	3.25867132	6.73841487
0.00851469	0.86675412	6.71311013
5.00072860	0.83980138	6.71652251
3.24203259	11.76349945	5.16910472
8.22873725	11.76491639	5.18015073
8.88384946	9.22783241	5.07643210
3.88353196	9.19575680	4.96507758
7.50676537	4.22612939	5.03607825
2.51282597	4.23173305	5.03644271
8.19541015	6.75945050	4.93007718
3.19465840	6.75481993	4.93658514
5.66827587	12.42277056	4.89958509
2.52643260	0.06057193	7.02101763
3.22717134	1.48013488	4.84181176
8.21863294	1.47738784	4.84262484
1.39624940	9.88592843	4.77655820
6.39029755	9.88419202	4.80783827
5.01421628	4.84700148	4.72396609
0.02771911	4.86066826	4.74168980
0.73303309	7.31874820	4.71767242
5.71390909	7.28883471	4.71357097
5.74486381	2.18659894	4.51539284
0.75594787	2.18737033	4.51875917
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970

4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CH<sub>Cv</sub>->CH+Cv

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H	C	O	Fe
1	40	4	80

Cart

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5.20024748	9.59897490	8.12530892
4.60400051	2.56636046	8.22705474
9.60447407	2.59995530	8.22492051
1.70943727	7.86127218	8.48806676
6.77917195	7.45583879	8.41616859
9.17049357	9.28909183	7.39152251
2.21145963	4.26554229	7.20787035
7.18840026	4.24531610	7.19158966
3.43453493	11.82346934	7.17624796
8.35436880	11.91615526	7.21399702
-0.30802093	6.75760048	6.31961903
4.67481215	6.88135532	6.37071274
1.72988112	1.61853708	6.18326452

6.71916035	1.60960317	6.15793339
2.17809584	8.36302815	5.66180437
7.18606355	8.28191523	5.60465734
9.20107280	3.14325888	5.30387714
4.20351064	3.13981486	5.30276032
4.68168442	10.84021138	4.30410984
-0.32614289	10.82044984	4.27838607
6.72708434	5.69625709	4.02062057
1.73759185	5.71682007	4.02138428
7.18522064	12.34804657	3.63961776
2.18030264	12.35198500	3.63216795
9.23205929	7.20153288	3.34528702
4.24243423	7.20998675	3.37424218
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.68822092	7.16052220	9.56944406
4.75836659	2.39016735	9.39727697
9.73584158	2.43632845	9.40122508
1.80926624	7.66221596	9.65718584
2.40514229	10.23756232	6.94459561
-0.04441591	10.91908480	6.88261616
3.25777445	7.93147900	7.19686578
8.21192636	7.75157806	7.14315205
0.67273922	12.42419138	4.90323568
7.44270069	0.03518523	7.02545567
3.88781357	5.20270666	6.95333402
8.87038593	5.14745175	6.97893509
3.21256668	2.73034394	6.92626117
8.19702801	2.70805502	6.92139434
0.72302255	8.34365061	6.98785251
5.79995738	8.30169069	6.99179729
4.95715378	10.80689391	6.77232487

7.46593358	10.21581037	7.19518824
1.41289706	5.89512977	6.75291437
6.36046606	5.87005089	6.76245944
0.70691776	3.26648344	6.74364147
5.68440130	3.24566372	6.73760590
0.00446291	0.84871521	6.73709639
4.98985988	0.82038820	6.71441592
3.23384405	11.78165044	5.15394439
8.21278046	11.75097978	5.19585105
8.88655383	9.22570776	5.09182306
3.89895989	9.19530370	4.98361083
7.50721195	4.21761473	5.03801849
2.51995823	4.23646037	5.03356743
8.20493141	6.75225908	4.92048210
3.19431338	6.77233792	4.97837743
5.67190051	12.45332826	4.87441610
2.53498701	0.06342218	7.03017497
3.21778733	1.48605123	4.84334500
8.22988869	1.47203680	4.84376652
1.39350620	9.88075823	4.72255548
6.39431768	9.87073072	4.78491483
5.01494338	4.84488450	4.71980072
0.03445906	4.85656624	4.73661422
0.73574424	7.31774487	4.71607548
5.71726866	7.27899967	4.71475392
5.74179343	2.19180587	4.51031828
0.75402371	2.18541257	4.52411168
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903

2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH+Cv

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H	C	O	Fe
1	40	4	80

Cart

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5.88305581	9.95683315	8.10768940
4.60869251	2.57498351	8.22798886
9.60637952	2.62675626	8.22680158
1.69273636	7.71431575	8.46836462
6.82853276	7.27041746	8.36722891
9.17489165	9.30179836	7.38532270
2.21840861	4.26297900	7.19928991
7.17068517	4.26747990	7.17404457
3.44798575	11.79061511	7.19630317
8.39372807	11.92245520	7.18714364



-0.32218674	6.75499633	6.31219916
4.65711156	6.91588832	6.39476835
1.73864942	1.61404069	6.17885345
6.71854491	1.60773945	6.16956192
2.17760081	8.35481681	5.65645014
7.16029172	8.28485346	5.62496155
9.19714221	3.14546668	5.30404640
4.20517669	3.13616944	5.30392412
4.67855008	10.82692700	4.29601789
-0.32291727	10.81860813	4.28013228
6.72258194	5.70035370	4.01878876
1.73424531	5.70800092	4.01975562
7.18040342	12.35064579	3.63377939
2.18211413	12.35216718	3.62694935
9.22950569	7.20130737	3.34495913
4.24155130	7.20748596	3.36803743
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.59307755	7.07898573	9.52311005
4.77190345	2.40330642	9.39925928
9.73464961	2.47544660	9.40556880
1.64951971	7.48928880	9.63908104
2.44277096	10.19038948	6.94195497
-0.00573000	10.92057590	6.84997014
3.13405959	7.79900924	7.17392295
8.20279573	7.75245172	7.14837599
0.68132728	12.43091150	4.89685071
7.47375733	0.05003152	7.02982685
3.88626004	5.20695274	6.95436722
8.86077208	5.15531624	6.98764704
3.21599889	2.72437156	6.92623104
8.19145077	2.71934195	6.92453615

0.69429719	8.34017056	6.96723960
5.76022962	8.40092338	6.96005157
4.99055464	10.84379645	6.76170543
7.52271612	10.24197437	7.15352520
1.39842698	5.88346260	6.75582540
6.34902471	5.92234962	6.80043657
0.70462946	3.27460197	6.74037155
5.68254501	3.24900459	6.73501673
0.01560994	0.86406960	6.72737979
4.99441318	0.80955742	6.72096709
3.22704955	11.76781823	5.15810528
8.21896294	11.76349401	5.17716998
8.87978532	9.22364466	5.08155897
3.91636453	9.19377310	5.02872156
7.50286845	4.22890276	5.04283659
2.51978147	4.23170400	5.03241956
8.19899875	6.75879650	4.92249898
3.19297354	6.76294047	4.95057929
5.67821935	12.43735587	4.87964307
2.55427006	0.05452719	7.02765652
3.22762304	1.48131331	4.84337004
8.22420320	1.48480248	4.84264691
1.39581434	9.88000363	4.72191226
6.40508750	9.87127925	4.76500388
5.01290672	4.84523609	4.72156390
0.02480724	4.85835903	4.73158690
0.73485006	7.31731345	4.70932820
5.71191403	7.27549662	4.72162490
5.74636425	2.18910521	4.51234720
0.75588570	2.18875440	4.52281090
8.93206166	3.17824094	3.12792051
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899

5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
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# CO<sub>cν</sub> (state1)

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H	C	O	Fe
1	41	5	80

Cart

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4.61464310	2.59859987	8.22673504
9.60964312	2.65603001	8.22792141
3.65028974	8.58650722	8.78441564
1.67919135	7.20775463	8.36919138
7.07040501	7.05811941	8.42106004
9.18126134	9.27955884	7.38807519

2.20898641	4.25555173	7.18284796
7.16155950	4.25502649	7.16716904
3.45039526	11.79941785	7.19499329
8.41336530	11.91310639	7.18144033
-0.32659699	6.71751651	6.25932945
4.64680987	6.86700393	6.38875201
1.73862990	1.60724395	6.17673490
6.72100643	1.60399513	6.16447658
2.18453114	8.36149018	5.68033790
7.14695831	8.28823944	5.61313927
9.19750709	3.14310175	5.29560695
4.20336537	3.13524112	5.29767512
4.68045766	10.82623116	4.29484038
-0.31959422	10.81274353	4.27509869
6.72022760	5.69646322	4.01884073
1.73839344	5.71217298	4.01833308
7.18251676	12.34892874	3.63037651
2.18627440	12.35183222	3.62813021
9.22733459	7.20203706	3.33130037
4.24186498	7.21334886	3.38116325
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.76292113	6.94822480	9.56513535
4.75383614	2.43921757	9.40271679
9.72363201	2.51603682	9.40886061
1.34140164	6.97600133	9.49422129
3.78300322	9.02044044	9.86213486
2.46276750	10.17358930	6.95906628
0.01281485	10.90005146	6.84361938
3.16983850	7.77868467	7.27301084
8.19879443	7.74287335	7.12386839
0.68421459	12.43077257	4.89222622

7.49300860	0.05277873	7.03070061
3.89846941	5.17214598	6.98412757
8.84195334	5.16889408	7.02608720
3.20978490	2.71410827	6.92142957
8.19272097	2.71781732	6.92011680
0.67825902	8.28626080	6.94745017
5.68878465	8.43180393	6.97264791
5.02026109	10.90272509	6.75895629
7.54347224	10.23480127	7.13176422
1.39475023	5.88876787	6.79057954
6.37064201	5.92585393	6.82820797
0.69782263	3.27255625	6.73160003
5.67656281	3.24595989	6.72978744
0.01731917	0.86152421	6.72013951
4.99639275	0.81560996	6.71656516
3.22614255	11.75679167	5.16464092
8.22503924	11.76202497	5.17519942
8.87427555	9.22304834	5.08045999
3.91128792	9.19071082	5.04263761
7.50404552	4.23200759	5.04679722
2.51982370	4.23729669	5.03773717
8.18929188	6.76410556	4.90435762
3.19223087	6.77617871	4.98156794
5.68254204	12.44010282	4.87558413
2.55420144	0.04428671	7.02663170
3.23334939	1.47518749	4.84253553
8.22778439	1.48072096	4.84107171
1.40025755	9.87531727	4.73856029
6.40610382	9.87958180	4.76674502
5.01035645	4.85072388	4.72179175
0.02282458	4.87252320	4.75116900
0.74747474	7.32794775	4.69801615
5.70556265	7.27764294	4.73980354
5.74721316	2.18864809	4.50904036
0.76002255	2.18788504	4.51862094
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308

1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CO<sub>Cv</sub> (state2)

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9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
1	41	5	80

Cart

6.64938988	7.16226332	9.31262792
6.75517278	7.32992315	8.23149855
4.60579968	2.57894953	8.21983474
9.60380114	2.63857050	8.22436023

4.38404950	8.98381200	8.29507387
1.94952397	7.43703428	8.45804440
0.89834103	11.31412996	8.51112306
9.15191365	9.25277916	7.41304323
2.19571172	4.24393311	7.19263955
7.16895488	4.25505553	7.20322140
3.47228905	11.83558774	7.12663158
8.36653730	11.88566859	7.20758674
-0.32354395	6.71437710	6.29285480
4.65581603	6.79754119	6.28770537
1.72995286	1.58954954	6.19096883
6.71918950	1.62042153	6.15770331
2.20758204	8.35425278	5.67733229
7.16708212	8.29087041	5.58098548
9.19595658	3.14074535	5.29633352
4.19625092	3.13006079	5.29030858
4.68228668	10.81117487	4.27617767
-0.32339499	10.80478292	4.25898310
6.72477015	5.69015505	4.01478123
1.73532059	5.70524391	4.01693166
7.18688952	12.34921507	3.63956507
2.18195649	12.34975632	3.64251570
9.22885723	7.20096099	3.33608954
4.23810532	7.21340128	3.35323374
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.19241104	11.45659647	9.64691093
4.74416845	2.40221184	9.39339441
9.70490111	2.46928347	9.40279126
1.57980736	7.20335938	9.56425671
4.34241507	9.53697122	9.35791492
2.45150189	10.20952608	6.98632374

-0.01961833	10.89690812	7.02543655
3.23337953	7.81278599	7.18510106
8.17110231	7.74483232	7.11049727
0.67938348	12.39929106	4.93143758
7.48645931	0.05319732	7.02313197
3.87684488	5.16953217	6.99606487
8.85197119	5.15508239	7.04356334
3.20313867	2.70438059	6.91757181
8.19082305	2.71687171	6.91795150
0.69102300	8.28591734	6.96191997
5.68751493	8.30308611	7.00323504
5.01878362	10.80501225	6.73682646
7.49912844	10.19552699	7.09305344
1.41510379	5.90106279	6.80496669
6.35635779	5.91033489	6.90496878
0.69626236	3.25353706	6.73468111
5.67317204	3.26004389	6.73555492
-0.00825426	0.84848809	6.71532114
5.00894668	0.82965094	6.70812972
3.24188717	11.75364001	5.16037558
8.22949115	11.74265289	5.19603747
8.89350463	9.22376675	5.09614757
3.88890848	9.18809315	4.98435455
7.50191103	4.22860790	5.05338560
2.51351198	4.23086093	5.04385661
8.20300356	6.75568849	4.90549714
3.19526489	6.76283514	4.93825489
5.68070376	12.41926702	4.88478396
2.55968422	0.05494561	7.07847300
3.22793793	1.45290447	4.85148127
8.22310229	1.47137328	4.84285331
1.39313411	9.88024063	4.77077369
6.38624126	9.85287955	4.77575367
5.01386886	4.85532402	4.74452910
0.02821897	4.87171912	4.76694807
0.74313461	7.32535725	4.70435681
5.72112682	7.28165466	4.71721940
5.74150396	2.18447083	4.51403973
0.75602261	2.17388471	4.52082796
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337



3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CO<sub>CV</sub>->C<sub>CV</sub>+O

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
1	41	5	80

Cart

6.71491244	7.07986060	9.29640059
6.83799061	7.15655452	8.20773376
4.60467669	2.58299553	8.21309436
9.58573218	2.63279662	8.23504348
4.25320032	9.29882970	7.45382394
1.83011935	7.46179150	8.42386238
0.95787372	11.28797023	8.47426170
9.13867686	9.26682313	7.40012025
2.18799189	4.24985505	7.20012920
7.17280399	4.24373922	7.20230572
3.45186758	11.94572336	7.13641375
8.35788323	11.91513628	7.21618175
-0.32037580	6.72199387	6.27654162
4.66218967	6.73532761	6.27361302
1.71879853	1.59908339	6.19095014
6.71895816	1.65168961	6.13331058
2.18657616	8.30169478	5.63726222
7.14966161	8.28848140	5.58473691
9.19539697	3.14402413	5.30036743
4.19160424	3.13424140	5.28905875
4.67711838	10.82980025	4.28766900
-0.32972095	10.79804408	4.26454073
6.72234075	5.69276860	4.01695666
1.73213800	5.70326024	4.01448219
7.18496618	12.34982715	3.63945189
2.17600004	12.34841588	3.63928378
9.22516316	7.20080046	3.32787055
4.23712934	7.20602424	3.34004344
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.23590460	11.37647017	9.62629314

4.74546121	2.39907159	9.38575743
9.72992777	2.47658209	9.41001769
1.59738099	7.24747182	9.57606786
5.69092691	9.78186259	8.23146728
2.55178526	10.24904271	7.17322738
-0.04243957	10.91271095	7.01388750
3.20117437	7.78328069	7.16522048
8.21317152	7.72880530	7.10753393
0.66048418	12.40536551	4.92227162
7.49204839	0.11825050	7.01426906
3.86385191	5.16159815	7.01122901
8.84803499	5.17091129	7.05036207
3.19221366	2.70861344	6.91671539
8.19772297	2.72444317	6.92081912
0.70373870	8.29723202	6.97390049
5.75144571	8.21821612	7.01636533
4.99981611	10.94430937	6.79719714
7.44569043	10.24137042	7.22815384
1.39880026	5.90209904	6.81200057
6.36859521	5.88423130	6.85984978
0.69054441	3.26302577	6.73772361
5.66751208	3.27840511	6.73436850
-0.01845887	0.86424736	6.71639213
5.00642292	0.89170508	6.67682405
3.22757777	11.77194234	5.16669462
8.20888132	11.74049553	5.20745185
8.86637321	9.25454745	5.14376587
3.87719571	9.23474526	5.06674567
7.50168367	4.22676288	5.04520377
2.51039126	4.23597777	5.04507789
8.19274018	6.76892178	4.89585319
3.19822113	6.76783563	4.92535875
5.67014795	12.44491027	4.86600893
2.52640015	0.07255378	7.07848089
3.21490415	1.46440440	4.84380587
8.22639484	1.48251726	4.83351721
1.39143059	9.89983556	4.86195655
6.39160408	9.88664657	4.77615326
5.00384193	4.85880236	4.73586616
0.02183331	4.87055114	4.76302731
0.73191086	7.31285498	4.70376431
5.71523512	7.29554724	4.71515096
5.73897205	2.20148380	4.50449077
0.75483597	2.18374139	4.51875206

8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# O

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
1	41	5	80

Cart

6.62754039	7.18902823	9.29724976
6.73748738	7.30696537	8.20918209
4.60638555	2.59789053	8.22980420
9.61711950	2.63314244	8.22344251
4.18049585	9.26779288	7.37673075
1.82917372	7.40553227	8.39536137
1.00777729	11.17986684	8.44938759
9.13000929	9.28934973	7.36753737
2.19603830	4.25936709	7.19903196
7.17711398	4.25421547	7.19876489
3.42982618	11.94876332	7.16035870
8.49671763	11.97728899	7.13098315
-0.35271662	6.74660158	6.28759717
4.64525038	6.72264955	6.24684422
1.74083655	1.63427961	6.16343725
6.72949204	1.59687945	6.17578114
2.15976232	8.28045523	5.58543557
7.14620353	8.28203782	5.54582007
9.19334018	3.12721885	5.29163192
4.20590114	3.13017779	5.29870537
4.66379897	10.78843384	4.24869424
-0.32207598	10.79479042	4.26257908
6.71823271	5.67814422	4.00972823
1.72681403	5.68541311	4.01330460
7.17402746	12.34816129	3.64309508
2.19154383	12.34786176	3.63959361
9.22264347	7.19913806	3.32890013
4.23091034	7.20032362	3.31784055
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183

7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.23967473	11.26166822	9.61167739
4.75723908	2.42324282	9.40134839
9.77129407	2.45695713	9.39428311
1.56690921	7.17710874	9.53756644
6.23899810	11.32005927	8.24477679
2.51391472	10.26116670	7.17406491
0.02700029	10.90070057	6.95174803
3.16086949	7.75323008	7.12263724
8.14724545	7.77162947	7.09945562
0.67909789	12.41440704	4.89989920
7.53521528	0.09888577	7.12622896
3.86271010	5.16719945	7.02491347
8.84397559	5.17370907	7.02885456
3.20904494	2.72043558	6.92332561
8.19621374	2.71224689	6.92624187
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7.52349784	10.32339653	7.25324955
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3.20091629	10.75315189	2.92137337
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3.24625349	5.59719324	2.75910425
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0.73558354	11.29866314	2.69921899
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0.03281343	8.84247589	2.64073300
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-0.26345146	4.52631235	0.98044425
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1.51178777	2.71004343	0.73384589
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1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
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7.45328903	1.12937152	0.40848067
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4.75647831	8.73880577	0.18583304
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1.22782551	11.34892962	9.64021925
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9.74566406	2.46765193	9.39915247
1.58261060	7.30244763	9.55852331
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9.65447807	0.51179242	2.92767382
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3.20091629	10.75315189	2.92137337
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3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
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0.70104283	6.28061676	2.47308970
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3.99426270	2.08401227	0.94984233
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2.50702286	12.16127491	0.88189071
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3.93891239	7.14167833	0.77916235
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3.24189639	9.65808487	0.74752367
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1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
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9.62246061	2.63825466	8.23266307
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6.79756558	7.54444076	8.42367842
1.83088900	7.34545635	8.38504471
9.15299096	9.29482799	7.35713384
2.20196263	4.25873425	7.18423100
7.19525290	4.26405515	7.20027031
3.50896628	11.97679430	7.13692639
8.42659601	11.94629762	7.16981103
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4.64739271	6.77529870	6.30869497
1.75218080	1.57609218	6.20085667
6.74180849	1.63101769	6.17084278
2.16309080	8.29232759	5.59684995
7.15313806	8.27971865	5.58448498
9.20267048	3.13639748	5.30293183
4.21012996	3.13201596	5.29741792
4.67344350	10.80178487	4.26491123
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2.18855787	12.34952413	3.64105947
9.22831010	7.20145790	3.33603409
4.23693029	7.20149493	3.33709584

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6.73540354	9.72874641	2.00704742
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5.69167990	3.29381387	6.73654388
0.00593203	0.89526769	6.70215285
5.01660118	0.91615586	6.66383894
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9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
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7.18588972	5.31081581	0.60368013
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9.60675203	2.63138054	8.22265624
4.20126944	9.29794516	7.40833830
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1.87658999	7.27314953	8.39056121
9.10959613	9.29892302	7.31535683
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7.18485834	4.25790785	7.20400297
3.41369361	11.92574788	7.19505995
8.46375829	11.95879802	7.17376423
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6.72326773	1.61562802	6.17973452
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5.69815154	8.31454393	6.94186297
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7.49688380	10.31208976	7.17777246
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6.36820039	5.88877822	6.78371540
0.69012613	3.28712151	6.72858736
5.68485405	3.27262173	6.74083899
0.01250212	0.90384419	6.67711100
4.99457758	0.87517847	6.71276683
3.24355818	11.76055662	5.18305360

8.21643354	11.78108831	5.16767533
8.88144084	9.24044604	5.10823973
3.89146070	9.23240541	5.09429371
7.50659888	4.22880737	5.04066544
2.51350331	4.23720655	5.04353502
8.19812018	6.75663148	4.91101591
3.19833494	6.76582501	4.91789596
5.66509763	12.42122502	4.89822307
2.50969236	0.08206732	7.04399171
3.23342841	1.47999872	4.84195438
8.21300685	1.47849093	4.84291367
1.40629578	9.90044537	4.81393856
6.39515032	9.89875761	4.83806081
5.01139823	4.85260704	4.73980703
0.02537300	4.86097585	4.73849205
0.72445605	7.30122404	4.72074968
5.70932420	7.28237823	4.69953697
5.74701859	2.18918564	4.51818459
0.75915969	2.19187124	4.50922646
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071



2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

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H	C	O	Fe
2	41	4	80

Cart

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0.52998117	9.78882421	8.30172204
4.60162151	2.63521566	8.23155537
9.60194873	2.62753401	8.21555897
4.15660586	9.26866340	7.41855451
6.79671899	7.48694132	8.42034240
1.88562336	7.24344951	8.38567336
9.27670145	9.33666070	7.78933562
2.19588811	4.24586641	7.18429473
7.17574144	4.26551520	7.19481085
3.35718375	11.90146956	7.22118030
8.44835161	11.92626325	7.11873101
-0.33271160	6.79797009	6.31546516
4.67715621	6.73655917	6.29514971
1.73112850	1.62531052	6.14293058
6.71082853	1.59127807	6.20622768
2.16120252	8.27783956	5.63715668
7.19478680	8.34201523	5.67586795

9.18370845	3.13475249	5.29122679
4.20765826	3.14595187	5.30174824
4.65825504	10.79417186	4.26508113
-0.30792255	10.84985776	4.31487637
6.72629546	5.71759573	4.01584387
1.73459414	5.70223072	4.01751251
7.16011538	12.35119493	3.62938481
2.20122095	12.34956428	3.63801344
9.22880762	7.21063740	3.35322967
4.23983650	7.20272275	3.34221645
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.65099363	6.96189016	9.52440132
4.72248767	2.48745295	9.41054824
9.72439407	2.45996853	9.39051821
6.61749301	7.26960898	9.58114101
2.41645420	10.20751473	7.22267945
0.01366280	10.90991155	6.71618439
3.21711902	7.73361031	7.14649560
8.22136693	7.84996790	7.19468444
0.69016215	12.46153553	4.86187685
7.50681559	0.04561118	7.06194698
3.87226932	5.15172613	7.00623485
8.86357513	5.16790440	6.98186032
3.20540557	2.71316503	6.91608194
8.18082266	2.72165281	6.91648293
0.74753396	8.26761008	7.00736638
5.70287998	8.31532447	6.98663489
4.92008936	10.89668520	6.95245384
7.53631830	10.23728282	7.10632268
1.37094897	5.87099675	6.77670319
6.40453712	5.92759242	6.81325069

0.68293843	3.27677521	6.72868413
5.68545046	3.26186643	6.74169757
-0.00302836	0.89018353	6.66637181
4.97479643	0.84719007	6.72948615
3.21960118	11.73382212	5.20756622
8.20749649	11.78606331	5.14983586
8.86868718	9.21038410	4.97831906
3.87294409	9.23568896	5.11819687
7.50196193	4.24248012	5.03866382
2.51537655	4.22603176	5.03461648
8.18667253	6.77426682	4.95166952
3.20882200	6.76467108	4.91572814
5.64534859	12.40936186	4.91029074
2.47723266	0.07558529	7.03164003
3.24623199	1.47544343	4.83746587
8.19715459	1.47388055	4.84484467
1.40030041	9.86437785	4.77263279
6.38365322	9.89382310	4.81951824
5.02141191	4.87116196	4.75942424
0.02005373	4.85414094	4.73156069
0.72391047	7.29148568	4.71002104
5.72910266	7.32866106	4.71233887
5.74518331	2.18351251	4.52534275
0.75100893	2.19905429	4.50465792
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970

4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for  $CCH_{cv}+H \rightarrow CCH_2_{cv}$

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H	C	O	Fe
2	41	4	80

Cart

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0.88268140	10.97115964	8.23914614
0.39476443	9.66744891	8.46510248
4.60028639	2.61783101	8.22889348
9.59438331	2.58158734	8.21779884
4.18995560	9.25497262	7.39714567
6.81285761	7.36572568	8.39787228
2.41901139	7.09415359	8.64249067
9.17588707	9.28952031	7.84870687
2.18589205	4.22933399	7.18226553
7.18538983	4.25161093	7.19294800
3.40791803	11.89571523	7.19446189
8.37955441	11.88600778	7.17563563
-0.33374101	6.78368368	6.32656428

4.68574814	6.71986510	6.27454955
1.72788910	1.59594199	6.16165571
6.70983318	1.60675012	6.17799154
2.15579516	8.26121162	5.63337503
7.19354719	8.33790810	5.66533061
9.18815971	3.12790416	5.29422224
4.20431979	3.13157854	5.29759329
4.66032536	10.77726837	4.26556985
-0.30995365	10.82043652	4.27511139
6.72668291	5.70461021	4.01663704
1.73368694	5.68938566	4.01617992
7.17583452	12.34615537	3.64011190
2.19297280	12.34480090	3.64575847
9.23122298	7.21064648	3.35672191
4.23955026	7.20272585	3.33832241
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.99844730	6.82445397	9.70747541
4.72442570	2.46460780	9.40750543
9.72133003	2.40700649	9.39343425
6.59185489	7.12370843	9.54749243
2.50414399	10.19676551	7.18145773
-0.02595945	10.91674050	6.87906261
3.21834236	7.71100752	7.17229502
8.21135196	7.80192479	7.18228518
0.68303036	12.41417292	4.90295767
7.49058777	0.04864725	7.02893021
3.85880863	5.16412348	7.03022610
8.88028702	5.15196119	6.99033277
3.20243952	2.70230218	6.91704112
8.18871269	2.71053362	6.91711908
0.68078253	8.36103290	6.93812033

5.72186477	8.29577097	6.98006105
4.98531578	10.88593675	6.89941905
7.50430913	10.17880134	7.03882689
1.38523439	5.87478260	6.76742238
6.40601351	5.90143939	6.80048070
0.68388370	3.24618648	6.73325552
5.68168092	3.25806966	6.73938205
-0.00379090	0.84666397	6.70341719
4.98690008	0.84667705	6.71987196
3.23273644	11.73287131	5.19390351
8.22689069	11.75139531	5.17728613
8.88823467	9.20323765	4.99936755
3.87372447	9.21050627	5.15355314
7.50481207	4.23099075	5.04152839
2.51619278	4.22037046	5.04347601
8.18877792	6.76208060	4.94507754
3.20847510	6.75458448	4.91593627
5.65571561	12.40999213	4.89618278
2.49829126	0.05005563	7.04726592
3.23166240	1.46169682	4.83751849
8.20817285	1.46585382	4.84098241
1.39553374	9.88043759	4.81760462
6.38017969	9.87794451	4.78399980
5.01488648	4.86472001	4.76351775
0.02256009	4.84224582	4.72827324
0.72667441	7.27226752	4.71473425
5.73074755	7.31787339	4.70921056
5.74327024	2.18295372	4.51726849
0.75297877	2.17853308	4.51124865
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300

0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CCH<sub>2</sub> cv

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H	C	O	Fe
2	41	4	80

Cart

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0.09384119	9.18581328	8.95227136
4.60912664	2.65371586	8.23493271
9.60526721	2.58195758	8.21697063
4.20478827	9.27284729	7.38894486
6.83581667	7.43840556	8.40128808
2.49430499	7.05979148	8.66023823
9.12821898	9.31329499	7.91746292

2.18831428	4.24957441	7.17438531
7.19371548	4.26632045	7.18949601
3.39776000	11.89722087	7.18890546
8.39372970	11.89386103	7.15192977
-0.33065465	6.82095051	6.33301565
4.69036933	6.74339370	6.27979799
1.73163801	1.61896364	6.15832608
6.71555044	1.62301894	6.18118300
2.13790421	8.29572837	5.69815885
7.19237872	8.34418188	5.64406861
9.19039336	3.14313840	5.29581605
4.20627682	3.13997114	5.30224071
4.66672784	10.79287934	4.26761544
-0.30977439	10.83619500	4.29087011
6.72262020	5.70464404	4.01287998
1.73519283	5.70703499	4.02176179
7.16980422	12.35154233	3.63120324
2.19410920	12.34798345	3.63525005
9.23472642	7.21264344	3.36128175
4.24069520	7.20597782	3.34546830
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
2.12176353	6.71150297	9.71972690
4.72705029	2.51015758	9.41543069
9.74105693	2.40805684	9.39182178
6.62939659	7.16421226	9.54700065
2.51794449	10.18641689	7.07886051
-0.01766709	10.88193471	6.74324534
3.23170436	7.72765756	7.17711467
8.19803788	7.81584402	7.14235600
0.68349751	12.43780158	4.87964108
7.50099166	0.06465221	7.01994279



3.86264582	5.18370649	7.02338498
8.88511017	5.17350109	6.97680219
3.20860546	2.72343804	6.92070072
8.19729183	2.72669661	6.92014429
0.64022501	8.43726961	6.99304682
5.73001200	8.31799439	6.96737645
4.99652855	10.91162182	6.89212825
7.55361333	10.19058688	7.06358745
1.38646238	5.89434176	6.75993050
6.40533297	5.91044030	6.79236295
0.68777239	3.26046191	6.73138786
5.68674638	3.27138886	6.74102177
0.00418013	0.85565532	6.70546730
4.98897720	0.85677965	6.71513288
3.24144559	11.75824377	5.17643186
8.21232888	11.77512622	5.15840546
8.87477817	9.19206336	4.95070962
3.87888683	9.20420862	5.11612894
7.50402828	4.23500084	5.03609245
2.51855076	4.22954433	5.03713084
8.19535867	6.74738592	4.93467376
3.20021914	6.76660781	4.92378434
5.65631690	12.42341085	4.89219048
2.50629835	0.06041699	7.01192092
3.23083066	1.47941532	4.83896225
8.20823092	1.48312639	4.84115907
1.40291699	9.86347748	4.76646957
6.38911890	9.89471400	4.78647015
5.01193575	4.86935406	4.76217678
0.02802293	4.84904503	4.71915038
0.72558581	7.29977801	4.73606077
5.73140829	7.31576070	4.70707103
5.74428624	2.19003323	4.51872451
0.75144570	2.18820396	4.51131125
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308

8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

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1.23323252	11.27483516	7.99321671
8.75782284	8.75521603	9.12749057

4.59632870	2.57022878	8.21203130
9.58269773	2.56116565	8.22516976
4.18808681	9.28942448	7.40446973
6.87055634	7.08976080	8.38627984
1.76814202	7.62959792	8.41693363
9.37094187	9.26837303	7.97826436
2.19359510	4.22711537	7.20311687
7.17974925	4.24887673	7.18000019
3.45155341	11.93129074	7.18283175
8.40079765	11.84333821	7.18705681
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4.67422961	6.72590612	6.30950761
1.73076628	1.56773542	6.17885810
6.72590799	1.60254933	6.16988183
2.18456318	8.27155298	5.57344029
7.21611635	8.34502640	5.71634529
9.19504917	3.12404105	5.30032930
4.20393247	3.13099347	5.29005221
4.67598564	10.79572133	4.26541675
-0.30166175	10.79562264	4.26179310
6.73305364	5.71172413	4.02287386
1.73601034	5.68425112	4.01364130
7.18821747	12.34513080	3.64163964
2.19423621	12.34163181	3.64375871
9.23438167	7.21547854	3.37438644
4.24506325	7.19978836	3.34760747
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
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1.64110215	7.39238974	9.58353960
4.72412454	2.39559698	9.38691239
9.69874779	2.38091655	9.40051707
6.44443841	6.95841591	9.49666366

2.54088557	10.26855756	7.22708232
-0.02560993	10.79969194	6.93894767
3.18397233	7.78050576	7.12326123
8.24269304	7.79211297	7.28078175
0.68738049	12.40522766	4.91149190
7.51874652	0.03705115	7.02289140
3.86530582	5.14710721	7.00309916
8.88233187	5.15080565	7.00869723
3.19861740	2.69078843	6.91008695
8.19271014	2.70727763	6.91588084
0.72194699	8.32001947	6.94367997
5.69092551	8.31259675	6.95985821
5.01545846	10.89516270	6.87244746
7.52140968	10.15941628	6.97792822
1.38349858	5.86768670	6.79829460
6.41909427	5.91273368	6.80808416
0.69333178	3.22844628	6.74802562
5.68121859	3.25890487	6.73164083
-0.00147098	0.81355008	6.71710539
5.00674026	0.86792234	6.69955875
3.24728574	11.74489026	5.18604500
8.25162071	11.73895477	5.17556614
8.89933498	9.17679099	4.99423365
3.90694222	9.22339931	5.10837921
7.51011932	4.23202874	5.04285839
2.51456838	4.21850024	5.04441227
8.19315958	6.76799473	4.97722292
3.22113608	6.74513255	4.92116058
5.67546064	12.41450003	4.89201383
2.50692436	0.02531727	7.07344904
3.23133889	1.45203127	4.84019637
8.22162833	1.46287964	4.84018698
1.40523499	9.88952093	4.85222952
6.39802860	9.86681664	4.76344076
5.02152521	4.86130213	4.74446035
0.02603395	4.84050467	4.74677291
0.73107057	7.26075399	4.71411160
5.74157564	7.32301740	4.71748136
5.74790756	2.18329008	4.51379798
0.75853740	2.17611905	4.51838751
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382

8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
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# TS for CCH<sub>2</sub> cv+H->CCH<sub>3</sub> cv

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	-0.26724249		10.12018310	9.01899668
	4.61018866		2.61448432	8.22424729
	9.59298981		2.57132085	8.22263103
	4.19252230		9.28139598	7.41173745
	6.85073683		7.47751247	8.44643750
	1.74851890		7.60469226	8.41965297
	9.26958925		9.24585921	7.96481088
	2.18840913		4.24097811	7.20188327
	7.18229510		4.25751740	7.19757684
	3.41578017		11.91994396	7.18644307
	8.38778833		11.86063911	7.16663489
	-0.34483184		6.79977998	6.31377210
	4.66318894		6.75488914	6.31798995
	1.73086619		1.59498846	6.17764109
	6.71982186		1.61651350	6.17613725
	2.16677207		8.28561636	5.60289239
	7.19262271		8.34153806	5.67976509
	9.19132886		3.13380439	5.30120604
	4.20409257		3.13642150	5.29962540
	4.66967358		10.81078637	4.26926282
	-0.30399280		10.80593671	4.25587933
	6.72563530		5.70961458	4.01853993
	1.73388951		5.69265245	4.01504826
	7.18620461		12.34688386	3.64524313
	2.18910410		12.34825559	3.64558818
	9.22896904		7.21089592	3.35799601
	4.24222848		7.20076553	3.34925223
	5.47292232		2.23055553	2.34193015
	0.48302215		2.23055553	2.34193015
	6.73540354		9.72874641	2.00704742
	1.74550355		9.72874641	2.00704742
	7.98876715		3.77819967	1.47019899
	2.99886727		3.77819967	1.47019899
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	4.22357798		11.29064846	1.28800344
	5.52626467		6.13002825	0.45987183
	0.53636485		6.13002825	0.45987183
	7.45328903		1.12937152	0.40848067
	2.46338916		1.12937152	0.40848067

4.75647831	8.73880577	0.18583304
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1.62575020	7.37738605	9.58649209
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9.73460450	2.38281854	9.39503443
6.58903981	7.23100331	9.58269572
2.53999336	10.23317953	7.13360163
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3.16965319	7.77619966	7.13629068
8.21949780	7.83040618	7.20006049
0.68341469	12.40616008	4.92019945
7.50547603	0.05390835	7.02276658
3.86000917	5.15863446	6.99424829
8.86663889	5.16520698	6.98511660
3.20195574	2.70860232	6.91950584
8.19514989	2.71997983	6.92211007
0.68375549	8.30631385	6.95191297
5.69933514	8.31047991	6.97992169
4.99812454	10.90131078	6.87347493
7.48388427	10.17125416	6.97384632
1.36756247	5.87339812	6.78819039
6.39040523	5.90918224	6.80143505
0.68965537	3.24559528	6.74027430
5.68399405	3.26614494	6.73759043
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8.25783946	11.74199150	5.18162376
8.89093531	9.19904975	4.98737347
3.88787457	9.22288413	5.08099462
7.50178982	4.23139914	5.03952879
2.51242340	4.22109814	5.04138356
8.18268385	6.76770842	4.94658084
3.20876426	6.75298583	4.92461545
5.67367627	12.42112591	4.89397580
2.48214120	0.03379088	7.06108968
3.22479087	1.46819849	4.84132510
8.21903379	1.46821376	4.84382336
1.38924637	9.89728850	4.86057659
6.38227093	9.87044357	4.75834225
5.01764681	4.86029986	4.74558884
0.02220798	4.84657450	4.73500390
0.72635233	7.27577932	4.70625566
5.72454330	7.31642347	4.71806191

5.74332075	2.18393550	4.51868364
0.75463230	2.17795906	4.51752665
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
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# CCH<sub>3</sub> cv

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H	C	O	Fe
3	41	4	80

Cart

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9.30201910	9.50703498	9.52328331
4.62541951	2.62707453	8.22793472
9.60912478	2.59065188	8.22859402
4.20866260	9.28472036	7.40130722
6.81947419	7.56329713	8.43320321
1.77005752	7.56218450	8.42142934
9.26126183	9.24642856	8.03961155
2.19938915	4.25037775	7.19340481
7.19717893	4.25948713	7.19118635
3.40997724	11.90617190	7.19089213
8.41390689	11.85999740	7.16821881
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4.67233017	6.76366879	6.31968985
1.73762477	1.60978738	6.16928493
6.73032918	1.61078295	6.17844625
2.17497304	8.29558395	5.62499722
7.20054268	8.34408054	5.67032723
9.19694457	3.13493904	5.30299551
4.20872846	3.13663846	5.30259995
4.67336450	10.81491049	4.26719163
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6.72472750	5.70591945	4.01700700
1.73527969	5.69765357	4.01764723
7.18064497	12.34839439	3.64087475
2.18973044	12.34823248	3.64090849
9.23180121	7.21211890	3.36327960
4.24340100	7.20128951	3.35265236
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899

9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.68946387	7.25386487	9.57393239
4.75617490	2.47158924	9.40529898
9.75132998	2.42404823	9.40211840
6.62355681	7.31403382	9.58505889
2.54149671	10.21221871	7.09644885
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3.18842578	7.77561382	7.13784483
8.22503293	7.83124132	7.17382915
0.67942697	12.41543256	4.90244370
7.52355258	0.05284103	7.02095986
3.87456050	5.15763394	6.98132384
8.87909248	5.16634597	6.97145708
3.21401436	2.71553850	6.92250958
8.20799303	2.72043768	6.92399677
0.68399246	8.34052833	6.99500253
5.71742871	8.32274174	6.97163277
5.00906561	10.91177725	6.87623514
7.54885980	10.16940233	7.04257859
1.37484579	5.88406337	6.77962931
6.39356227	5.90537748	6.78522745
0.70054458	3.25041156	6.73846102
5.69585638	3.26652636	6.73682693
0.01555844	0.82761173	6.71879592
5.00122292	0.85806157	6.71675034
3.24219383	11.76143155	5.17772269
8.23565195	11.75386099	5.17264282
8.87931140	9.19019805	4.96101628
3.89512633	9.22197426	5.06475463
7.50693808	4.22664498	5.03371376
2.51759960	4.22334776	5.03660068
8.18811972	6.75113374	4.94078532
3.20800346	6.75528231	4.92824009
5.67258497	12.42352515	4.89663438
2.50736549	0.05332170	7.02452661
3.23041724	1.47211179	4.84190446
8.22158093	1.47365543	4.84286405

1.40000927	9.87373810	4.80691783
6.39104137	9.88419718	4.77866069
5.02024269	4.85646636	4.73941530
0.02863900	4.84542718	4.73022158
0.72741152	7.28922268	4.71974111
5.72701678	7.31693346	4.71443410
5.74788643	2.18373937	4.51922097
0.75744530	2.18208457	4.51529206
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943

7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CCH<sub>3</sub><sub>CV</sub>->CCH<sub>3</sub>+Cv

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	41	4	80

Cart

9.00069530	9.33992377	10.00419744
-0.08215179	10.87579745	9.88650296
0.77525324	9.33192934	10.21046718
-0.04515584	9.80355772	9.64569162
4.60995313	2.58891129	8.22211679
9.58881737	2.55226980	8.22510119
4.19121608	9.28199670	7.40171620
6.76155285	7.98471394	8.49799209
1.80257282	7.40209812	8.41084217
0.12854057	9.56990861	8.18883832
2.19696458	4.24074241	7.18559930
7.20080635	4.25709325	7.20956870
3.37187158	11.90355555	7.20190702
8.43082733	11.80945135	7.17230904
-0.31249463	6.87673344	6.38233845
4.68787515	6.75170456	6.32768807
1.72841847	1.59775023	6.16136576
6.72061655	1.60948743	6.18176550
2.19636644	8.28460325	5.62884577
7.16866467	8.35060338	5.64843543
9.19429421	3.13776265	5.30305281
4.20954041	3.13854689	5.30268093
4.66757228	10.81808372	4.27709059
-0.30715734	10.82813260	4.29684622
6.72699247	5.71041379	4.02093370
1.73747117	5.69821158	4.02256001
7.17352668	12.35101335	3.63238117
2.19468958	12.34738725	3.63793135
9.23464763	7.21044406	3.38002290
4.24241761	7.20291065	3.35114300

5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.73466447	7.07082307	9.55808663
4.73196970	2.42096663	9.39991085
9.74134566	2.37444592	9.39749160
6.84054315	7.87386112	9.68378648
2.50490542	10.19972948	7.15005035
-0.03630396	10.75615687	6.77733039
3.22938230	7.74485320	7.14662429
8.24132588	7.92200964	7.17701976
0.68215648	12.44102662	4.88000957
7.53109429	0.05435277	7.02859397
3.88344948	5.13886329	6.97952963
8.87544316	5.19823537	6.95595044
3.20386446	2.69977634	6.91857765
8.20179991	2.72201078	6.92542594
0.79612660	8.30892147	7.03163142
5.71929034	8.34382709	6.98367112
4.95946548	10.91019537	6.87073674
7.40075869	10.22779586	6.94843634
1.37330701	5.87249093	6.76900729
6.40784867	5.88773059	6.74801391
0.69349429	3.23697357	6.73840096
5.69559707	3.25833894	6.74558289
0.00390796	0.80716474	6.71991858
4.99472166	0.84203187	6.73402516
3.22983075	11.75323913	5.18626487
8.22911697	11.77279670	5.15513485
8.88808022	9.18729858	4.97403363
3.89655736	9.21453422	5.07262596
7.50950306	4.22946947	5.03304223
2.51608898	4.21622937	5.03889377

8.18641618	6.76226146	4.97544215
3.21241234	6.75020167	4.92494095
5.66757365	12.42284125	4.90158183
2.45707867	0.01634020	7.01833261
3.23630203	1.46902452	4.84158381
8.21132463	1.48126808	4.84271466
1.40423406	9.85956972	4.78623923
6.38457603	9.87574986	4.72247515
5.02288720	4.85207357	4.73713969
0.02715882	4.84421880	4.72289962
0.72929568	7.28254834	4.72723258
5.72507717	7.30792426	4.71702943
5.74397303	2.18292131	4.52412151
0.75251348	2.18677650	4.51139459
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367

6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CCH<sub>3</sub>+Cv

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	41	4	80

Cart

-0.49647790	9.64502977	9.77463151
0.44011636	11.14233773	9.90163080
1.22785675	9.56272545	10.21064360
0.49379367	10.08906339	9.58248600
4.59750056	2.60289770	8.22359177
9.57774086	2.55977822	8.22697789
4.15651011	9.29384328	7.38631930
6.74767428	8.14352848	8.50740645
2.07049614	7.01901693	8.42596740
0.81787055	10.02244036	8.12915174
2.15871677	4.25723040	7.16453466
7.20136644	4.25676738	7.21133666
3.38578843	11.91284786	7.19911951
8.44105152	11.77157052	7.18086040
-0.31557742	6.88600766	6.43099581
4.68255793	6.74614094	6.31448340
1.71943075	1.60263224	6.16104748
6.72103236	1.60323727	6.18684623
2.16748780	8.27930191	5.62634435
7.16348415	8.34290383	5.63169805
9.18843290	3.13186269	5.30657120
4.20133014	3.14205811	5.30619966
4.66347899	10.81400978	4.28149656
-0.30848016	10.82566245	4.29849567

6.71965055	5.70180748	4.02099079
1.73081191	5.69519617	4.01912488
7.16855284	12.35240921	3.62513919
2.19384596	12.34925796	3.63090528
9.23126166	7.20937626	3.37421079
4.24035915	7.20490165	3.34949157
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.74242768	6.95729319	9.56950055
4.71102293	2.45516891	9.40570311
9.73497283	2.38558688	9.39965461
6.83307864	8.16378167	9.69754603
2.49410221	10.23234236	7.18205336
0.00296452	10.85231515	6.70691149
3.22080090	7.73889163	7.15024911
8.12237409	7.77932296	7.16196405
0.69122165	12.43826007	4.86919238
7.54316718	0.03502384	7.02247044
3.85503034	5.16657250	7.01709179
8.86698381	5.20696961	6.96597482
3.18762732	2.71317980	6.92160688
8.19208014	2.71631975	6.92641773
0.71181258	8.45767020	6.92744791
5.68937085	8.36964904	6.95926328
4.95777463	10.91340382	6.84592273
7.43059758	10.17435748	6.92871109
1.39948858	5.94514229	6.83250639
6.39625329	5.87116222	6.73388874
0.67803196	3.23651940	6.73571337
5.68482757	3.26654013	6.75058602
-0.00175913	0.80221470	6.71301751
4.99863619	0.85485677	6.73970250



3.21934625	11.75238392	5.18287769
8.21618268	11.76964932	5.14895999
8.90636168	9.18560462	5.02608648
3.88293696	9.21364096	5.07921211
7.50808101	4.22498019	5.02995126
2.50817588	4.22972242	5.04946250
8.17972022	6.75052699	4.95400144
3.20876389	6.75235774	4.92455128
5.66568987	12.42340659	4.90027251
2.47737596	0.04502299	7.01683039
3.23510590	1.48032136	4.84101577
8.20891833	1.47931346	4.84281210
1.42189409	9.86569064	4.74700972
6.38157200	9.87828362	4.71326581
5.00871584	4.85557363	4.74402087
0.01835903	4.84179245	4.71844821
0.72102061	7.26859200	4.73200360
5.72319841	7.30894229	4.71044461
5.74266099	2.18506488	4.52995342
0.75067929	2.18576506	4.50937811
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233

7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CCH<sub>3</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	42	4	80

Cart

5.94647339	8.11635619	10.08880279
6.22847726	11.30810194	7.97086827
7.67776730	7.68845774	10.16210023
6.43965947	6.40395516	10.14010280
9.15643639	9.30467701	7.35047676
6.70276456	7.39539678	9.73903920
4.61603909	2.61986727	8.23061992
9.61576449	2.64187071	8.22510967
4.19685298	9.29333218	7.36728555
0.99593415	11.27274510	8.45909051
1.80009055	7.60497345	8.41286059
6.77560584	7.40854856	8.25123121
2.19965834	4.26722460	7.20385981
7.18233306	4.28428590	7.20377155
3.46530388	11.96139454	7.16483105
8.42600800	11.96694909	7.18070318
-0.33145519	6.75954151	6.28260610
4.66289502	6.74301871	6.26685078

1.74100714	1.62978255	6.17878014
6.73534619	1.63836644	6.17586012
2.17458614	8.28739508	5.57629341
7.16698571	8.29795103	5.53027191
9.19834266	3.14361235	5.29809606
4.20781986	3.13795917	5.30287494
4.67080144	10.81478211	4.26322156
-0.31709272	10.82086879	4.26281910
6.72149391	5.69059447	4.00698346
1.73141576	5.69280760	4.01179046
7.17888818	12.35069123	3.63520531
2.18932213	12.35125701	3.64046860
9.22662205	7.20088301	3.32409275
4.23525994	7.20236639	3.32369764
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.59810699	7.42393942	9.57650703
4.77064857	2.45066535	9.40330431
9.75012007	2.47531270	9.40065504
1.23630007	11.35133902	9.62124503
2.54853700	10.29161181	7.19416046
0.00823129	10.94286840	6.97711154
3.17440799	7.78693756	7.11961926
8.16306230	7.79658847	7.08378771
0.68439413	12.41994782	4.91260807
7.50568787	0.09434834	7.05919097
3.86595703	5.17797362	7.01325324
8.85384439	5.18628390	7.02072933
3.21292656	2.72765242	6.92686287
8.20028886	2.73862210	6.92313483
0.69758505	8.31827396	6.92808424
5.69986576	8.30478241	6.95186429

5.00289278	10.91732197	6.89719664
7.51004718	10.29961400	7.16396660
1.37977606	5.90239623	6.79344420
6.36773108	5.95380569	6.93901239
0.70004257	3.29003033	6.73684544
5.68888483	3.29814841	6.74573685
0.00425756	0.90947215	6.68635326
5.01209919	0.90712213	6.68988475
3.24269632	11.77191201	5.18146018
8.22960957	11.77693967	5.18296109
8.88781695	9.25867529	5.10117999
3.87788593	9.25479786	5.10469975
7.50535005	4.24008761	5.05002854
2.52232873	4.23353677	5.04176675
8.20165995	6.75875640	4.89800141
3.20621052	6.76202215	4.90560425
5.67106889	12.42784556	4.89051877
2.54570246	0.10593379	7.07408522
3.23484956	1.47324071	4.84879199
8.22247391	1.48113946	4.84541169
1.40156607	9.91216918	4.84317655
6.38900576	9.90378634	4.81804370
5.01610430	4.86426458	4.75701365
0.02455387	4.85877305	4.74160253
0.72845808	7.29543734	4.69199786
5.71846055	7.29091226	4.69815334
5.75292260	2.19913927	4.51824409
0.76269717	2.19205050	4.51582535
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300

7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for  $C_{cv} + CCH_3 \rightarrow CCCH_3_{cv}$

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9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	42	4	80

Cart

0.19488182	9.38557485	10.13362647
6.21664972	11.33966580	7.98695113
0.36918017	11.14889961	9.91336296
1.80946757	10.13224012	10.14607858
9.15404823	9.35276712	7.40315630
0.81441130	10.17048604	9.67536798
4.60408418	2.61961636	8.23391853
9.60722285	2.60103750	8.21473076
4.18815817	9.29711301	7.36550344
6.77807292	7.72559475	8.45165556

2.38200443	7.16858946	8.63557924
0.93701919	10.00787758	8.19404912
2.19484638	4.26805017	7.18754205
7.19181576	4.26801578	7.20927418
3.39268723	11.92072156	7.20365023
8.45129168	11.98078461	7.15281045
-0.31762444	6.79738376	6.34481047
4.68743324	6.76359932	6.28801619
1.74408584	1.64280823	6.15401123
6.72128311	1.62194389	6.18553753
2.17119699	8.28148422	5.62827755
7.17008950	8.29251269	5.58924573
9.19684638	3.14060335	5.29632534
4.21231092	3.14609300	5.30724130
4.66549377	10.78457503	4.26434484
-0.31783963	10.84128798	4.28604026
6.72822824	5.70050007	4.01342443
1.73488395	5.70365398	4.01750798
7.16666795	12.35188716	3.62430398
2.19768666	12.34893898	3.63323803
9.23157557	7.20226796	3.34344201
4.23776590	7.20466576	3.33433723
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.95129180	6.93569060	9.70601039
4.73607661	2.45461915	9.41096775
9.74943046	2.41484613	9.38687085
6.66602888	7.56374513	9.62787248
2.50555259	10.24480920	7.15604167
-0.00382872	10.94855517	6.81203426
3.23209890	7.74524745	7.16989672
8.18925831	7.83181029	7.14244683

0.69278567	12.44270584	4.87430926
7.50702196	0.08949884	7.06226018
3.87045286	5.19025157	7.01759438
8.86923464	5.18343290	6.98781433
3.21438048	2.73540208	6.92404572
8.19681639	2.73282808	6.92086509
0.70643054	8.41455030	6.95405368
5.72845105	8.33363105	6.94722754
4.97067572	10.92688842	6.92509619
7.50104252	10.31860004	7.16999370
1.39986824	5.91997089	6.77480107
6.40207503	5.90567365	6.76635233
0.69481266	3.29127448	6.73299154
5.69187149	3.27482380	6.74728342
0.01182202	0.91826393	6.66475820
4.99176657	0.86957044	6.71658157
3.23923277	11.75435514	5.18434606
8.20770212	11.79385018	5.15896635
8.88683571	9.24733502	5.08793420
3.88941578	9.22280725	5.14201056
7.51183472	4.23602852	5.03777011
2.52101140	4.23699071	5.04185647
8.20488955	6.76493433	4.93281257
3.20873397	6.76430742	4.91899696
5.65520857	12.41902640	4.89712856
2.50644511	0.09437147	7.02090660
3.24224030	1.48654133	4.83951761
8.20522584	1.48569457	4.84106344
1.40690451	9.89431373	4.78918660
6.39609997	9.90435289	4.83108708
5.01684078	4.86033005	4.74735052
0.02653221	4.85606076	4.72463820
0.72655998	7.29502383	4.71718993
5.72090486	7.29962953	4.69788005
5.74885368	2.19300879	4.52035696
0.75911193	2.19853657	4.50676774
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265

6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CCCH<sub>3</sub> CV

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9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	42	4	80

Cart

0.17258935	9.44180689	10.49854960
6.22690057	11.26012947	7.95549206



0.62146058	11.10291964	10.03179334
1.85077000	9.82255641	10.00452647
9.19398474	9.33650665	7.83320382
0.79165443	10.03806736	9.81101624
4.59862222	2.66053726	8.23980791
9.61013046	2.65894518	8.22393369
4.14734640	9.26413763	7.37787573
6.79767994	7.39825242	8.39376667
2.36362805	7.09621481	8.61887045
0.41407866	9.77744851	8.38344112
2.18832283	4.24712468	7.17415031
7.18395613	4.26232568	7.18741031
3.36443491	11.89885158	7.21406670
8.43815770	11.91696087	7.12957496
-0.34954978	6.79644953	6.32562471
4.67846311	6.73367301	6.27377322
1.73427333	1.62332664	6.14747223
6.71496495	1.59192028	6.20514584
2.14480821	8.27141874	5.63456395
7.18306860	8.33823663	5.65679251
9.18686623	3.13184914	5.29249875
4.20765887	3.13607529	5.30395367
4.65531745	10.77878736	4.26614298
-0.31160544	10.83806496	4.30408535
6.72250880	5.70624449	4.01501669
1.73269274	5.69355088	4.01663035
7.16298494	12.35129554	3.63017474
2.19865610	12.34755812	3.63797210
9.22529536	7.20926816	3.35022153
4.23749471	7.20399200	3.33457903
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304

1.91014722	6.81599467	9.66985209
4.71477527	2.52753081	9.42059732
9.71832482	2.51333528	9.40480663
6.58810594	7.15992369	9.54762119
2.41603696	10.20305058	7.18058211
-0.00346182	10.89970876	6.74451127
3.19849090	7.71842170	7.16757718
8.20108278	7.83627525	7.17717544
0.69004035	12.44062280	4.87304383
7.50213666	0.04062279	7.06022564
3.85911742	5.17445056	7.02168196
8.87738375	5.15972016	6.98123164
3.20651402	2.71905277	6.91900771
8.18627556	2.71699248	6.91887977
0.65937090	8.36496816	6.92628887
5.70487572	8.30520458	6.97967767
4.92879020	10.89180652	6.94778294
7.50648521	10.23034886	7.09292645
1.37714003	5.88409153	6.74816277
6.40166573	5.91518154	6.80149559
0.68247872	3.27405854	6.72823299
5.68530938	3.26282798	6.74376080
0.00226256	0.87811190	6.67514792
4.97595057	0.84801055	6.71811327
3.22801877	11.73560416	5.19804553
8.20599723	11.77515795	5.15383596
8.86947543	9.20555541	4.98682210
3.86833235	9.21705361	5.15544840
7.50375479	4.23434465	5.03777150
2.51661701	4.22301790	5.03477282
8.18444000	6.76407536	4.94702470
3.20457981	6.76198164	4.91408028
5.64827685	12.40741572	4.90627423
2.48080645	0.06322190	7.01977059
3.23969340	1.47451928	4.83640704
8.20244486	1.46967753	4.84601726
1.40042279	9.86936636	4.76299622
6.37998997	9.89149420	4.80642385
5.01371719	4.86590281	4.76453675
0.01809219	4.84770282	4.71834346
0.72140012	7.28666101	4.70094059
5.72661916	7.32062645	4.70704185
5.74808183	2.18250854	4.52375930
0.75173276	2.18951479	4.50594958

8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CCH<sub>3</sub>+CH<sub>Cv</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
5	42	4	80

Cart

5.93165874	8.07522833	10.12325773
6.20334985	11.25585981	7.92503958
4.26972037	9.46639884	9.02069629
7.66922480	7.65267911	10.17192140
6.43794426	6.36664500	10.10357019
9.14881671	9.29794530	7.36010133
6.69220682	7.37389318	9.74221880
4.61563454	2.62427817	8.22753541
9.61770828	2.65712051	8.22066232
4.23720227	9.26719203	7.93466538
0.95425833	11.26688230	8.47625429
1.85283910	7.56569227	8.42297515
6.74936474	7.44796788	8.25727862
2.19982762	4.27719104	7.19332083
7.17322312	4.29091756	7.19730611
3.47373468	11.90526732	7.12227868
8.40989723	11.95339841	7.17902915
-0.32851063	6.75557429	6.28370945
4.65019573	6.79492378	6.27058785
1.73860399	1.62612464	6.19269797
6.72999158	1.62465684	6.18252146
2.20119256	8.33715796	5.63672484
7.16427062	8.29905271	5.53488717
9.19885612	3.15023851	5.29687454
4.20221416	3.13908385	5.30070858
4.68294233	10.82490665	4.27657673
-0.32020242	10.82159191	4.26246955
6.72253489	5.69325889	4.00720278
1.73138702	5.70466824	4.01296078
7.18203060	12.35034022	3.63380105
2.18495034	12.35292263	3.64099088
9.22911748	7.20001049	3.32541775
4.23614718	7.21151743	3.33716186
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899

2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.59412547	7.36450838	9.57116778
4.76247639	2.45364979	9.40197686
9.72992400	2.48897391	9.39891955
1.26803047	11.34070564	9.61685720
2.59313810	10.20621318	7.09749664
0.00019528	10.93651204	6.99605260
3.20874637	7.81945137	7.14357362
8.14761206	7.79525989	7.08542848
0.68131492	12.41746145	4.91738852
7.48541637	0.06271521	7.05845459
3.87499801	5.18556482	6.99449289
8.84808938	5.18572605	7.01994409
3.21025426	2.73231253	6.92548379
8.19189875	2.73852778	6.92048340
0.69815443	8.31887377	6.94093776
5.65565298	8.33036691	6.96340043
4.98525193	10.81110361	6.83379661
7.49531320	10.28129682	7.15565187
1.39392096	5.92378314	6.79715668
6.35529148	5.96147094	6.93983556
0.69822078	3.29452940	6.73673570
5.68423698	3.29042658	6.74241959
0.00079650	0.90128147	6.69121062
5.00100077	0.88300290	6.68667716
3.24698856	11.76837696	5.16324164
8.22900279	11.77030518	5.18400861
8.88951159	9.25446428	5.09864887
3.87432926	9.20622395	4.97485368
7.50473779	4.24185119	5.04760506
2.51795546	4.23785135	5.03899991
8.20699271	6.76302084	4.89847779
3.19467348	6.76024907	4.91613011
5.67662430	12.43417509	4.88954914
2.55818134	0.08755917	7.05662412
3.23072580	1.47333944	4.85157703

8.22458862	1.48047738	4.84936463
1.39810015	9.90426212	4.79917130
6.38918263	9.88892119	4.79317596
5.01622550	4.86259293	4.74947375
0.02684837	4.87261061	4.75063373
0.73831165	7.32829420	4.69367756
5.72182814	7.28797634	4.69955264
5.75164431	2.19827723	4.51908793
0.76175332	2.18913101	4.52176361
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943

1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CCH<sub>3</sub>+CH<sub>CV</sub>->CHCCH<sub>3</sub> CV

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9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
5	42	4	80

Cart

8.99898530	9.50102893	9.07876344
0.91143963	9.68404564	10.32086764
6.25516460	11.27502774	7.92740817
0.40208082	11.34579378	9.88257226
2.12030366	10.90372188	9.87226551
9.15568744	9.30336592	8.00791288
1.10860205	10.53260484	9.65006062
4.60402383	2.59959631	8.22315726
9.60673485	2.58263746	8.21338783
4.19905730	9.28810495	7.41240923
6.84869966	7.65807849	8.46143844
1.79062436	7.39714526	8.44106997
1.00537028	10.16413410	8.19830877
2.19499484	4.26780207	7.18875066
7.19109415	4.26255358	7.20007973
3.40128705	11.89981011	7.16608204
8.47494293	11.89550645	7.12549773
-0.32257003	6.84241649	6.34676410
4.67442775	6.75803008	6.32957262
1.73702594	1.61348441	6.16788598
6.72539449	1.59730223	6.19830882
2.16772277	8.30596850	5.67608339
7.19283512	8.33786397	5.65644912
9.19536068	3.14283560	5.29560242
4.20768898	3.14542788	5.30418207
4.67250172	10.80164739	4.26723174
-0.30914248	10.82822333	4.29082712
6.72762390	5.70874336	4.01603888
1.73586714	5.71528206	4.02320601

7.17092426	12.35164766	3.62416213
2.19253205	12.35018482	3.63098995
9.23748489	7.21414112	3.37039251
4.24177295	7.20396736	3.36163652
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.70223464	7.13815737	9.60609897
4.72273319	2.42328878	9.40025242
9.74883687	2.39218518	9.38627376
6.68849060	7.48951471	9.63105567
2.52733973	10.21403100	7.09067769
-0.03223092	10.79596940	6.77466494
3.21359069	7.76181181	7.16452345
8.22731095	7.84950051	7.16084803
0.68593127	12.43165234	4.88185719
7.53380839	0.04761774	7.05034629
3.87746636	5.15471604	6.99675887
8.87010805	5.18338246	6.97226382
3.20291879	2.71624510	6.91775245
8.19707482	2.72290630	6.92047610
0.71308944	8.38528446	7.11382113
5.71967279	8.31703236	6.97801182
4.97963442	10.90038125	6.89701143
7.52436811	10.22624369	7.05998445
1.36760998	5.91702524	6.83045716
6.40250115	5.91297130	6.79498948
0.69324078	3.27553738	6.73441034
5.69248274	3.26380558	6.74661055
0.00537371	0.87725721	6.68028311
4.99239045	0.85757445	6.71848918
3.23963231	11.75260914	5.17239237
8.22141546	11.77823992	5.14869736



8.87670133	9.19297077	4.96248024
3.89331989	9.21587388	5.07351836
7.50623670	4.23451609	5.03887255
2.51557398	4.24025920	5.04534080
8.19186941	6.75917927	4.94042685
3.20051355	6.76658030	4.93624292
5.66597193	12.42265288	4.89652587
2.48844351	0.03663549	7.00908557
3.23673856	1.47800340	4.84061371
8.21197792	1.47936833	4.84585461
1.39974307	9.86585378	4.77976849
6.39371509	9.87941419	4.76963531
5.02024954	4.86310710	4.74487326
0.03147519	4.85886024	4.73114829
0.72568337	7.30651312	4.75599542
5.72439290	7.31425619	4.71716489
5.74795003	2.18758538	4.52593711
0.75939233	2.19442699	4.51286697
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071

8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CHCCH<sub>3</sub> cv

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9.97980000	0.00000000	0.00000000	
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0.00000004	0.00000004	19.64040000	
H	C	O	Fe
5	42	4	80

Cart

8.79285974	9.27052976	9.12519880
0.84381933	9.44851619	10.41743291
6.21183185	11.26443617	7.93965332
0.73965915	11.17721017	9.96341648
2.26393360	10.29522870	9.74306581
9.32120735	9.29591779	8.14975083
1.16916996	10.20280565	9.68509302
4.59333810	2.62485257	8.23274490
9.59392914	2.67019001	8.22937210
4.16613045	9.25168570	7.40061557
6.71440662	7.63585448	8.42491098
1.88437659	7.18916386	8.38947270
0.67492688	9.83945599	8.30600411
2.18935381	4.23014933	7.18006921
7.17418505	4.24979371	7.20092112
3.35570086	11.88381907	7.19478326
8.43988713	11.89514992	7.12832273
-0.33939186	6.79910889	6.34432034
4.67665309	6.71154540	6.29107032
1.72414805	1.60663324	6.14791167

6.71045747	1.58011238	6.20630192
2.17016566	8.26490764	5.65296220
7.18059703	8.33987974	5.65616613
9.18098221	3.12459338	5.29266783
4.20159756	3.13356201	5.30505205
4.65844905	10.78696111	4.26397341
-0.31410472	10.82692137	4.30828836
6.72047701	5.70462811	4.01275595
1.73161642	5.69576457	4.01924384
7.16211185	12.35065270	3.62757554
2.19575798	12.34734231	3.63820868
9.23017974	7.21078062	3.36990556
4.23684839	7.20331083	3.34364213
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.70115972	6.92254613	9.54406103
4.70137252	2.48723645	9.41344100
9.70467055	2.53986428	9.41089927
6.67063504	7.44353795	9.60218426
2.43132363	10.18039977	7.17525452
-0.05231375	10.82273303	6.75624074
3.22277144	7.70470652	7.14807278
8.22896728	7.86388085	7.16647943
0.68319336	12.42818414	4.87627406
7.50266677	0.03313380	7.06223440
3.86664393	5.12913922	7.00140372
8.86114471	5.15346544	6.97296715
3.19548271	2.69176465	6.91481950
8.17806967	2.71113676	6.91963495
0.75895846	8.25234192	7.05113226
5.69862993	8.30715481	6.96670194
4.92313796	10.88045458	6.92506652

7.47469627	10.22585093	7.06025383
1.36257748	5.86044452	6.79250296
6.40299463	5.90737797	6.80265999
0.67718668	3.26064230	6.72900657
5.68086476	3.24985956	6.74850712
-0.00834548	0.86551319	6.67417042
4.97216215	0.83627058	6.72563491
3.21971743	11.72419920	5.19520072
8.20958083	11.77635019	5.15106543
8.86901625	9.18869972	4.96323831
3.87278629	9.21597436	5.10291103
7.49638121	4.22653119	5.03326539
2.51024846	4.21400321	5.03349696
8.17714561	6.75554153	4.95755805
3.20568771	6.75314397	4.91488164
5.64968182	12.40124741	4.90920472
2.46622145	0.03899433	7.00564443
3.23630960	1.46385680	4.83297575
8.19777070	1.46446911	4.84640182
1.38880151	9.84499139	4.78784576
6.38363249	9.88456990	4.79174661
5.01709557	4.85953689	4.76248841
0.01910029	4.84617487	4.73375488
0.72135183	7.28060181	4.73413763
5.72412100	7.31464647	4.70598114
5.74146521	2.17538927	4.52819561
0.75000713	2.18673201	4.50537176
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903

2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for H+CCH<sub>2</sub>cv->CHCH<sub>2</sub>cv

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9.97980000	0.00000000	0.00000000	
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H	C	O	Fe
3	41	4	80

Cart

8.10443883	9.30925348	9.67928573
9.27701511	7.89161310	9.68651454
0.11079949	10.56911505	8.42412682
8.85290782	8.73397952	9.12485444
4.60808477	2.58116856	8.22039393
9.58762847	2.57239712	8.22589166
4.19763202	9.26068305	7.42791354
6.82569536	7.25602510	8.38426905
1.79854787	7.53038604	8.41467239
-0.36279580	9.30869641	8.08745435
2.19560276	4.22011079	7.20196732

7.18435217	4.24733230	7.18945755
3.39048616	11.89476434	7.19596583
8.40647648	11.82619628	7.18549619
-0.32908751	6.81501304	6.33734250
4.68058686	6.71705188	6.30048151
1.72965237	1.57723731	6.16693889
6.71662375	1.59809808	6.17803397
2.19186726	8.27896020	5.59422327
7.20878545	8.34761018	5.71858095
9.19232754	3.12745986	5.29888206
4.20664246	3.13070056	5.29945243
4.67472790	10.80379103	4.26744228
-0.30396466	10.80672608	4.27975235
6.73235614	5.71255073	4.01987585
1.73638733	5.68639126	4.01780824
7.18280990	12.34728839	3.64025548
2.19323130	12.34476645	3.64484093
9.23311790	7.21504743	3.37725392
4.24399547	7.20136159	3.34750748
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.68811220	7.25891007	9.57517439
4.73576370	2.41188340	9.39663273
9.71400369	2.40205863	9.40205677
6.47896115	7.00585084	9.50356827
2.53471762	10.19653366	7.12767627
-0.06228555	10.78216505	6.89169134
3.20568148	7.74638114	7.12730594
8.26182329	7.86336774	7.27819513
0.68453099	12.41431478	4.90419136
7.51761072	0.04389901	7.03511791
3.86933178	5.13378091	6.99722330

8.88592739	5.15212446	6.98644133
3.20284778	2.68722778	6.91686411
8.19314650	2.70829872	6.91878513
0.75560387	8.28116061	6.96657639
5.69527797	8.29285663	6.97857831
4.98265015	10.88645483	6.88594351
7.40716172	10.19739380	6.93481652
1.37679411	5.85178544	6.78119572
6.42150332	5.90906749	6.80496632
0.69108227	3.22858608	6.74158393
5.68776424	3.24592683	6.73668455
-0.00276298	0.80952990	6.71616913
4.99279366	0.83557234	6.72483464
3.24426113	11.74778342	5.18695640
8.24711243	11.74990088	5.17167099
8.89215969	9.17432356	4.97186384
3.89826403	9.21190299	5.07052726
7.50727711	4.23131183	5.04006279
2.51502265	4.21030261	5.04127771
8.19216716	6.77145764	4.98915967
3.21624003	6.74202928	4.91720493
5.67406363	12.41246793	4.90154025
2.46402436	0.00382844	7.04339313
3.23127999	1.45949164	4.83871372
8.21548999	1.46509644	4.84141239
1.39547704	9.88023807	4.83022038
6.39224180	9.85286401	4.74314684
5.02660250	4.85975882	4.75690565
0.02504524	4.84003057	4.73449414
0.73162502	7.26705172	4.71077564
5.74063403	7.31861533	4.71687448
5.74409687	2.17770772	4.51794890
0.75407990	2.17622713	4.51477873
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425

3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CHCH<sub>2</sub> cv

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9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	41	4	80

Cart

8.20083476	9.09566440	9.84661906
9.26914033	7.61125557	9.64975978
-0.23880815	10.36346905	8.51776236
8.90396336	8.54574969	9.21365382
4.61325052	2.59854906	8.21992226



9.59345949	2.57646609	8.22400762
4.21638888	9.25900363	7.45027245
6.77868366	7.33996026	8.36953740
1.83283762	7.47392116	8.41807208
-0.29705329	9.21906131	8.24329684
2.19896429	4.22380152	7.19530567
7.19483560	4.25358788	7.19149357
3.38576842	11.88839188	7.19495176
8.39383335	11.82748642	7.16808969
-0.32752040	6.84090120	6.35181909
4.69126096	6.72725008	6.30121635
1.72920086	1.57932993	6.16471884
6.71662591	1.60735434	6.17621477
2.20103107	8.28571828	5.61961566
7.20330540	8.37053861	5.70774081
9.19516539	3.13521816	5.29526936
4.20787814	3.13502037	5.29736950
4.67609042	10.81368294	4.26884456
-0.30113615	10.80959095	4.27819015
6.73608033	5.72224671	4.02232011
1.73849393	5.69595719	4.02064555
7.18224313	12.34896574	3.63894778
2.19300375	12.34664637	3.64556773
9.23543343	7.21448059	3.38281762
4.24582101	7.20325062	3.35073872
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.72314691	7.16635889	9.56955039
4.73390508	2.43432962	9.39695870
9.72034312	2.41266766	9.40129734
6.46562253	7.01807189	9.48032570
2.54932913	10.17884329	7.11040339

-0.06616413	10.74823221	6.84556150
3.22802409	7.74375045	7.13639136
8.28457837	7.92594273	7.28537120
0.69081301	12.40636633	4.91309339
7.51151899	0.05924250	7.03988193
3.87667469	5.13453948	6.98719162
8.89746447	5.15931596	6.97472065
3.20502889	2.68943026	6.91472858
8.19784594	2.71527006	6.91787473
0.78148215	8.28418391	6.99869633
5.70814508	8.30006096	6.97950741
4.97572694	10.88923543	6.88389153
7.35841843	10.23466473	6.90109053
1.38096287	5.85411229	6.77205065
6.42867103	5.91121246	6.79162301
0.69423205	3.23028300	6.73678170
5.69288397	3.25309760	6.73581437
0.00145028	0.80550732	6.72817845
4.99193717	0.83621499	6.72802422
3.24665989	11.75147347	5.18483621
8.25202950	11.76528770	5.16271813
8.89546616	9.18389250	4.97325084
3.89673409	9.21070499	5.04843121
7.51109087	4.23909055	5.03827724
2.51640771	4.21363656	5.03829886
8.19569272	6.78501130	5.00401852
3.21686681	6.74712733	4.91909067
5.67728540	12.41788620	4.90384227
1.70297911	12.66163921	7.03677774
3.22899908	1.46316552	4.83666767
8.21705004	1.47200827	4.84172579
1.40064618	9.87247959	4.81748160
6.39336734	9.85751091	4.71539823
5.03064727	4.86312560	4.75408873
0.02737892	4.84678201	4.72850062
0.73289392	7.27984644	4.72138621
5.74363638	7.32228599	4.71593269
5.74331591	2.18005989	4.51851434
0.75287001	2.17451088	4.51533508
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337

3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# H+CHCH<sub>2</sub>cv

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9.97980000	0.00000000	0.00000000	
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0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	41	4	80

Cart

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9.28119165	7.65544819	9.61981457
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6.19669164	11.29420430	7.98583891
8.91113562	8.58691892	9.18586798
4.60629923	2.64813279	8.22858719
9.60104365	2.64177011	8.22279527
4.16648319	9.25677294	7.38246442
6.76996647	7.33568235	8.37760722
2.35000662	7.21369153	8.64440645
-0.29494353	9.27674339	8.21639239
2.18889054	4.24036800	7.18080774
7.18925907	4.26447972	7.18477347
3.37395762	11.90227197	7.21307477
8.42065005	11.87312339	7.14652160
-0.34728487	6.83639761	6.35512986
4.69048927	6.72377920	6.26967118
1.73225854	1.60281218	6.16020198
6.71717267	1.60144075	6.19168939
2.17693891	8.27650617	5.58197381
7.19761810	8.38578859	5.71559804
9.18927044	3.13367779	5.28547317
4.20695558	3.13835285	5.29692149
4.66554474	10.78979088	4.26315418
-0.30501725	10.81035487	4.27383440
6.73207952	5.72594356	4.02243405
1.73391101	5.68983111	4.01574772
7.17734972	12.34886948	3.64277437
2.19378147	12.34685979	3.64599522
9.22652477	7.21291577	3.37012097
4.24180586	7.20341789	3.33338034
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067

4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.92412606	6.96775908	9.71309372
4.72121017	2.49672289	9.40785086
9.70894020	2.49460456	9.40355723
6.43256263	7.03123622	9.48810789
2.51254035	10.20240414	7.11502449
-0.07185259	10.78184289	6.86740449
3.19515778	7.71566059	7.15479541
8.25995143	7.91685844	7.28587250
0.69164600	12.40413513	4.91346149
7.50347770	0.05405202	7.07318315
3.85886905	5.17140606	7.01931513
8.89645266	5.16014568	6.98483446
3.20594191	2.71169625	6.91458102
8.19098482	2.72026230	6.91333194
0.70980361	8.36716348	6.89327165
5.69993323	8.29667628	6.97308659
4.94648909	10.89183611	6.94279173
7.35339647	10.26385477	6.95949216
1.36941392	5.87365222	6.75287449
6.43259094	5.92651306	6.78942823
0.68611550	3.25620949	6.72704837
5.68939346	3.26297932	6.73607373
0.00453693	0.84161797	6.70421267
4.98188803	0.84918626	6.71852805
3.24772427	11.75103941	5.18995934
8.24826865	11.76485570	5.16298596
8.88562864	9.19589306	4.99550603
3.88759921	9.21509922	5.12863721
7.50826368	4.24526573	5.03800367
2.51597215	4.22364509	5.03982491
8.18837280	6.79330903	4.99982148
3.21543499	6.75627761	4.90731204
5.66921007	12.40787020	4.91123932
2.46814460	0.02544261	7.03655552
3.22801713	1.46792623	4.83795800
8.21200282	1.46391871	4.84632375
1.39640195	9.88777089	4.79904467
6.38880037	9.87052064	4.73815565
5.02237854	4.87401920	4.76661942
0.01568761	4.85144322	4.71880483
0.72270847	7.27773649	4.70258470
5.74099235	7.33666806	4.70634950

5.74423925	2.18021065	4.52171820
0.75140339	2.17741911	4.51182492
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CHCH<sub>2</sub><sub>cv</sub>->CHCH<sub>2</sub>+Cv

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9.97980000	0.00000000	0.00000000	
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H	C	O	Fe
4	41	4	80

Cart

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9.34014027	7.78086322	9.46619807
0.39192461	10.40092899	8.88358447
6.21801098	11.26336785	7.98877592
8.97273911	8.68765953	8.95691031
4.60522591	2.64617639	8.23112437
9.60321397	2.62727552	8.22280613
4.16484218	9.24887743	7.39322924
6.77262152	7.31980879	8.41726525
2.40714887	7.16806521	8.67154780
0.02078944	9.49938772	8.31393962
2.18523997	4.24560605	7.17489386
7.19281195	4.25407629	7.18231226
3.38839159	11.89411516	7.21190812
8.42335180	11.85994261	7.15775256
-0.34058710	6.85519370	6.35536205
4.67475907	6.71838738	6.26985908
1.72787643	1.61476866	6.15589342
6.72473766	1.58900003	6.19264866
2.14730922	8.27556422	5.62015013
7.20490439	8.36757137	5.72159660
9.18926524	3.12956429	5.28861054
4.20895372	3.13580169	5.29770938
4.66563384	10.77612951	4.26191275
-0.30779164	10.80792585	4.27436291
6.73002066	5.71464843	4.01979009
1.73298741	5.69225121	4.01992923
7.17637318	12.34704722	3.64299751
2.19748314	12.34337729	3.64080912
9.22824254	7.21228435	3.36489019
4.24029123	7.20313060	3.33693515
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899

2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.97729337	6.90455755	9.73389765
4.72336547	2.49488018	9.41018954
9.72122660	2.47977222	9.40278901
6.43262580	7.06935315	9.53612928
2.51061022	10.19553810	7.13523946
-0.01946588	10.84811751	6.85541359
3.19315977	7.70704423	7.16556929
8.18023562	7.78533508	7.24910976
0.68682942	12.41920029	4.89401840
7.50641275	0.03079784	7.07034184
3.86143802	5.16386992	7.02693538
8.88731196	5.16763531	6.97150586
3.20808735	2.71380277	6.91616222
8.19430667	2.71198272	6.91562764
0.67748245	8.42629776	6.89433544
5.68741901	8.28251767	6.97330759
4.95959741	10.87871215	6.95233360
7.41675847	10.21044081	7.01641373
1.36317533	5.88088535	6.74568807
6.40840762	5.90195649	6.79346409
0.68589809	3.25506488	6.72716437
5.68930255	3.25563718	6.73627921
0.00779747	0.83599388	6.70471623
4.99008512	0.84370961	6.71673197
3.24553085	11.74026394	5.19144639
8.23729393	11.75144150	5.16997960
8.89376401	9.19328383	5.02662622
3.88010104	9.20998471	5.14659024
7.50620038	4.23524494	5.03763614
2.51683771	4.22256516	5.04059042
8.19247695	6.77147643	4.96549463
3.20661242	6.76054350	4.91096848
5.66579354	12.40178493	4.91025753
2.50207697	0.05456832	7.01231133
3.23361961	1.46604393	4.83907521



8.21503838	1.45613457	4.84870070
1.39762060	9.88185819	4.78507386
6.38637931	9.86914024	4.76953693
5.01602634	4.87064248	4.76126905
0.01911313	4.84166625	4.71339316
0.71983134	7.27277845	4.70729533
5.73761043	7.33055587	4.70681193
5.74728752	2.17729255	4.52092745
0.75198702	2.18042274	4.50902195
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943

1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CHCH<sub>2</sub>+Cv (state1)

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	41	4	80

Cart

8.64624070	8.95294722	8.75207630
0.09543800	8.11125817	9.53934495
1.39481880	10.17522053	9.02643673
6.20882251	11.26320873	7.95924922
-0.21598293	8.74967315	8.70523571
4.61066156	2.62261323	8.22929208
9.60346815	2.58591487	8.21676759
4.16589811	9.24729146	7.37382113
6.75579491	7.47655477	8.41668349
2.67703131	6.98463083	8.70769139
0.60395824	9.86773620	8.29551539
2.19058616	4.24153896	7.16588426
7.19750473	4.24903846	7.20188787
3.37069012	11.89402502	7.22104269
8.45708106	11.82429693	7.16069846
-0.33790446	6.81805101	6.36386872
4.69936803	6.70802165	6.26382384
1.73055377	1.60903727	6.14695493
6.72235422	1.58373897	6.19331566
2.14638346	8.24197823	5.65328246
7.19113045	8.37898871	5.68884199
9.18853758	3.13178007	5.28980693
4.21393816	3.13852360	5.30251450
4.65477929	10.77296128	4.26624391
-0.29818945	10.83373577	4.30018614
6.73184171	5.71754504	4.02089074
1.73294008	5.68979628	4.01666869
7.16604798	12.35042365	3.63287588
2.20464010	12.34569300	3.63683866

9.22709964	7.20979222	3.36885659
4.23764200	7.20317142	3.33464271
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
2.34264826	6.64856028	9.78225015
4.72906655	2.47048881	9.40964127
9.73987758	2.42444820	9.39255836
6.58440338	7.25744962	9.58149975
2.48173888	10.19583129	7.18718470
0.01341839	10.87652090	6.75789929
3.23798496	7.68142536	7.16838051
8.22603703	7.87657704	7.21713233
0.69708891	12.44645578	4.86796584
7.52783520	0.03591559	7.07293843
3.87124271	5.15895880	7.03172717
8.89098326	5.15793850	6.97753673
3.20952525	2.70545967	6.91776725
8.19474928	2.70423836	6.91753641
0.63910765	8.44645013	6.87662846
5.71625717	8.29803500	6.97849753
4.93049323	10.88238733	6.94760715
7.36075446	10.25663518	6.91406768
1.37760554	5.88841346	6.75801554
6.43213478	5.91036913	6.80502197
0.68880425	3.24973598	6.72809526
5.69755437	3.25212338	6.74295908
0.00663818	0.83173774	6.70737333
4.99329818	0.83675588	6.73678620
3.23075873	11.72409168	5.20255576
8.23350963	11.77868487	5.15099334
8.89274261	9.21078091	5.02034819
3.87125605	9.19865109	5.16452757

7.50900197	4.24067168	5.04150651
2.52062540	4.22015790	5.03976673
8.18367794	6.78361744	4.98116449
3.20468579	6.75485733	4.90941575
5.66142653	12.39727271	4.91524782
2.48156339	0.04640251	7.00759884
3.24919557	1.46753975	4.83992684
8.21067129	1.46264837	4.84650954
1.41325836	9.86040383	4.78049173
6.37839080	9.86657928	4.71185876
5.02247155	4.87043611	4.77567680
0.01902043	4.84885811	4.72525141
0.71583681	7.27608226	4.71953142
5.73438596	7.32868098	4.70463254
5.74884726	2.17711298	4.52520936
0.75249523	2.18871064	4.50652777
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235

8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CHCH<sub>2</sub>+Cv (state2)

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	41	4	80

Cart

8.63733705	8.94207696	8.77334629
0.06451334	8.05031703	9.55083359
1.40088611	10.11386153	9.09007451
0.38106121	12.33476959	7.85369447
-0.23293440	8.71677525	8.73284632
4.61589749	2.62755306	8.22697024
9.59746166	2.55671049	8.22454299
4.17823764	9.25929974	7.36882713
6.72873293	7.49091117	8.42165275
2.67241970	6.99181879	8.70239882
0.60631846	9.82779030	8.36075867
2.18676951	4.24611352	7.16777773
7.20442021	4.25191504	7.20775636
3.40311199	11.91133960	7.19921466
8.34647375	11.77653760	7.18565524
-0.33761524	6.82945763	6.36601924
4.69404334	6.71570855	6.26107458
1.73063383	1.62630916	6.13553610
6.72521140	1.61344247	6.17035575
2.13761702	8.25218779	5.64998490
7.18497711	8.36486036	5.68009240
9.18982853	3.13811777	5.29224872

4.21473100	3.13885787	5.29499830
4.65839371	10.77676972	4.27204846
-0.30343298	10.83387472	4.27563776
6.73120275	5.71654454	4.02114342
1.73106207	5.69250946	4.01661842
7.17494430	12.34997782	3.63436762
2.19868019	12.34534769	3.63970302
9.22835444	7.21015909	3.36826840
4.23783994	7.20275508	3.33510283
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
2.33897781	6.65816704	9.77738562
4.73353140	2.47358035	9.40585430
9.73860436	2.43543592	9.40551996
6.57338689	7.25502318	9.58490447
2.49980996	10.21912462	7.19998316
0.01984369	10.95640533	6.90813696
3.23152213	7.69579202	7.16448087
8.22127088	7.86606694	7.22373836
0.68647356	12.44305520	4.88175419
7.50394411	0.05249247	7.02890722
3.86559765	5.17244920	7.03551453
8.89317315	5.16183691	6.97324380
3.21656771	2.71844053	6.91446832
8.20725021	2.70913638	6.91940786
0.63083836	8.47291832	6.88590672
5.71468646	8.30595287	6.97828027
4.96463687	10.89345706	6.88517335
7.37094896	10.19795773	6.85503401
1.37414350	5.89609940	6.76262785
6.42746512	5.90735797	6.80223570
0.69520260	3.23802934	6.72841765

5.70027239	3.26334737	6.74078033
0.03332058	0.79028045	6.80171977
5.00660576	0.85129786	6.72018173
3.23690331	11.73973589	5.18934898
8.24338117	11.77425615	5.16600680
8.90788159	9.22199329	5.03760071
3.86032994	9.20036882	5.15802556
7.50959401	4.24216686	5.04253469
2.51939526	4.22347332	5.04081767
8.18610980	6.78640144	4.97887209
3.20027238	6.75680268	4.90951561
5.66375539	12.40771019	4.89333538
2.52909562	0.09912101	7.01231481
3.24688702	1.46849698	4.83808368
8.21916988	1.46836471	4.84436138
1.39876306	9.89624806	4.83162048
6.37507159	9.85330964	4.68307201
5.01969579	4.87210503	4.77493160
0.02080280	4.85022219	4.72534234
0.71574135	7.27674393	4.72621689
5.73225431	7.32310236	4.70616963
5.74988840	2.18368163	4.51861415
0.74536116	2.18217980	4.50902845
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425

-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for H+CHCH<sub>2</sub>->CH<sub>2</sub>CH<sub>2</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	41	4	80

Cart

8.67947524	9.03416884	8.82407547
0.08220173	8.06964285	9.54434237
1.53183630	9.97618217	9.05036920
0.37903453	11.36038714	8.31882383
-0.22161051	8.74819507	8.73784539
4.60521008	2.61295924	8.22762168
9.59384737	2.55445845	8.21503904
4.19755795	9.25348219	7.36927743
6.71990752	7.49777029	8.41979525
2.68761460	6.99105797	8.70576569
0.68226585	9.81381831	8.34661203
2.18565947	4.24040517	7.17009945
7.19674516	4.25223129	7.20822528
3.39283680	11.89856696	7.19456253
8.39139146	11.80237277	7.17818919



-0.33291902	6.82275977	6.36490756
4.69665964	6.70937917	6.25999654
1.72753308	1.60705152	6.15549706
6.71725608	1.60942687	6.17738336
2.14861955	8.25605733	5.65725529
7.18874799	8.36402393	5.67834323
9.18948137	3.13603392	5.29518413
4.21210518	3.13905918	5.30076440
4.66168017	10.78686543	4.27351931
-0.29750433	10.82128333	4.28173862
6.73127679	5.71364130	4.01950417
1.73305419	5.69254591	4.01813373
7.17869449	12.34804604	3.63795624
2.19793283	12.34763911	3.64036094
9.22983604	7.20990025	3.36978093
4.23849373	7.20338907	3.33615685
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
2.35783935	6.65823671	9.78286223
4.72779053	2.45242003	9.40668605
9.74158765	2.37057703	9.38854155
6.58727837	7.25081401	9.58448608
2.52612354	10.18813622	7.13574518
0.03160682	10.97039233	6.88399007
3.24588984	7.68683147	7.16462281
8.22015731	7.85372818	7.21628822
0.68705866	12.43801187	4.88605622
7.51455263	0.05403159	7.03820770
3.86597799	5.16387171	7.03473780
8.88824611	5.16335829	6.97078023
3.20675012	2.70863161	6.91788730
8.19593552	2.71330696	6.91968264

0.63442516	8.45433757	6.88532506
5.72423234	8.30356682	6.97556285
4.97110867	10.89755332	6.88249533
7.37734451	10.21292824	6.86245072
1.38008625	5.88905985	6.75490418
6.42499257	5.90393376	6.79955132
0.68689048	3.24278656	6.73123052
5.69227153	3.25891463	6.74360941
-0.00529842	0.82611680	6.71025201
4.99670191	0.84424762	6.73037980
3.23862530	11.74626186	5.18788069
8.25285951	11.76196058	5.16484569
8.90963639	9.20670361	5.03789137
3.87413697	9.19614120	5.14085978
7.50648922	4.23970733	5.04162442
2.52028545	4.22209641	5.04105182
8.18620360	6.78027004	4.97305453
3.20145506	6.75664224	4.90953511
5.67107490	12.40925399	4.90031949
2.48814204	0.05302275	7.03084939
3.23797917	1.47316762	4.83758799
8.21469178	1.46901537	4.84301567
1.40680225	9.88190019	4.80792667
6.37846214	9.85511386	4.68856712
5.01825555	4.87051765	4.77083232
0.02036458	4.84868872	4.72270517
0.72164991	7.27666079	4.72384667
5.73362369	7.32025287	4.70467504
5.74580691	2.18268948	4.52091496
0.75245719	2.18704385	4.50856566
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899

5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>2</sub>CH<sub>2</sub>

1.000000000000

9.97980000	0.00000000	0.00000000
-0.76395804	12.66177393	0.00000000
0.00000004	0.00000004	19.64040000

H	C	O	Fe
4	41	4	80

Cart

8.70235570	8.88476116	8.98387484
0.12794369	7.80798285	9.44932196
1.58213867	9.80832650	9.14223901
0.10202299	10.75224793	8.69164304
-0.21671010	8.60501322	8.78917998
4.61528712	2.63095793	8.23018053
9.60371459	2.59271905	8.22203824
4.19307511	9.25573449	7.37471321

6.69038313	7.54881521	8.44171630
2.73441588	6.94948248	8.71324472
0.64109513	9.77237602	8.56696169
2.19085863	4.24892035	7.15971364
7.20698798	4.25490929	7.20357675
3.39242761	11.89458752	7.19709904
8.39115450	11.81402370	7.16818593
-0.33979678	6.84075700	6.37182409
4.69660936	6.71801362	6.25910306
1.72708932	1.61436609	6.14540555
6.72397396	1.61601609	6.17415325
2.14018930	8.27083560	5.69413045
7.18223670	8.37127779	5.68049374
9.19280113	3.14068933	5.29383917
4.21413644	3.14166044	5.30162446
4.66068320	10.78951090	4.27706484
-0.29655463	10.83021682	4.29928663
6.72883764	5.71466597	4.01965543
1.73499963	5.70153988	4.02244857
7.17306649	12.35073785	3.63559822
2.19709225	12.34888103	3.63659601
9.22946010	7.21047926	3.37185018
4.23884473	7.20438833	3.33853014
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
2.42207661	6.58028379	9.78454647
4.74286218	2.48173926	9.40967527
9.75004262	2.43754009	9.39846476
6.55966110	7.29593269	9.60430025
2.51893625	10.18932099	7.12619550
0.02055665	10.91149393	6.74861180
3.25051501	7.68380561	7.17411774

8.19806033	7.84549309	7.21626045
0.69352625	12.44252366	4.87891880
7.51109453	0.05784316	7.03243949
3.87448603	5.16774232	7.02956256
8.89375644	5.16850469	6.95855880
3.21267634	2.71582925	6.91984065
8.20404480	2.71739026	6.92012326
0.61026618	8.49535359	6.92036279
5.72282241	8.31572936	6.97704774
4.96864388	10.89913619	6.88011008
7.38252301	10.22319462	6.87338357
1.37866073	5.89447185	6.73276808
6.42117445	5.89864428	6.78934208
0.69196105	3.24793913	6.72740872
5.69762697	3.26506030	6.74154920
0.00448621	0.81845380	6.72085835
5.00282140	0.84763183	6.72901636
3.23303570	11.74351473	5.18458320
8.24182372	11.78199900	5.15445817
8.89126348	9.20416490	5.01457976
3.87195171	9.19292907	5.14671103
7.51005689	4.24150065	5.03600094
2.52330996	4.22288226	5.03453672
8.18743189	6.77513295	4.97297678
3.19732901	6.76373913	4.91284109
5.66612546	12.41524964	4.90016871
2.51856805	0.07937760	7.00615547
3.24232186	1.47965309	4.83518343
8.21539190	1.47642640	4.84087555
1.41536483	9.85864541	4.75842664
6.37932328	9.86653891	4.69584106
5.01590621	4.87222875	4.76679023
0.02298363	4.85192850	4.71489165
0.71687869	7.29896673	4.73881467
5.73431169	7.32203476	4.70588375
5.74773298	2.18621747	4.51908278
0.75290257	2.19049968	4.50627935
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265

2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>2</sub>CH<sub>2</sub>+H

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
5	41	4	80

Cart

8.70818721	8.86481413	8.97767652
------------	------------	------------

6.21405185	11.24802708	7.94713284
0.13518976	7.79414473	9.44800926
1.58250290	9.80056044	9.13966177
0.10286340	10.73459193	8.67228423
-0.20925930	8.58851044	8.78251902
4.61209408	2.62809045	8.23219455
9.60967904	2.59328508	8.21779773
4.18256867	9.24521268	7.37426440
6.69989102	7.52741635	8.43757681
2.75517673	6.94919822	8.72512584
0.64608130	9.75710600	8.55656103
2.19406454	4.24956722	7.16270706
7.20776779	4.24905967	7.19998938
3.38022552	11.88797492	7.20437208
8.43113163	11.83840468	7.12669507
-0.34117699	6.83355296	6.37121044
4.69869590	6.71198348	6.25539065
1.73104916	1.62109828	6.13944984
6.72772921	1.59245229	6.18829316
2.14319295	8.26707153	5.69239222
7.18722119	8.38244721	5.68701529
9.19284981	3.13912584	5.29124682
4.21747829	3.14280009	5.30367941
4.65859153	10.78594198	4.27276145
-0.29385524	10.82460083	4.29947914
6.73033943	5.71460164	4.01936171
1.73525678	5.70056622	4.02287095
7.17058202	12.34993571	3.63359407
2.20018287	12.34973277	3.63239523
9.22842573	7.20964704	3.37137032
4.23841576	7.20459096	3.33617351
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304

-0.23342146	8.73880577	0.18583304
2.45175089	6.58027294	9.79818484
4.74525831	2.47506469	9.41042466
9.75279668	2.43401174	9.39411032
6.55617745	7.28103188	9.60102075
2.50833976	10.18241650	7.11802225
0.02495958	10.89143397	6.72354158
3.25111489	7.67479239	7.17533812
8.19606960	7.84179762	7.21605335
0.69698592	12.44448570	4.87257031
7.51402305	0.04077931	7.06614216
3.87805300	5.16218861	7.03008345
8.89368684	5.16200911	6.95839543
3.21622537	2.71539619	6.91994494
8.20157652	2.70606154	6.91845839
0.61577671	8.47710732	6.91619774
5.72107285	8.29977227	6.97293665
4.94286273	10.88324178	6.92435393
7.37309813	10.24732297	6.92195754
1.37841659	5.89121556	6.72783438
6.42289635	5.89653093	6.79425292
0.69252130	3.25712220	6.72696923
5.70112574	3.25724381	6.74239670
0.01242513	0.83650312	6.70294359
4.99635422	0.84330942	6.72451967
3.23199620	11.73880154	5.18795203
8.24197986	11.78055061	5.14507351
8.88877343	9.20751100	5.02747548
3.87831017	9.19352185	5.14970418
7.51064897	4.24013474	5.03742922
2.52446232	4.22192712	5.03389780
8.18657569	6.77679867	4.97219083
3.19870935	6.76482806	4.91101011
5.66477917	12.41033139	4.90829792
2.51662204	0.07963544	7.00210642
3.24755452	1.48048623	4.83544876
8.21717728	1.46807083	4.84381526
1.41734495	9.85062992	4.74795557
6.38021476	9.87322474	4.71213359
5.01766805	4.87341552	4.76790572
0.02138900	4.85218060	4.71222978
0.71676834	7.29856447	4.73413347
5.73591602	7.32699841	4.70089876
5.75228899	2.18453177	4.52127360



0.75442980	2.19438946	4.50568443
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH+H (state1)

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
2	41	4	80

Cart

6.63798469	7.20613877	9.30233364
6.22408752	11.30173483	7.96766998
6.75509172	7.33051952	8.21532413
4.61251780	2.63667564	8.23247778
9.61135845	2.63545473	8.22366671
4.19214301	9.27868297	7.37638513
1.80129628	7.51841502	8.40442625
0.97825650	11.26286927	8.48185858
9.14892456	9.29260758	7.36665118
2.19282911	4.26049209	7.19964290
7.17516433	4.27001915	7.19689574
3.45782497	11.95117950	7.16816420
8.42058191	11.95660634	7.18248979
-0.34059835	6.75293292	6.28503341
4.65148363	6.73131630	6.25665061
1.73706304	1.62202704	6.17805212
6.72939635	1.62765544	6.17259496
2.16852549	8.28555473	5.58512049
7.16231271	8.29903756	5.54638746
9.19462350	3.13806404	5.29577301
4.20336824	3.13441047	5.29866097
4.66810383	10.80907183	4.26397603
-0.31868217	10.81060345	4.26054746
6.71991090	5.68978403	4.00976118
1.72832166	5.69113883	4.01242428
7.17915896	12.34866726	3.63684216
2.18851357	12.34994283	3.64179340
9.22494995	7.20077951	3.32749063
4.23322070	7.20217603	3.32299880
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344

5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.22782551	11.34892962	9.64021925
4.74737952	2.47673712	9.40810582
9.74566406	2.46765193	9.39915247
1.58261060	7.30244763	9.55852331
2.54313793	10.27878311	7.19520878
0.00380219	10.93142440	6.99550158
3.16857573	7.77205151	7.12224325
8.16047106	7.78190819	7.09854517
0.68179461	12.41213993	4.91620073
7.50170834	0.08510540	7.05861047
3.85975217	5.17203237	7.01987193
8.84474847	5.18237567	7.03156088
3.20741068	2.72205223	6.92309498
8.19566081	2.72883819	6.92103655
0.69130676	8.30769748	6.93963482
5.69261047	8.28768676	6.95920706
4.99425825	10.90476599	6.90002690
7.50318652	10.28780498	7.17258452
1.36900708	5.89473358	6.79932034
6.35834098	5.92803846	6.90343119
0.69418008	3.28226220	6.73419836
5.68103372	3.28693980	6.74097743
0.00106129	0.89926037	6.68645682
5.00524890	0.89661962	6.68865066
3.23948979	11.76525550	5.18339606
8.22923360	11.76763336	5.18513050
8.88441459	9.25270476	5.11048696
3.87485832	9.24846519	5.10820115
7.50292717	4.23381159	5.04737136
2.51788710	4.23109422	5.04254571
8.19459480	6.76190654	4.90101685
3.19946414	6.76236621	4.90252326
5.66855148	12.42359898	4.89166077
2.53890169	0.09755682	7.07631299
3.23202385	1.46729518	4.84777453
8.22070217	1.47398982	4.84393681
1.39744574	9.90686126	4.84832837
6.38484774	9.89907849	4.81884548

5.00938448	4.86342162	4.75315868
0.01957058	4.85809723	4.74624366
0.72304843	7.29368767	4.69669270
5.71522143	7.29431508	4.69769979
5.75009291	2.19530798	4.51561155
0.76086093	2.18793099	4.51447329
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013

5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

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1.000000000000

9.97980000	0.00000000	0.00000000
-0.76395804	12.66177393	0.00000000
0.00000004	0.00000004	19.64040000

H	C	O	Fe
2	41	4	80

Cart

-0.12965310	2.33423476	9.13106756
7.78490733	1.59742931	8.17565853
9.69422423	2.47059074	8.05363569
4.24730690	2.41074692	8.37352870
7.21380006	4.25188597	7.16787489
4.20861545	9.30748994	7.37230038
6.00815867	11.41071986	8.46137055
6.76108151	7.70497948	8.43789894
9.19680990	9.32810248	7.36233429
1.74072672	1.62705711	6.08403878
1.79150319	7.73243085	8.44914318
3.40053976	11.91763094	7.20867506
8.46699999	11.97123982	7.14940213
-0.33541322	6.78068317	6.32787771
4.66611069	6.78178808	6.32001509
2.18529133	4.26251870	7.19179876
6.70210072	1.53369101	6.11732362
2.17792711	8.29256429	5.59317920
7.16577098	8.28291851	5.58075112
9.20111749	3.14549604	5.23485637
4.20523733	3.14445898	5.29821880
4.67706759	10.81802248	4.26867663
-0.31680942	10.83159150	4.27185296
6.72855557	5.67766285	4.01820465
1.73449701	5.69436591	4.01524005
7.17543510	12.35387999	3.64145012
2.19139414	12.34832060	3.63330044
9.22932449	7.19976823	3.34140694
4.24144469	7.20293493	3.34276333
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742

1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.64283850	7.52672583	9.60941577
4.72736429	2.33794084	9.45277645
1.65715725	7.55479201	9.61970267
6.18453556	11.38243111	9.64119480
2.53556793	0.12936447	7.03860064
7.55372480	10.31736337	7.20237646
3.18565098	7.80097666	7.13115030
8.17264544	7.81883607	7.13000098
2.53061396	10.24908305	7.10580046
5.67528824	12.42316180	4.92071879
1.38485173	5.90650683	6.76761168
6.37491935	5.88988733	6.78601561
3.20896801	2.72690877	6.94641127
8.15141062	2.65088258	7.00173278
0.72031947	8.35050209	6.94485700
5.70586126	8.32320911	6.93436345
5.00107666	10.95240646	6.97902497
0.69120892	12.44074888	4.88424066
8.88463722	5.15456334	6.99504103
3.86575765	5.16861381	6.96383667
0.68381139	3.29681366	6.71398431
5.68686866	3.28175278	6.69742050
8.22886264	1.48135168	4.86033801
5.74905926	2.19859677	4.50408479
3.24421348	11.77353415	5.18815533
8.22280136	11.78250139	5.18442283
8.87367425	9.25216248	5.09353067
3.90362283	9.23602495	5.08999060
7.51811833	4.18851430	5.08047037
2.52069182	4.20438851	5.03636631
8.20054167	6.74516715	4.92888982
3.20792080	6.75213256	4.92167116
4.97229504	0.87836721	6.70914953

3.24227188	1.49326212	4.82785208
0.75135810	2.19775530	4.49846857
0.04769571	10.94882392	6.84006140
1.40367674	9.89188315	4.79943510
6.39886298	9.91549418	4.85753899
5.02219546	4.84881764	4.71951126
0.03106801	4.86068764	4.72268514
0.72344780	7.29406723	4.70760768
5.72086422	7.27592449	4.70383363
0.07420868	0.92860661	6.80397950
7.55690506	0.13767221	7.17770493
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453

0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CH+H->CH<sub>2</sub>

1.000000000000

9.97980000	0.00000000	0.00000000
-0.76395804	12.66177393	0.00000000
0.00000004	0.00000004	19.64040000

H	C	O	Fe
2	41	4	80

Cart

-0.08240744	2.27536249	9.13239449
8.08518107	1.95213674	8.33708333
9.67140757	2.37549830	8.06576259
4.25559479	2.40959880	8.36618891
7.21052267	4.26623918	7.16342490
4.20384284	9.30637290	7.36897556
6.00025294	11.32485758	8.46783512
6.76302875	7.69916821	8.43806912
9.19607585	9.33010162	7.36779497
1.74012722	1.62421318	6.08804405
1.79384728	7.72780492	8.45184943
3.40194757	11.92208508	7.21005151
8.47939175	11.96894613	7.15825223
-0.33461170	6.79305277	6.32351877
4.66048422	6.78261308	6.31847308
2.17474203	4.25854114	7.19902894
6.70630380	1.57746101	6.14459669
2.17669178	8.29428753	5.59109451
7.16281557	8.28620806	5.57891204
9.20262321	3.15155764	5.24137939
4.20059502	3.14779990	5.30084897
4.67584786	10.81628347	4.26720358
-0.31640102	10.83014788	4.27439296
6.72597335	5.68237292	4.01699394
1.73454660	5.69377768	4.01497839
7.17742997	12.35252879	3.64499007
2.19380236	12.34756640	3.63334762



9.22937129	7.19943446	3.33903552
4.24051840	7.20224332	3.34110258
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.63820349	7.51722886	9.60870022
4.73826220	2.32489213	9.44434958
1.65220828	7.54987455	9.62068760
6.22165820	11.39591532	9.63695475
2.53361078	0.12762165	7.04344965
7.55915943	10.32482004	7.21203551
3.18181021	7.80043849	7.13171654
8.16955214	7.82287379	7.13048237
2.53099672	10.25106969	7.10157168
5.67604867	12.42375885	4.92379693
1.38025387	5.90246881	6.77025833
6.36811511	5.89830499	6.78463634
3.20162631	2.72629048	6.94930160
8.16146894	2.68152916	6.97981715
0.71938265	8.35069030	6.94657443
5.70413484	8.32375343	6.93358322
5.00192611	10.95410600	6.99223355
0.69296496	12.44069174	4.87968800
8.87867410	5.17811661	6.98918395
3.85890636	5.16815979	6.96560713
0.67015811	3.28077052	6.72854144
5.67764671	3.29491285	6.70363288
8.22176593	1.48550360	4.85310386
5.74666155	2.19695061	4.51126922
3.24601136	11.77224780	5.18937138
8.22388321	11.77765314	5.18539646
8.87477991	9.25461409	5.10392268
3.90670079	9.23812199	5.09815644

7.51491624	4.19589962	5.07483723
2.51227574	4.20578068	5.04269846
8.19804312	6.75237682	4.92598331
3.20504029	6.75468806	4.92007247
4.97822876	0.88101436	6.70822587
3.24310436	1.49295026	4.83151324
0.74957286	2.19732415	4.50042126
0.05410301	10.94380060	6.83278419
1.40486676	9.89180221	4.79692370
6.39801671	9.91933359	4.85983522
5.01580763	4.85077341	4.71716029
0.02823315	4.86278669	4.72191575
0.72292312	7.29455258	4.70711582
5.71737340	7.27677059	4.70360297
0.06203783	0.91765723	6.77028502
7.55714461	0.14590093	7.14428831
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235

8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>2</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
2	41	4	80

Cart

6.12015810	6.93373031	9.22278539
7.67055632	7.61500395	8.78194205
6.62548959	7.27241167	8.30911342
4.62252971	2.61626457	8.22131627
9.60199124	2.64000542	8.22965953
4.21564155	9.29746745	7.37637333
1.78914458	7.56152122	8.40875496
0.99687457	11.27682791	8.47968019
9.16406828	9.29614365	7.31544238
2.19944865	4.25738119	7.19740410
7.18027620	4.27863194	7.19433577
3.47258706	11.96103783	7.15478923
8.38079215	11.92875208	7.21965296
-0.32633193	6.77007163	6.29527190
4.65536789	6.73832054	6.27788290
1.73477761	1.61363719	6.18633574
6.73211774	1.65565029	6.15645602
2.18193765	8.28599143	5.58619332
7.14942830	8.31132905	5.58743047
9.19648810	3.14018993	5.30038967
4.20233374	3.13575368	5.29518533
4.67157931	10.81685293	4.26775834

-0.32274663	10.78745308	4.26236468
6.72290364	5.70028571	4.01539724
1.73231576	5.69332242	4.01117883
7.18427736	12.34852967	3.63493982
2.18276714	12.34906953	3.64308359
9.22522411	7.20163351	3.33425639
4.23684189	7.20152181	3.33007466
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.25531630	11.34368763	9.63852973
4.76365038	2.44415405	9.39532137
9.74038576	2.48066251	9.40568814
1.61103506	7.33609961	9.56869068
2.56737368	10.28614696	7.20335317
-0.00838975	10.94036944	7.01512390
3.18417853	7.78431164	7.12545228
8.17067258	7.75706966	7.16043278
0.67504884	12.40303414	4.92184378
7.50299535	0.09927692	7.01800958
3.86753454	5.16988397	7.00219650
8.86431844	5.18629843	7.01378034
3.20839366	2.71872801	6.92059093
8.20226067	2.74065005	6.92184680
0.72402723	8.31367861	6.93574753
5.70887533	8.31421232	6.96337024
5.02149110	10.92402151	6.83249585
7.49491748	10.25192393	7.06906482
1.38720665	5.89545432	6.78836850
6.39371207	5.93256135	6.85202585
0.69992091	3.27229405	6.73610253
5.68367052	3.29581390	6.73699662
-0.00534091	0.87807277	6.70524292

5.01715143	0.90334779	6.68626374
3.23994496	11.77299129	5.17421770
8.23349885	11.76240682	5.18743104
8.89421552	9.22394929	5.15739843
3.88278402	9.24515240	5.10096327
7.50724374	4.23864822	5.04051129
2.51820930	4.23052082	5.03878907
8.18886137	6.77434314	4.92417592
3.20579310	6.76024178	4.91007504
5.67310308	12.43518544	4.87761345
2.54493261	0.09470987	7.07953765
3.22692680	1.46623768	4.84615077
8.22470347	1.48218474	4.83955105
1.40514290	9.91097485	4.85782521
6.38496172	9.89450834	4.78587811
5.00991809	4.86041683	4.73584390
0.02258389	4.85655684	4.74307259
0.72446960	7.29229430	4.69771206
5.71674878	7.29839756	4.70767160
5.74770736	2.19883323	4.51206902
0.75983349	2.18178179	4.51778787
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233

3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>2</sub>+H (state1)

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	41	4	80

Cart

6.12822649	6.96459876	9.23421757
7.68368578	7.61280239	8.77767687
6.22780717	11.29339456	7.96481232
6.63337466	7.27391813	8.30900513
4.61781273	2.61894182	8.22947131
9.61164229	2.64552779	8.22679559
4.18657720	9.29401261	7.36077101
1.80412066	7.56344571	8.41593365
0.98971550	11.26977292	8.48656883
9.15472453	9.30965229	7.31542057
2.20523558	4.26253184	7.19940863
7.18556775	4.27040678	7.18371482
3.45533072	11.95962216	7.16119904
8.42044003	11.96503280	7.18010235
-0.33575409	6.77977903	6.30201613
4.64416103	6.74759880	6.27213974
1.74301831	1.62672270	6.17102488

6.73521647	1.62829553	6.16780643
2.16673638	8.28656621	5.57492211
7.13988324	8.30244183	5.58069460
9.20025820	3.13685673	5.29505688
4.21065969	3.13685696	5.29794389
4.66862084	10.81090082	4.26852236
-0.32327608	10.79325978	4.26111516
6.72279700	5.69491808	4.01372914
1.73118025	5.68883721	4.01202963
7.18118272	12.34819701	3.63456082
2.18760085	12.34931884	3.63805840
9.22485353	7.19987538	3.33460014
4.23453318	7.20055034	3.32596468
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.24554752	11.34440633	9.64411730
4.77038922	2.45354213	9.40313124
9.75529255	2.48867475	9.40282587
1.59551891	7.33923496	9.56994738
2.54004178	10.29041092	7.18388295
0.00674818	10.94109826	7.00671445
3.16738383	7.78238285	7.11921404
8.16079272	7.77291153	7.15876574
0.67865147	12.41465055	4.91067776
7.50034996	0.08879995	7.06040993
3.87278720	5.17281306	7.00388207
8.86791169	5.18077559	6.99925272
3.21723242	2.72361714	6.92360522
8.20433388	2.72894389	6.92014732
0.71456937	8.31937425	6.93441029
5.69371087	8.30230061	6.96169484
4.99429231	10.91921465	6.88962561

7.50319443	10.30100654	7.13289904
1.37785910	5.89257331	6.78411709
6.38276471	5.92415102	6.86595212
0.70357512	3.28502048	6.73200975
5.68908346	3.28426581	6.73687039
0.00721795	0.90242534	6.68580609
5.00822997	0.89996751	6.68366034
3.23778167	11.76872419	5.17804782
8.23344198	11.76733288	5.18031427
8.87898046	9.23666132	5.16702787
3.88047303	9.24731264	5.11459076
7.50740417	4.23545407	5.04523670
2.52138753	4.22776157	5.04151953
8.18501016	6.77293858	4.92432227
3.19895047	6.76131319	4.90507378
5.67053222	12.42841349	4.88719392
2.53844300	0.10738246	7.07703606
3.23404196	1.47226264	4.84428984
8.22566514	1.47475050	4.84143315
1.39600027	9.90690452	4.83718739
6.38347813	9.89599075	4.80796570
5.01166790	4.85934126	4.73655336
0.02184492	4.85157553	4.72918704
0.71526662	7.28539572	4.70142025
5.71083727	7.29237138	4.70518091
5.75386364	2.19644278	4.51097373
0.76450538	2.18997704	4.51086772
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903



2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>2</sub>+H (state2)

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	41	4	80

Cart

0.15321932	1.53308991	8.60709055
9.57030300	3.09640455	9.16137188
7.85500261	1.52801888	8.14190088
9.73097091	2.53503734	8.22649123
1.79463871	7.70576161	8.44649162
4.60054322	2.63290535	8.22396424
4.21415150	9.28645344	7.39220140
6.74803544	7.61899024	8.42664665
5.97430112	11.30759375	8.48334998
7.17513313	12.34980878	3.64451134
2.18055274	4.27474209	7.19051847

4.66421699	6.75899471	6.30493236
3.40081870	11.91750930	7.21709897
8.45369174	11.94505743	7.13290692
-0.33071681	6.78323269	6.31758167
6.68485091	1.57260631	6.10876533
4.19190520	3.14292735	5.30576295
7.19379852	4.23485209	7.20003396
2.18493402	8.29406284	5.59679407
7.16625165	8.28088788	5.59329472
9.19743771	3.15487615	5.27367486
1.74901007	1.63237174	6.14266700
2.19312359	12.34678145	3.64434695
9.22836608	7.19982564	3.33758258
6.72768659	5.67205697	4.01739478
1.73484622	5.70270834	4.01270539
9.19271244	9.31128533	7.38703117
4.24093429	7.20358603	3.33798010
-0.31341015	10.82248394	4.27384813
4.67827735	10.80606338	4.26342898
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.20366859	11.34879225	9.64981203
1.64407250	7.53796213	9.61585287
4.74155781	2.47071324	9.40014396
6.63724802	7.40137090	9.59322342
2.53686522	10.23072416	7.10618953
0.04091191	10.91985903	6.82981256
3.18736940	7.78568645	7.13398062
8.17382889	7.80008961	7.13479676
7.53830569	0.13567959	7.12405915
8.22924258	1.48277375	4.87047107
3.85999529	5.16514349	6.98870514

8.85796073	5.15503665	6.94874408
3.19576652	2.73195414	6.91822249
8.17046736	2.65490090	7.02127387
0.72036039	8.34901243	6.94655329
5.70153697	8.29405883	6.94284987
4.99501264	10.93968574	7.00059508
8.24260202	11.79626799	5.17742333
1.38064944	5.91911790	6.77776538
6.37942416	5.87765489	6.78800475
0.66699865	3.32428800	6.72101595
5.67621421	3.25991613	6.72510374
5.73396545	2.19222528	4.49965485
4.96385401	0.87725994	6.70023629
0.68301878	12.44615828	4.88821626
3.24986213	11.75968203	5.19171356
8.87148329	9.24318417	5.09057810
3.91146834	9.23135573	5.09850925
7.50752717	4.18198848	5.07453479
2.50487993	4.22783072	5.03215575
8.19685045	6.74655322	4.92321257
3.21024168	6.75786389	4.91612767
3.23346163	1.47835158	4.83401918
7.55427425	10.29782104	7.19878783
5.66970775	12.41988737	4.92002376
2.51837047	0.08719545	7.03175856
1.40418352	9.89110944	4.80192978
6.40060847	9.91437125	4.87503666
5.01796321	4.84943485	4.74134821
0.02392065	4.86489265	4.70553012
0.72544766	7.30160689	4.70469200
5.72401797	7.27874654	4.69903539
0.74469683	2.18961586	4.52642074
0.04104047	0.91333765	6.77843016
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425

3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CH<sub>2</sub>+H->CH<sub>3</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	41	4	80

Cart

0.05681819	1.41710289	8.59467727
9.75313118	3.04278403	9.16141847
8.10073087	1.90682132	8.34273161
9.69175178	2.44631787	8.23972889
1.79437805	7.70344495	8.44864782

4.59872009	2.63632596	8.23045560
4.20406613	9.29362896	7.37715666
6.75861074	7.60544150	8.42157811
5.97672720	11.29249284	8.47678251
7.17656803	12.35079430	3.64426179
2.17897419	4.27007233	7.19497435
4.65824779	6.76793859	6.30767060
3.39952736	11.92577416	7.21270060
8.45538944	11.95109138	7.13210867
-0.33381058	6.79502839	6.31808526
6.69632289	1.60524926	6.13450890
4.19670695	3.14411299	5.30604150
7.19498424	4.24573474	7.19798960
2.17767386	8.29529390	5.59408974
7.16191261	8.28614486	5.58610395
9.20413874	3.15616843	5.27629443
1.75565378	1.63859807	6.13784187
2.19488292	12.34712168	3.64054369
9.22841256	7.19934260	3.33708889
6.72508825	5.67629391	4.01715978
1.73518025	5.70135182	4.01370478
9.18922999	9.31863211	7.38624699
4.24003566	7.20218745	3.33755540
-0.31547645	10.82370409	4.27585318
4.67573064	10.80879025	4.26432924
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.22783727	11.36996072	9.63849898
1.63982713	7.52333848	9.61673410
4.74878970	2.46841686	9.40454384
6.62223962	7.37323904	9.58354765
2.52908755	10.24086388	7.10149509

0.03914240	10.92314568	6.82576471
3.18032392	7.79023775	7.13307105
8.16916865	7.80892162	7.13239857
7.53230654	0.14601238	7.11035798
8.22222149	1.49077067	4.86015692
3.85951166	5.16918153	6.98723632
8.85773810	5.17185720	6.95036998
3.19948744	2.73450799	6.92258998
8.17986212	2.68394124	6.99823735
0.71635288	8.34959494	6.94876384
5.70033943	8.30279971	6.93980335
4.99298983	10.94479527	7.00039796
8.23935466	11.79319486	5.17572365
1.37453015	5.90888805	6.77384517
6.37202408	5.88437319	6.78854094
0.66752813	3.29859811	6.72946947
5.67152716	3.27021753	6.72763963
5.73851162	2.19129630	4.50469252
4.97332140	0.88158153	6.69978377
0.68297071	12.44604802	4.87994581
3.24940215	11.76442297	5.18931965
8.87189955	9.24683432	5.09763494
3.90968137	9.23662729	5.10563105
7.50765077	4.18690233	5.07121805
2.50452506	4.22726522	5.03789807
8.19412120	6.75056073	4.92230481
3.20594283	6.76093951	4.91591585
3.23783207	1.48260094	4.83498250
7.55031449	10.30798570	7.20021267
5.67314255	12.42090151	4.92114834
2.51760682	0.09438765	7.02908939
1.40361171	9.89234044	4.79983397
6.39902908	9.91633024	4.86490593
5.01352729	4.85114295	4.73364327
0.02543448	4.86277494	4.70786011
0.72171277	7.29886186	4.70610403
5.71882435	7.27867535	4.70115965
0.74977711	2.19331490	4.51702458
0.04440101	0.90122827	6.72882299
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337

3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

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H	C	O	Fe
3	41	4	80

Cart

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7.72667773	7.56818170	9.07883632
6.00858497	8.02256856	8.99438798
6.74975911	7.29689778	8.58883987
4.62896792	2.60948873	8.22371035
9.60245911	2.64824538	8.23313462
4.17610576	9.33229924	7.33497403
1.79875903	7.58262846	8.40804901
0.98730992	11.27256151	8.47744587
9.15818628	9.31016217	7.32918960
2.20782568	4.26215071	7.19846528
7.19887704	4.26839665	7.18440185
3.46624862	11.97549167	7.15624118
8.37584831	11.93631171	7.21032404
-0.31755217	6.77637907	6.30536741
4.64942499	6.76388056	6.31945974
1.73966718	1.62088134	6.17816514
6.73471249	1.65406162	6.14947348
2.17304421	8.28830267	5.56295311
7.15961643	8.30059497	5.61153333
9.20162985	3.14031257	5.29873266
4.21153410	3.13988557	5.29877224
4.67088845	10.82043952	4.27359933
-0.32147496	10.80484552	4.26300585
6.72641956	5.70125930	4.01365258
1.73474319	5.69014298	4.01116912
7.18268464	12.34934981	3.63320615
2.18391400	12.35008095	3.63824120
9.22651106	7.20090567	3.33518387
4.23995229	7.19827394	3.33953440
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304



-0.23342146	8.73880577	0.18583304
1.24629061	11.33443702	9.63798648
4.77718562	2.43804008	9.39755227
9.74601872	2.50332311	9.41054946
1.59570752	7.35528346	9.56412792
2.54591116	10.31355546	7.18660112
-0.00880435	10.95272813	7.00338741
3.17441672	7.80295830	7.11599791
8.18428972	7.76845772	7.14071780
0.67714334	12.41700364	4.91473285
7.49753972	0.10376310	7.02307766
3.87894511	5.17028385	6.99404390
8.88278618	5.17166721	6.96804265
3.21758181	2.72283292	6.92418531
8.21288100	2.73523301	6.91890469
0.71480468	8.32693014	6.92511052
5.71128092	8.35763710	6.96281428
5.01630798	10.93988721	6.82728688
7.49866526	10.25579655	7.04233909
1.39308640	5.89693225	6.77556331
6.40243395	5.93155050	6.84680231
0.70926386	3.27431273	6.73486131
5.69425558	3.28995864	6.73620355
0.00060901	0.88135374	6.70471185
5.01642533	0.90852911	6.68233416
3.23513028	11.77780539	5.17296625
8.23263618	11.77358771	5.18256208
8.89538428	9.23232085	5.12849909
3.89282370	9.24652155	5.11898203
7.50499044	4.24061499	5.04463954
2.52182650	4.22609066	5.04051068
8.18710880	6.76895554	4.92157695
3.20843586	6.75501488	4.91756329
5.67205431	12.43661037	4.87611254
2.54022575	0.10902143	7.08355578
3.23060556	1.47522968	4.84388778
8.22546019	1.48518819	4.83581911
1.40264954	9.91370143	4.84709406
6.38841672	9.88547529	4.78800474
5.01564419	4.85751866	4.73085496
0.02681614	4.84854679	4.72310081
0.72307654	7.28295848	4.69924522
5.71188347	7.29124664	4.72727112
5.74910407	2.20010966	4.50782352

0.76245320	2.18654162	4.51365114
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>3</sub>+H

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0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	41	4	80

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6.22565650	11.26855905	7.98318624
6.03570986	7.95052258	9.02347296
6.77380500	7.23869973	8.59332250
4.60762748	2.59519966	8.22685752
9.60990282	2.64749427	8.22508116
4.14995003	9.30165536	7.35725777
1.81799171	7.43933813	8.39613029
0.96272634	11.26022129	8.49057875
9.14398948	9.29679743	7.34344711
2.20348082	4.25141345	7.19241594
7.19469031	4.24505631	7.17466199
3.44436956	11.95546683	7.16957430
8.41351752	11.95160192	7.17783910
-0.32869736	6.76084987	6.30488214
4.64376483	6.74826784	6.31159718
1.73804127	1.61641395	6.16389193
6.73169381	1.60898983	6.16636783
2.16574616	8.28012973	5.57277313
7.15447875	8.28665313	5.61514294
9.19724205	3.12701457	5.29033529
4.20975770	3.13145655	5.29810175
4.66539547	10.79636763	4.26388240
-0.32349119	10.78674405	4.26026859
6.72299980	5.69409408	4.01451074
1.73159198	5.68631418	4.01225205
7.18007067	12.34534521	3.63640924
2.18853245	12.34736248	3.63913382
9.22508382	7.19983695	3.33673637
4.23793493	7.19871521	3.33768972
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899

9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
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1.21816054	11.34730987	9.64703678
4.77635139	2.42965062	9.39847852
9.73599454	2.50215509	9.40395520
1.56929584	7.17206389	9.53482069
2.52440848	10.29068036	7.18480051
-0.00081904	10.92918257	7.00064966
3.16712998	7.77105577	7.12079696
8.17165386	7.75661878	7.14238593
0.67747141	12.40792820	4.91014080
7.49381187	0.07222501	7.06771907
3.87500555	5.15512981	6.99629795
8.87763189	5.15123222	6.96449486
3.21448714	2.71107655	6.92129426
8.20388688	2.70976986	6.91277499
0.70166708	8.30542326	6.94018574
5.70463106	8.33750398	6.97131195
4.98521668	10.91402778	6.91144033
7.49857204	10.27991073	7.12503058
1.38264594	5.88413061	6.77711511
6.40132128	5.90664568	6.82137030
0.70206159	3.27316426	6.72857908
5.69153364	3.26446318	6.73393154
0.00285698	0.88850312	6.68406123
5.00223913	0.88936586	6.68585108
3.23577445	11.75743882	5.18238504
8.23013635	11.75823987	5.18098409
8.88260732	9.22887377	5.14808937
3.88960168	9.23991196	5.13936929
7.50232068	4.22798085	5.04232732
2.51940637	4.21841721	5.03838043
8.18226579	6.76176727	4.92043436
3.20457854	6.75266661	4.91277608
5.66724007	12.41188374	4.89504218
2.52994365	0.10267975	7.07747114
3.23368826	1.46437452	4.84133851
8.22150875	1.46279881	4.83771921

1.39459811	9.89839869	4.84588288
6.38411899	9.88183488	4.81940528
5.01204854	4.85103845	4.73281380
0.02144219	4.84360460	4.72191258
0.71768263	7.27955479	4.70350910
5.70684853	7.28750235	4.72630418
5.75143984	2.18855203	4.50972681
0.76155161	2.18313534	4.50721122
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943

7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
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# TS for CH<sub>3</sub>+H->CH<sub>4</sub>(g)

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9.97980000	0.00000000	0.00000000
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H	C	O	Fe
4	41	4	80

Cart

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8.46117930	6.99528932	9.49921312
6.94915547	8.39918185	8.12760125
7.04380185	8.02346432	9.86887007
7.45384118	7.28015252	9.17264934
4.61895784	2.60118127	8.21458216
9.59969084	2.66023385	8.23646882
4.15972242	9.34856872	7.40636758
1.75761491	7.57361513	8.40306820
0.99194384	11.29599132	8.45970545
9.16750563	9.28567407	7.33468278
2.20149672	4.26737046	7.19590095
7.18925285	4.27697402	7.18023993
3.46101793	11.98600480	7.15865656
8.37620432	11.92646284	7.21716747
-0.33144546	6.78487416	6.30002085
4.64570477	6.79187551	6.34144100
1.73036675	1.61995294	6.18532667
6.73359467	1.65513773	6.15492036
2.16410166	8.29351841	5.57227272
7.15100349	8.28198066	5.58439702
9.20254894	3.13945281	5.30291326
4.20321032	3.13783314	5.29405588
4.67219354	10.82091196	4.26948693
-0.32551139	10.79270322	4.26540817
6.72112065	5.69639638	4.01822393
1.73545161	5.69826155	4.01099018
7.18454275	12.34801132	3.63733376
2.18206273	12.34891927	3.64233452
9.22696076	7.20207577	3.33108563

4.23419348	7.19873188	3.33295895
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.20945158	11.38525046	9.62829476
4.76546922	2.42318053	9.38798826
9.72872518	2.51250925	9.41482675
1.58073309	7.33322258	9.56042943
2.53689794	10.33232756	7.21579162
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3.17426666	7.82466431	7.13055288
8.11958503	7.76708567	7.19311318
0.67190352	12.41046664	4.91658151
7.49891779	0.10153063	7.02627905
3.87584747	5.17491521	6.98324927
8.86275874	5.18043655	6.96309997
3.20692306	2.72513469	6.91945839
8.20694837	2.74120219	6.92251862
0.70677422	8.31325162	6.92817149
5.64692122	8.40535610	6.86392664
5.01094286	10.94838809	6.85408174
7.49435271	10.24531630	7.10394535
1.38641797	5.90331506	6.78208909
6.37662468	5.89451321	6.67711669
0.70151690	3.27524063	6.73678629
5.68556765	3.29474884	6.73337880
-0.00703827	0.87718998	6.70565639
5.01562103	0.91409651	6.68426790
3.23678190	11.77803313	5.17545708
8.22683882	11.76017795	5.19112236
8.88404954	9.22782604	5.14533855
3.87636441	9.25509030	5.10843833
7.51143435	4.22281146	5.02364105

2.51612873	4.23337454	5.04040162
8.19628836	6.76960891	4.93242957
3.20738265	6.76067917	4.92683629
5.67193638	12.43037064	4.88229985
2.53197729	0.10393073	7.08434160
3.22207750	1.47079863	4.84543604
8.22460151	1.48067602	4.84186627
1.39799666	9.92054637	4.86292716
6.39209479	9.89792314	4.78982504
5.00384702	4.84784228	4.70769544
0.02600007	4.85247776	4.72935063
0.72217026	7.28683234	4.69742156
5.70339992	7.29689098	4.69256042
5.74539280	2.19502793	4.51058436
0.75861197	2.18426111	4.51599184
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367



3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

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H	C	O	Fe
5	41	4	80

Cart

4.58716098	5.68963881	14.80811165
5.95447946	6.37191510	15.74222659
1.24241092	11.32171557	7.98905213
5.43374630	7.15063468	14.21690404
4.39403403	7.24716066	15.67140776
5.09204768	6.61470652	15.10970557
4.62970330	2.64418950	8.22643154
9.60645803	2.67077325	8.24186313
4.19012007	9.31649872	7.38196551
1.76574669	7.57139676	8.41500455
6.76010122	7.61012810	8.42643410
9.17214501	9.30112804	7.38365504
2.19600002	4.26495275	7.19606382
7.18626688	4.27362304	7.19714860
3.44917722	11.96826818	7.17337159
8.38505876	11.93748762	7.21559797
-0.34044372	6.78129369	6.30988626
4.64778014	6.78772918	6.31587772
1.73608093	1.61528487	6.18488965
6.72922190	1.64982531	6.15860400
2.16521477	8.29142078	5.59124960
7.15583429	8.29722219	5.59581772
9.19794143	3.13854982	5.30715512

4.20409819	3.13753651	5.29881453
4.66823046	10.81901483	4.26913263
-0.32307852	10.81554276	4.26331924
6.72046293	5.69817744	4.01488243
1.73068204	5.69649157	4.01240168
7.18121301	12.34948531	3.63915970
2.18445846	12.34825122	3.63988355
9.22670446	7.20177904	3.33650535
4.23702370	7.20022065	3.33883766
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.59495382	7.37184391	9.58113971
4.76102594	2.48443732	9.40250450
9.73069049	2.52936139	9.42054021
1.59034026	7.31774470	9.56591110
2.53381566	10.29895452	7.19378567
-0.01782951	10.93486139	6.93846872
3.16903510	7.80725803	7.13466687
8.16051463	7.79228972	7.13209893
0.67513268	12.41902977	4.90506316
7.49937104	0.10246337	7.02664216
3.86438917	5.17711342	6.98387427
8.85825378	5.17366480	6.98666032
3.20991502	2.72840006	6.92364332
8.20544117	2.73903986	6.92604043
0.70203787	8.32808349	6.94694544
5.69542377	8.34195410	6.94910373
5.00722203	10.93279741	6.85325861
7.50357531	10.25254924	7.11220471
1.37463570	5.90048155	6.78348149
6.36108413	5.90315604	6.77325305
0.70044772	3.27435181	6.73983154

5.68622477	3.29324159	6.73331465
-0.00040642	0.87835687	6.70897439
5.00524882	0.90226571	6.68753315
3.23544409	11.77507503	5.17617980
8.22846350	11.76935552	5.18802811
8.88236339	9.23993680	5.08979070
3.88070143	9.24266581	5.09176135
7.50550051	4.22864550	5.03473392
2.51364654	4.22847229	5.03765390
8.19036283	6.76155170	4.91810174
3.20229184	6.75916201	4.92323021
5.66955750	12.43263234	4.88541979
2.51649725	0.08613020	7.07226250
3.22479553	1.47370341	4.84569159
8.22111823	1.48377818	4.84161227
1.40008830	9.90556409	4.83901500
6.38725614	9.89807842	4.80809770
5.00996737	4.85159287	4.72609173
0.02355475	4.85099843	4.73503787
0.71914255	7.29004519	4.70482692
5.70734242	7.29472042	4.70721717
5.74464712	2.19397853	4.51157213
0.75753038	2.18713609	4.51828699
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425

-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

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H	C	O	Fe
1	40	5	80

Cart

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4.63159187	2.64672341	8.22661270
9.61926587	2.62867445	8.22574919
4.15829256	9.29758898	7.38439699
1.82396978	7.41792270	8.40604949
6.97468787	7.34358915	8.46688077
9.15446840	9.29252643	7.38775510
2.20060726	4.26319538	7.19529134
7.18677267	4.24998709	7.18748106
3.41401103	11.96235523	7.18439583
8.50998507	11.97547730	7.13950683
-0.33461643	6.75688746	6.29006525
4.65329300	6.75380574	6.30426378
1.74913379	1.63156761	6.16724910
6.73257863	1.59232050	6.17572726

2.16906799	8.28755724	5.59216499
7.14995250	8.26812970	5.58486293
9.19699365	3.12917465	5.29706057
4.20727440	3.13214201	5.29549962
4.66879859	10.78314114	4.24750961
-0.32245953	10.78681955	4.26456255
6.72028092	5.68979288	4.01318314
1.73057960	5.69564520	4.01422655
7.17630335	12.34827377	3.64430736
2.19438585	12.34722921	3.63838887
9.22691909	7.20260757	3.33117590
4.23518041	7.20074926	3.32989564
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.55909287	7.13537611	9.55985035
4.75999007	2.48954591	9.40280429
9.76690334	2.45678161	9.39814069
1.57773320	7.16566934	9.54567946
6.23529398	11.33500415	8.24554254
2.48935623	10.27242991	7.16631698
0.01960728	10.88824004	6.87517133
3.16979092	7.77095767	7.13429647
8.15895758	7.76678801	7.14269378
0.68213267	12.41683160	4.88591599
7.54338378	0.10225856	7.12468478
3.87261556	5.16094886	6.99782294
8.85070888	5.17568828	7.00712551
3.21452819	2.72607228	6.91996355
8.20226806	2.71120799	6.92454307
0.70275334	8.31111049	6.96298989
5.66657895	8.30797930	6.92366581
4.93956615	10.93424844	7.02928840

7.54038993	10.32354755	7.28160412
1.38007888	5.89808851	6.79472503
6.37589171	5.89020108	6.78273012
0.69833339	3.28915726	6.73443500
5.69073777	3.27282402	6.72784695
0.01880697	0.91964107	6.66440128
4.98587218	0.90253391	6.68103510
3.25029523	11.74996770	5.18786039
8.23238350	11.75566857	5.18508874
8.86045534	9.23880283	5.13956692
3.90238492	9.24821080	5.15031803
7.50980668	4.22227147	5.03760415
2.51955847	4.22992322	5.03574886
8.20032751	6.75889391	4.91244632
3.20819464	6.76421115	4.91319646
5.67177893	12.39304525	4.92862329
2.50911431	0.08843011	7.05535300
3.23868981	1.46422807	4.84516751
8.21644670	1.46421985	4.84277191
1.39991675	9.88668745	4.81899587
6.38969032	9.90571202	4.87806291
5.01187815	4.85223831	4.73473307
0.02021172	4.85456949	4.74270311
0.72591642	7.29462289	4.70451954
5.71413258	7.28230916	4.69693204
5.75474073	2.18155233	4.51286059
0.76433243	2.19197570	4.51037063
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903

2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

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9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
2	40	5	80

Cart

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1.20795803	11.31655782	7.95879589
4.18387327	9.31385836	7.36914001
4.63441350	2.66178055	8.22543120
1.78640475	7.55869049	8.41929832
9.69447570	3.39787528	8.30365335
6.73509518	7.53801604	8.39621465
9.15633038	9.30821240	7.39150260
2.22910364	4.30124835	7.16657955
7.16496456	4.28627176	7.16299154
3.40995947	11.97584652	7.18716538

8.51311832	11.95361956	7.09524216
-0.34705530	6.77674695	6.31369224
4.64803751	6.79343287	6.29167979
1.72884176	1.65352204	6.18705831
6.71694649	1.61201888	6.15745142
2.16494610	8.29450371	5.58998233
7.14997517	8.28113841	5.58327740
9.20394645	3.12653972	5.30440625
4.20295412	3.13727867	5.29385923
4.66701401	10.80700100	4.25123662
-0.32056704	10.80494662	4.26859098
6.72294799	5.68597772	4.01502591
1.72910243	5.70167874	4.01478517
7.17154928	12.35403654	3.63963813
2.18974151	12.34964257	3.64089494
9.22441080	7.20026853	3.33318180
4.23430177	7.19941945	3.32200147
5.47292217	2.23055554	2.34193027
0.48302217	2.23055554	2.34193027
6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348
4.22357812	11.29064837	1.28800348
5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
6.24441922	11.36807974	8.23806617
6.55700171	7.26497731	9.54319941
4.75386681	2.50019968	9.40195616
1.59114516	7.32344907	9.57193158
9.63949494	3.52251287	9.48547001
2.50214972	10.28725710	7.17569130
0.02588014	10.89178151	6.85488319
3.16374315	7.79993209	7.13204415
8.15284331	7.79704860	7.12873471
0.67847767	12.43238591	4.88759302
7.57574372	0.16422425	7.15780460
3.88544337	5.18901966	6.98974699
8.85059288	5.17657739	7.00712515



3.20942829	2.73899210	6.92346952
8.20562663	2.74136375	6.97589629
0.69636416	8.33327406	6.95388501
5.68024759	8.31323258	6.92897871
4.95059634	10.96172771	7.02570950
7.53165946	10.32933868	7.28106224
1.38793354	5.93399138	6.77043127
6.35972474	5.91545845	6.76312902
0.69931657	3.36205022	6.73378876
5.67953456	3.28593740	6.72019496
0.00436885	0.93665250	6.69616932
4.98108207	0.91607997	6.67966916
3.24549637	11.76527513	5.18945654
8.22699367	11.76833795	5.17604373
8.85821545	9.24716919	5.11364077
3.89299604	9.26693988	5.13902314
7.50928892	4.20110704	5.05415582
2.51516130	4.23314405	5.03440994
8.19249388	6.75396875	4.91892975
3.20235048	6.77496628	4.91007471
5.66884992	12.40935309	4.93137725
2.50328473	0.10684010	7.05694205
3.22524296	1.47539331	4.84894907
8.20960936	1.48466571	4.85571357
1.39812793	9.89612998	4.81560003
6.38412583	9.91369796	4.86465568
5.01356204	4.85365811	4.72959029
0.01850271	4.85764980	4.73082722
0.71496627	7.30088840	4.70252957
5.71185161	7.29447468	4.68786317
5.74840756	2.18905073	4.50892286
0.75311127	2.19035852	4.52399277
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422

5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946
7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# TS for O+H->OH

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-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
2	40	5	80

Cart

7.33080495	0.02323383	8.69223256
1.22583312	11.32889963	7.96444811
4.19135774	9.30458326	7.38001486
4.62237011	2.66002225	8.22759522
1.79798987	7.53439410	8.41935704
9.63280236	2.84987392	8.25942635

6.74435463	7.56854490	8.40935046
9.16296307	9.32063938	7.38252108
2.20571300	4.28229694	7.19037115
7.18454502	4.27042780	7.18918964
3.42485802	11.97469866	7.18973821
8.48145526	12.00274110	7.16279538
-0.34183240	6.78566196	6.31127466
4.65199276	6.78194296	6.29714053
1.74969042	1.64866191	6.16923031
6.74643059	1.60170658	6.18043202
2.16917106	8.29348724	5.59459691
7.15250460	8.28111618	5.58317593
9.19716235	3.12611197	5.29808894
4.21041902	3.13840708	5.29475608
4.66659797	10.79377434	4.24939471
-0.32036537	10.80514366	4.27018973
6.72357397	5.69423546	4.01359708
1.73244213	5.70332859	4.01446772
7.17699310	12.34901290	3.64808377
2.19470502	12.34758335	3.64013765
9.22767394	7.20064883	3.33433095
4.23684296	7.20053504	3.32777474
5.47292217	2.23055554	2.34193027
0.48302217	2.23055554	2.34193027
6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348
4.22357812	11.29064837	1.28800348
5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
6.21948000	11.35640402	8.34802161
6.57983831	7.30452933	9.56002508
4.74551882	2.49812401	9.40429808
1.58361239	7.29601980	9.56739095
9.70120482	2.76214270	9.44461049
2.51496828	10.29171491	7.18592756
0.01109545	10.92389188	6.88496503
3.17007320	7.79545396	7.13692016

8.15554233	7.80616089	7.13047053
0.68294510	12.42684590	4.88580389
7.53755566	0.11986887	7.12306751
3.87287629	5.18171472	6.99139066
8.85572546	5.18278840	6.99538140
3.21653506	2.74130586	6.91823160
8.20545125	2.73579989	6.93590692
0.70180252	8.33414788	6.95589040
5.68709504	8.30748443	6.93486064
4.96915296	10.95669441	7.00803711
7.53653466	10.34050542	7.31074640
1.37845805	5.91770406	6.79030976
6.36739271	5.90194346	6.77371039
0.69995249	3.31660892	6.72923985
5.69073995	3.28744045	6.72880703
0.01565681	0.93222210	6.65513245
5.00404684	0.90932534	6.68973894
3.24537525	11.76105219	5.18991327
8.23268648	11.75985870	5.18741619
8.86938900	9.24873660	5.12339096
3.89820680	9.26193100	5.14885230
7.51095936	4.22271525	5.04318670
2.51812688	4.23746896	5.03709423
8.19635984	6.76300069	4.91680936
3.20580371	6.77311604	4.91309981
5.65532978	12.40395400	4.90966746
2.51449499	0.10571231	7.05484334
3.23505123	1.47381208	4.84374757
8.22208629	1.45761834	4.85903719
1.40063093	9.89625611	4.82154289
6.38821406	9.91767741	4.88188443
5.01435747	4.85544153	4.73046474
0.02226352	4.85740115	4.73289922
0.72074370	7.29730517	4.70673250
5.71288485	7.29045656	4.69446402
5.75656594	2.18855396	4.51536190
0.76330879	2.19654524	4.50921899
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266

2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422
5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946
7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# OH

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9.97980000	0.00000000	0.00000000
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H	C	O	Fe
2	40	5	80

Cart

6.01359305	11.33014667	9.42361543
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1.22965600	11.29941472	7.97244131
4.18157844	9.29062880	7.38301479
4.63090479	2.59263959	8.21758364
1.79546059	7.52283122	8.41789260
9.60676741	2.60952361	8.22595624
6.74486714	7.56183172	8.40826246
9.16793358	9.30172661	7.39129261
2.20236006	4.26364236	7.20373534
7.19244651	4.25756793	7.20116961
3.42134392	11.97097437	7.18133064
8.47523224	11.97689521	7.13160910
-0.34433279	6.77811975	6.30660203
4.64559458	6.77138161	6.30008089
1.74559687	1.62794938	6.16896908
6.73022736	1.60694448	6.15102698
2.16432256	8.28967329	5.59081247
7.14671801	8.28126697	5.58888958
9.20284995	3.13687087	5.29756693
4.20865182	3.13683399	5.30022435
4.67202396	10.80193110	4.25975383
-0.32687615	10.80908121	4.27013585
6.72098923	5.69232448	4.01321115
1.73044748	5.69417751	4.01354662
7.17717989	12.34746952	3.64507235
2.19451022	12.34678121	3.64324718
9.22573444	7.19997497	3.33497379
4.23492580	7.20025996	3.33126266
5.47292217	2.23055554	2.34193027
0.48302217	2.23055554	2.34193027
6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348
4.22357812	11.29064837	1.28800348
5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
6.23243911	11.35660099	8.47602200
6.58485942	7.29648694	9.56245069
4.79727417	2.39944667	9.38688849

1.58079872	7.27934945	9.56693718
9.76793839	2.43310752	9.39741582
2.51118751	10.28192657	7.17420808
0.01046737	10.90596096	6.88776497
3.16341588	7.78553157	7.13306860
8.15351628	7.79287103	7.13297251
0.67735473	12.42535699	4.88956937
7.51554953	0.14252364	7.15187309
3.86945030	5.16867355	6.98874798
8.85836545	5.17073206	6.98540720
3.21594715	2.72682832	6.92578982
8.20665963	2.72188407	6.92069124
0.70107455	8.31759907	6.95347020
5.68279874	8.29847917	6.93382050
4.96715507	10.93946939	6.98784169
7.53905628	10.31143432	7.29746355
1.36917987	5.89239382	6.78846146
6.36407582	5.88527417	6.77364861
0.70086216	3.28711258	6.73838115
5.69427481	3.27804363	6.73338999
0.01106156	0.91911087	6.67443255
4.98800066	0.90860166	6.67334130
3.24797162	11.75903084	5.18577973
8.21882709	11.75726790	5.19636204
8.87139783	9.24142195	5.11017470
3.89127528	9.24702916	5.12523881
7.50850466	4.22356750	5.03519207
2.51833097	4.22768806	5.03864350
8.19157753	6.76088944	4.91638767
3.20080422	6.76140439	4.91423660
5.67348450	12.41424340	4.92024775
2.51060239	0.08902257	7.05635606
3.23393409	1.47169820	4.84355459
8.22218178	1.47322400	4.83573695
1.39625970	9.89175726	4.81600989
6.38509817	9.90700138	4.86261088
5.01186438	4.85016391	4.73102309
0.02203630	4.85215495	4.72975232
0.71850924	7.29134075	4.70537899
5.70863480	7.28599939	4.69538252
5.75124822	2.19501129	4.50761879
0.76353311	2.19547592	4.51158920
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412

9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422
5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946
7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# O+CH<sub>v</sub>

1.000000000000

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-0.76395804	12.66177393	0.00000000



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	H	C	O Fe
	2	40	5 80
Cart			
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	1.25875194		11.25386801 7.91706407
	4.21251008		9.24741570 7.95984693
	4.62863870		2.60400899 8.21909282
	1.81368788		7.49168518 8.42721683
	9.62293567		2.63471587 8.22044040
	6.73134123		7.55976890 8.42042454
	9.16564524		9.29843719 7.39546443
	2.20630291		4.27407058 7.18888311
	7.18510834		4.26161141 7.18777073
	3.43704944		11.90306812 7.13330625
	8.50662425		11.97442006 7.13564429
	-0.33826604		6.77548701 6.30779239
	4.63755611		6.81354481 6.30383223
	1.75345763		1.62212429 6.18000879
	6.73333221		1.59011744 6.17621500
	2.19189429		8.33992508 5.66484346
	7.14796552		8.27513529 5.59969588
	9.20053462		3.13964817 5.29570041
	4.20787723		3.14027527 5.29682354
	4.68084604		10.80186764 4.25729722
	-0.32256504		10.80231763 4.27097765
	6.72233395		5.69741691 4.01438521
	1.73147944		5.71095245 4.01679675
	7.17844025		12.34971081 3.63958931
	2.19282454		12.34946992 3.63557204
	9.23063171		7.20021755 3.34010216
	4.23718169		7.20890767 3.34574017
	5.47292217		2.23055554 2.34193027
	0.48302217		2.23055554 2.34193027
	6.73540357		9.72874639 2.00704745
	1.74550357		9.72874639 2.00704745
	7.98876734		3.77819959 1.47019894
	2.99886734		3.77819959 1.47019894
	9.21347812		11.29064837 1.28800348
	4.22357812		11.29064837 1.28800348
	5.52626486		6.13002817 0.45987182
	0.53636486		6.13002817 0.45987182
	7.45328915		1.12937154 0.40848067
	2.46338915		1.12937154 0.40848067

4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
6.20516953	11.30849177	8.20957999
6.57064805	7.27113779	9.56740031
4.77084182	2.42369291	9.39071406
1.58777054	7.21962840	9.56598463
9.76320214	2.45712113	9.39315343
2.55139179	10.19742030	7.11286233
0.01780475	10.89473415	6.86227586
3.19831137	7.81281744	7.16530561
8.14480423	7.78711186	7.13629686
0.68407286	12.42574360	4.88334834
7.53129932	0.09603817	7.12496534
3.88102227	5.17512499	6.97482987
8.85350136	5.17434786	6.98624839
3.21708592	2.73068145	6.91981717
8.20089489	2.71678349	6.92234011
0.70538347	8.31678299	6.97556035
5.63966732	8.33012761	6.96416215
4.94897671	10.83229703	6.96095897
7.54033795	10.31541503	7.28527033
1.38402650	5.91307079	6.79385687
6.35599975	5.89621399	6.78603556
0.70301197	3.29611599	6.73349205
5.69286892	3.26603818	6.73001019
0.02160889	0.91968943	6.66913046
4.98998847	0.87873143	6.68066632
3.25517187	11.74748682	5.16863235
8.22981947	11.76059864	5.18485072
8.86191047	9.24538568	5.12204343
3.87899038	9.21300604	5.01335467
7.50935693	4.22946933	5.03734921
2.51791467	4.23662271	5.03299125
8.19805839	6.76603870	4.91779449
3.19257131	6.76740453	4.92431569
5.67514738	12.40599808	4.91850243
2.53421992	0.06364683	7.04044100
3.24096110	1.46779136	4.84799654
8.22217765	1.46777158	4.84724354
1.39670828	9.88361803	4.77895664
6.38193030	9.89813089	4.87205717
5.01465017	4.85302475	4.72869119
0.02455961	4.86501673	4.73705209
0.72985109	7.32462217	4.71029901

5.71152448	7.28678613	4.70508975
5.75549053	2.18745866	4.51383208
0.76672980	2.19452179	4.51616594
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422
5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946
7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# TS for O+CH<sub>cv</sub>->OH+C<sub>cv</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
2	40	5	80

Cart

5.15228243	10.14678176	8.34332458
1.24819409	11.30215430	7.95501885
4.27943365	9.31565900	7.61834911
4.61926101	2.59771390	8.21680702
1.78849843	7.53504046	8.43071432
9.61913394	2.61681803	8.21838044
6.80779637	7.50392469	8.41500247
9.17800186	9.29577869	7.40555002
2.20195855	4.27349634	7.19889598
7.19742296	4.25077780	7.19693688
3.41682268	11.96137124	7.11098631
8.46795320	11.97006317	7.15737874
-0.32689500	6.77331408	6.30586944
4.65810929	6.80093486	6.32491036
1.73510368	1.62812910	6.17366865
6.73572577	1.57692362	6.17027073
2.19106277	8.32591400	5.65173401
7.15549749	8.27733555	5.60753140
9.20323747	3.14881288	5.29567190
4.20739971	3.14367629	5.29753031
4.68054662	10.84116146	4.30071671
-0.32479995	10.80756513	4.27379294
6.72540475	5.70159803	4.01585334
1.73869129	5.71568003	4.01749958
7.18856480	12.34821052	3.63910664
2.18027595	12.35178264	3.62486631
9.23129479	7.20021357	3.33940828
4.23961911	7.20621228	3.35019913
5.47292217	2.23055554	2.34193027
0.48302217	2.23055554	2.34193027
6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348

4.22357812	11.29064837	1.28800348
5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
6.12602453	11.13305990	8.33663250
6.59130718	7.23681625	9.55670486
4.76524129	2.41448353	9.38709435
1.63522591	7.28397743	9.58564169
9.75021299	2.43618709	9.39280702
2.52851458	10.26064988	7.14686051
0.01310691	10.90628522	6.88276333
3.21399644	7.84568347	7.18345026
8.17442595	7.77839864	7.13548873
0.67034356	12.43148625	4.88803319
7.47145541	0.05321805	7.18199992
3.88027337	5.17368490	6.97695420
8.86523771	5.16575790	6.98517641
3.20926310	2.73282129	6.91998549
8.19522072	2.70278326	6.92016002
0.72190684	8.31993124	6.98191961
5.69728904	8.29364124	6.96622516
4.94651754	10.93383481	6.76371134
7.55257350	10.30991748	7.32761283
1.39274721	5.91398980	6.79729097
6.37069360	5.87808674	6.77702745
0.69889612	3.29297285	6.73644775
5.69413251	3.27527326	6.73445149
0.00496535	0.90904648	6.68672172
4.97903589	0.91186905	6.66230331
3.22599590	11.78366384	5.15291701
8.22193197	11.75645475	5.20054729
8.86950064	9.24729282	5.12652374
3.88924334	9.23111315	5.04610274
7.51011994	4.22758522	5.03894167
2.51896007	4.24173718	5.03772780
8.20088894	6.76442896	4.91576486
3.20201302	6.77698772	4.94433356
5.68831816	12.45959975	4.88831518
2.50712289	0.08968664	7.05879811
3.22497775	1.48489877	4.84075671
8.23424433	1.47405440	4.84313498

1.40095208	9.89263282	4.80454351
6.39240883	9.89627405	4.84325067
5.01621156	4.85332914	4.72548786
0.03031384	4.86783956	4.73643338
0.73323609	7.31892723	4.71177141
5.71149331	7.28726730	4.71022721
5.75401183	2.20183139	4.51286468
0.76060055	2.19992479	4.51654591
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422
5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946

7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# OH

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9.97980000	0.00000000	0.00000000
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H	C	O	Fe
2	40	5	80

Cart

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1.23114035	11.29787560	7.97556568
4.18007592	9.28879967	7.38122387
4.63369123	2.59460578	8.21897912
1.80464958	7.50567474	8.41770307
9.60734005	2.60673880	8.22727420
6.75241553	7.55391515	8.40931881
9.17241221	9.29955070	7.39397927
2.20633252	4.26120882	7.20292864
7.19654529	4.25577326	7.20137754
3.42227539	11.97079487	7.18255285
8.47629763	11.97383850	7.12987932
-0.34293454	6.77734358	6.30733790
4.64666008	6.77056109	6.30075233
1.74818674	1.62704156	6.16661804
6.73162517	1.60912785	6.14924672
2.16452838	8.28791669	5.58920831
7.14680497	8.28012505	5.58891603
9.20569656	3.13485379	5.29686937
4.21205966	3.13507908	5.29935684
4.67170168	10.79898039	4.25767882
-0.32555690	10.80660073	4.27047672
6.72215818	5.68986735	4.01339107
1.73178780	5.69188478	4.01384600
7.17807909	12.34664838	3.64446068
2.19599782	12.34599731	3.64339422
9.22592390	7.19953387	3.33585555
4.23523007	7.19966071	3.33129715
5.47292217	2.23055554	2.34193027
0.48302217	2.23055554	2.34193027

6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348
4.22357812	11.29064837	1.28800348
5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
6.23778691	11.35500569	8.47602775
6.59294185	7.28292366	9.56249845
4.80333195	2.40252416	9.38783772
1.58051926	7.25266943	9.56245650
9.77648620	2.43227919	9.39798670
2.50969236	10.28212983	7.17154340
0.01343054	10.90464837	6.88766652
3.16486485	7.78226156	7.13286441
8.15639321	7.79145803	7.13284060
0.67835933	12.42571971	4.88836179
7.51959901	0.14549025	7.14999748
3.87433608	5.16663669	6.98984510
8.86316385	5.16855701	6.98497324
3.21981540	2.72492828	6.92627384
8.21125091	2.72056119	6.92195110
0.70385937	8.31411974	6.95441768
5.68571605	8.29593687	6.93652598
4.96559582	10.93713739	6.99856851
7.54316118	10.30768162	7.29338154
1.37140635	5.88810944	6.78593742
6.36597313	5.88232152	6.77424640
0.70436664	3.28434827	6.73651373
5.69736889	3.27681862	6.73221642
0.01394348	0.91601925	6.67380223
4.98936093	0.90738887	6.67052370
3.24997693	11.75698804	5.18634223
8.22062274	11.75545653	5.19508061
8.87306784	9.23988420	5.11403028
3.89375426	9.24771030	5.13293668
7.51047602	4.22118903	5.03708242
2.52087422	4.22550268	5.04026945
8.19108092	6.75918528	4.91691588



3.20116049	6.76074768	4.91394725
5.67357829	12.41361342	4.91992570
2.51108428	0.08806132	7.05666987
3.23592364	1.47097094	4.84278620
8.22427251	1.47207467	4.83601257
1.39670053	9.88950511	4.81455543
6.38505049	9.90310059	4.85621049
5.01344940	4.84875606	4.72935313
0.02359522	4.84984899	4.72720178
0.71802865	7.28808680	4.70630635
5.70818608	7.28390247	4.69686332
5.75335510	2.19472740	4.50546981
0.76555496	2.19513164	4.50923846
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422
5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591

1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946
7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# OH+H

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9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	40	5	80

Cart

6.44661093	1.45905293	9.10029099
6.22768448	11.13428541	7.90532706
1.24722174	11.29735935	7.96534984
4.17911828	9.25461577	7.38511018
4.58099365	2.94997148	8.23978976
1.78224465	7.51631952	8.41468500
9.59726807	2.60412535	8.21461039
6.78605525	7.50335409	8.41139360
9.17550638	9.27849402	7.38291659
2.19167915	4.23872935	7.17622720
7.19262340	4.24395761	7.19155310
3.44165650	11.89591212	7.14231111
8.40801283	11.93633979	7.18843428
-0.32996920	6.74887674	6.29834918
4.65834878	6.73700497	6.29977896
1.74118261	1.58788356	6.17228150
6.74278369	1.60291163	6.10483476
2.17145183	8.28062421	5.59790382
7.16533719	8.28507021	5.59718506
9.19888946	3.12986139	5.28238325
4.19824619	3.12540989	5.26503766
4.67778369	10.81987759	4.28535933
-0.32089776	10.79953006	4.26420081
6.72258265	5.69444435	4.01099882
1.73297165	5.69038411	4.00982082

7.17923893	12.34289372	3.66049014
2.18880212	12.34821386	3.63966669
9.22750521	7.20209286	3.33521478
4.23669425	7.20250114	3.33575556
5.47292217	2.23055554	2.34193027
0.48302217	2.23055554	2.34193027
6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348
4.22357812	11.29064837	1.28800348
5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
6.25158791	0.60651223	8.66133717
6.60468049	7.26503536	9.56635465
4.68441291	3.02542521	9.42925686
1.60131310	7.28679798	9.57200472
9.69182650	2.43030947	9.39288642
2.52614335	10.24399349	7.17616070
-0.00821835	10.90639828	6.91517839
3.17350785	7.75688769	7.13114534
8.17156240	7.76684718	7.13050347
0.67862108	12.41115453	4.90299218
7.49436963	0.11952344	7.24489467
3.86679938	5.14512251	7.00135829
8.85872360	5.15358814	6.99900435
3.22247407	2.70913774	6.91156502
8.19929511	2.71205736	6.89703808
0.70497585	8.29848666	6.95205695
5.70137560	8.28728016	6.95378561
4.98766471	10.83213794	6.81860405
7.51597429	10.25927117	7.16484589
1.37725217	5.88166629	6.79891300
6.37834148	5.88362438	6.78806534
0.69757446	3.25152100	6.73348418
5.69450924	3.28519415	6.68340251
0.00829834	0.87103809	6.71481604
5.10766541	0.85978181	6.99409483
3.25172807	11.78948696	5.18724883

8.23226674	11.74529897	5.19758771
8.88489145	9.22559259	5.09918907
3.88309083	9.22369940	5.07307541
7.50988102	4.22717798	5.03531336
2.51484525	4.22084387	5.04175772
8.19654829	6.75269926	4.91393182
3.20694889	6.74889821	4.91510696
5.67656100	12.44372387	4.93269080
2.53940492	0.07287587	7.08247145
3.21869653	1.46009930	4.83829700
8.24529537	1.44218694	4.84541984
1.40479768	9.89372004	4.83293795
6.39674606	9.88300720	4.80149817
5.00913182	4.86285846	4.72874711
0.02842232	4.85118777	4.74705093
0.72790606	7.28672762	4.70222392
5.71531054	7.29359660	4.70025545
5.73723520	2.17600058	4.49806418
0.76707829	2.18177166	4.51205760
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422
5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072

2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946
7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# TS for OH+H->H<sub>2</sub>O

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	40	5	80

Cart

6.27188870	0.31267350	9.43592197
5.93049269	11.47297708	8.23996366
1.23973108	11.33069795	7.96955670
4.19693264	9.31437190	7.38660209
4.62100367	2.74458867	8.23457221
1.77748019	7.58960702	8.41945907
9.60029350	2.62549319	8.22071728
6.76655563	7.57071176	8.41981987
9.16981732	9.31075086	7.38189393
2.18881536	4.27332752	7.19445618
7.18894042	4.26485641	7.19413838
3.46708482	11.96308831	7.17290566
8.39242452	11.95276184	7.14820004
-0.33562530	6.78411053	6.31197581
4.65176271	6.78004007	6.30804865
1.74215048	1.62740861	6.18157275
6.73967582	1.58628946	6.16121292
2.16875053	8.29371692	5.59227646
7.15812869	8.29873507	5.59527892

9.19617666	3.14136627	5.29515452
4.20810753	3.13737852	5.29407843
4.67620335	10.82780033	4.28022190
-0.32332795	10.81855405	4.26742051
6.72246929	5.70205191	4.01263571
1.73352053	5.70093412	4.01207280
7.17853251	12.34948992	3.64234706
2.18975991	12.35008167	3.63796284
9.22803152	7.20203323	3.33715027
4.23812134	7.20150169	3.33525814
5.47292217	2.23055554	2.34193027
0.48302217	2.23055554	2.34193027
6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348
4.22357812	11.29064837	1.28800348
5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
6.35525001	12.57952064	9.14229387
6.59072273	7.33718184	9.57446037
4.72412149	2.61873805	9.42033868
1.60541614	7.35123390	9.57417247
9.72989288	2.44999861	9.39282060
2.53836288	10.30266538	7.20282175
-0.01434733	10.93373586	6.91012186
3.17486149	7.80848684	7.13178319
8.16409847	7.79774522	7.13315543
0.67996742	12.42275705	4.89501712
7.47997552	0.13682845	7.25974455
3.86468402	5.17932998	6.99518604
8.85668052	5.17513230	6.98644142
3.21182469	2.74095495	6.91967414
8.19868778	2.72902736	6.90987458
0.70490907	8.33288099	6.94731967
5.69992553	8.32494941	6.94951371
5.00676705	10.90649836	6.86983311
7.49504903	10.27014790	7.12623980
1.37716217	5.91007133	6.78926932

6.36553061	5.90320821	6.78999628
0.69690823	3.28168042	6.73417792
5.68767211	3.29086468	6.72739970
0.01423777	0.88567562	6.68994487
4.98319644	0.91440247	6.65794616
3.23886094	11.77178860	5.17780238
8.22515525	11.77487216	5.18659856
8.88461753	9.23817721	5.08829680
3.88558107	9.24274049	5.09079271
7.50485300	4.23572212	5.03593398
2.51648194	4.23473546	5.03962427
8.19457257	6.76417999	4.91934912
3.20550569	6.76424993	4.91901935
5.68528779	12.43431408	4.91337908
2.52976340	0.08903023	7.05792432
3.22467458	1.47755086	4.84368917
8.22750537	1.46981276	4.84822199
1.40014083	9.90589066	4.83699306
6.39518423	9.89452624	4.79741744
5.01224476	4.85930576	4.73300772
0.02487067	4.85730633	4.73321380
0.72234243	7.29367271	4.70484619
5.71201993	7.29625688	4.70440497
5.75099941	2.19553783	4.50875986
0.76183092	2.19267351	4.51498492
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422
5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962

0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946
7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# H<sub>2</sub>O

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	40	5	80

Cart

6.28557143	0.98839795	9.43519389
5.94834392	12.15145013	9.68810804
1.26242619	11.30999875	7.97935042
4.21957089	9.29211435	7.40331851
4.62693961	2.43268076	8.16717458
1.79626493	7.59061444	8.43278663
9.55843580	2.55156818	8.22159909
6.78997752	7.56541524	8.43164932
9.19918909	9.27666218	7.40952796
2.19747484	4.23762617	7.22464772
7.18253796	4.23954278	7.21320240
3.46997241	11.93778597	7.14904307
8.38697656	11.90414372	7.18072323



-0.32126909	6.75242855	6.31383246
4.66373800	6.75783145	6.31315002
1.73356556	1.59625019	6.18480900
6.73658132	1.58294732	6.14323165
2.17816570	8.28288004	5.60336278
7.17321312	8.29636417	5.61496688
9.19719841	3.13761403	5.29727027
4.20645683	3.13890226	5.29971747
4.68005883	10.81833905	4.28139086
-0.31733775	10.80850281	4.26564104
6.72524966	5.69913936	4.01284859
1.73681474	5.69034872	4.01362104
7.18727762	12.34498324	3.64181789
2.18913297	12.34870438	3.63698287
9.23079407	7.20408217	3.34671774
4.24054113	7.20154004	3.34477113
5.47292217	2.23055554	2.34193027
0.48302217	2.23055554	2.34193027
6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348
4.22357812	11.29064837	1.28800348
5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
6.99171917	0.31342051	9.24915952
6.62929092	7.34831857	9.59309566
4.87197123	2.13623221	9.31980116
1.65417991	7.36475616	9.59579400
9.68870868	2.38181094	9.39800575
2.56063913	10.27467274	7.20049320
-0.00176733	10.91005703	6.92548950
3.19318997	7.79300761	7.13854208
8.18702387	7.76959975	7.14180413
0.68054924	12.41735187	4.90199370
7.48494791	0.09464775	7.20172510
3.86651170	5.15814475	7.00140571
8.85648360	5.15293611	6.99557229
3.21194873	2.70375505	6.93482256

8.19779712	2.71437480	6.90268732
0.72279125	8.30159876	6.96076875
5.71626311	8.30963017	6.96310405
5.02722849	10.88959394	6.79311368
7.52736000	10.20982390	7.07889120
1.38823653	5.87532723	6.79953080
6.36985221	5.87936500	6.81009783
0.69944447	3.24750796	6.75323984
5.68705448	3.25249524	6.73618571
0.00387188	0.85272311	6.71370730
4.99114658	0.88427038	6.64602991
3.23746716	11.76171073	5.16667729
8.23276171	11.75548975	5.19360605
8.89897833	9.21765740	5.07403420
3.89097575	9.22326205	5.07853417
7.50626791	4.23231459	5.03886254
2.51559099	4.22178148	5.04922224
8.19765019	6.75408183	4.92301967
3.20918827	6.75064596	4.92565973
5.69175340	12.43200312	4.90069836
2.53318652	0.06346417	7.06311111
3.22315995	1.47609319	4.84278433
8.23512757	1.45982085	4.84379972
1.40649659	9.89611810	4.84790382
6.39946066	9.87508739	4.77972675
5.01682710	4.85428755	4.74513795
0.03097309	4.84997210	4.74654274
0.72962406	7.28218305	4.71026139
5.71938727	7.29099889	4.71132785
5.74967891	2.19651682	4.50680305
0.76079002	2.18864248	4.52132364
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422
5.72548353	11.29866287	2.69921895

0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946
7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# OH+OH (state1)

1.000000000000

9.97980022	0.00000000	0.00000000	
-0.76395801	12.66177369	0.00000000	
0.00000004	0.00000004	19.64039993	
H	C	O	Fe
3	40	6	80

Cart

4.58217994	3.22329912	8.86056423
4.77205474	5.37888395	9.66844340
1.22357866	11.29728093	7.97091136
4.17936262	9.28010911	7.37324132
5.96638827	11.39441735	8.45260278
9.59240945	2.56009562	8.20547102
6.74669901	7.56579109	8.40930295

1.76985574	7.60796108	8.42449614
9.16700816	9.30041730	7.37815941
2.24904841	4.29379768	7.09416992
7.19260997	4.25612859	7.16222254
3.41822945	11.92609787	7.17147167
8.45043377	11.96032562	7.16295499
-0.35076332	6.78796345	6.30037699
4.62248947	6.70353838	6.27456808
4.19961809	3.13328091	5.24050885
6.74345791	1.57721481	6.15731252
2.16751548	8.28724105	5.58320264
7.15029022	8.27913591	5.57995769
9.19846087	3.14003771	5.28565357
1.74706292	1.61890764	6.16100711
4.67292954	10.80821129	4.26859777
-0.31777703	10.80328799	4.26397969
6.71162949	5.67794625	4.01586675
1.73716622	5.68820315	4.02153387
7.17548078	12.34699154	3.64553380
2.19370203	12.34366650	3.63392465
9.22545005	7.19937874	3.32805436
4.23184541	7.20117890	3.32764572
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
4.25347346	4.78026469	9.10010807
4.64052186	2.44846211	8.17893035
1.57080215	7.37286698	9.57495825
6.15242145	11.46402707	9.62743272
9.79243909	2.39479880	9.37198015
6.57471342	7.31733564	9.56675603
2.51817399	10.26749600	7.17456733
7.52131466	10.29269324	7.20785480

3.15724530	7.78062366	7.12994258
8.14644304	7.79633588	7.12870415
0.67936925	12.42702805	4.88614789
5.67313257	12.42186127	4.92218278
3.87988311	5.27557695	7.34260240
8.85678765	5.17027282	6.97258286
3.21632605	2.70484759	6.89895667
8.20618112	2.70864348	6.90539328
0.69878399	8.32653027	6.93540046
5.67713100	8.28620084	6.93135347
4.98878133	10.91522810	6.97623663
8.86673354	9.24252438	5.10627898
1.33892472	5.89326348	6.76002488
6.36893998	5.89957970	6.77411666
0.70971742	3.29279119	6.72708354
5.69914320	3.26211809	6.69627300
2.50250686	0.07069892	7.05469866
4.98293916	0.88640463	6.74446534
3.24373880	11.76656831	5.18766168
8.23584289	11.76430824	5.18184337
0.00400056	10.91346734	6.88974251
3.89057440	9.24075895	5.11176277
7.50184932	4.21643878	5.04165749
2.54234684	4.24001479	5.06918133
8.19129140	6.75030691	4.91542640
3.19682971	6.76398689	4.90863095
7.53431413	0.08615142	7.10476072
3.23698303	1.46183220	4.83317246
0.76715432	2.20223154	4.51102352
8.23330443	1.46094369	4.83810948
1.40436637	9.89641828	4.82043805
6.38906607	9.90747634	4.85707975
4.99866605	4.87364211	4.77752830
0.02660615	4.84993826	4.72176056
0.71537309	7.29790385	4.69406506
5.70933837	7.28240324	4.69383256
5.75642022	2.18746982	4.51479713
0.02559197	0.90200740	6.69456008
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337

7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# OH+OH (state2)

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	40	6	80

Cart

6.32011190	11.51609745	9.14200314
8.02489645	0.87310891	9.70556410
1.22699727	11.33147282	7.96257360
4.14888691	9.28241234	7.29983388
4.64148246	2.66476912	8.22394684
2.11958101	7.38645061	8.55425456
9.67358166	2.79064001	8.22603451
6.79845730	7.44903418	8.38016877
9.11905108	9.33479446	7.39146231
2.20347523	4.27727063	7.17667471
7.19095522	4.27320378	7.18350396
3.45927191	11.96625350	7.21310042
8.39774542	11.99130829	7.15401009
-0.33892752	6.78193668	6.30550390
4.66115273	6.75601820	6.26117232
1.76281307	1.64635762	6.16476087
6.73309896	1.61341194	6.12135738
2.15074114	8.28912669	5.56126086
7.15389529	8.28371326	5.56499132
9.20352565	3.13474346	5.27633805
4.20833641	3.13930344	5.28993440
4.67450750	10.79582239	4.25524930
-0.33334077	10.81676744	4.27065776
6.72286033	5.69667883	4.01050224
1.72938908	5.69915630	4.01189233
7.17611316	12.35273273	3.65931285
2.20104559	12.34567615	3.65025027
9.22414196	7.20104151	3.32078357
4.23596121	7.20343261	3.31482135
5.47292217	2.23055554	2.34193027
0.48302217	2.23055554	2.34193027
6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348
4.22357812	11.29064837	1.28800348
5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
7.32330975	0.45973858	9.16517435

6.16554465	10.65113426	8.63288370
6.53943267	7.22417109	9.52276592
4.76014599	2.51988643	9.40143952
1.64290289	7.22489814	9.62233533
9.73326253	2.62527735	9.41023530
2.49892371	10.30311853	7.15985356
-0.02325763	10.94456011	6.91362820
3.14935661	7.76687864	7.13223508
8.15933535	7.78937796	7.11875245
0.68657406	12.41870385	4.89383605
7.56909086	0.33143198	7.34053253
3.86344159	5.19634651	7.01085153
8.86610025	5.18715376	6.99823976
3.22419811	2.74266173	6.91466823
8.22628278	2.75355931	6.91600422
0.67085056	8.38341964	6.90719587
5.67780620	8.28462296	6.90357584
4.99929054	10.91559537	7.08073093
7.50690725	10.34310555	7.30075019
1.38211274	5.91258459	6.75953046
6.38103477	5.90318433	6.77229170
0.70460041	3.31128140	6.71397084
5.69624425	3.28697080	6.71467134
0.03623871	0.91323242	6.66584907
5.00792769	0.90596829	6.69730856
3.26418254	11.75626084	5.19889366
8.21755109	11.76145995	5.20799800
8.86817208	9.26479413	5.14529444
3.88148527	9.25235023	5.15278015
7.51366255	4.23295199	5.03523566
2.52115791	4.23527477	5.03148634
8.20478888	6.76851731	4.90743340
3.20640099	6.76943052	4.90284945
5.68150665	12.40152741	4.95276512
2.53135376	0.09671099	7.04647579
3.24237950	1.46583500	4.84442757
8.22715911	1.46139897	4.85445071
1.39270266	9.91137664	4.81999758
6.38153669	9.93150656	4.89786750
5.00936502	4.86334727	4.74064666
0.01976168	4.86391074	4.71994853
0.71776142	7.29856124	4.69457073
5.72182257	7.29075821	4.67718217
5.75041993	2.19329319	4.49871293



0.76557801	2.18618283	4.50396849
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422
5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946
7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# TS for OH+OH->H<sub>2</sub>O+O

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	40	6	80

Cart

6.36115178	11.82993910	9.08417231
8.01590766	0.81291283	9.66944882
1.24395750	11.31058505	7.95998288
4.17389503	9.25635533	7.34634255
4.63433296	2.64423805	8.22286011
1.94945375	7.35626174	8.44285154
9.65228377	2.67147774	8.21312512
6.77101388	7.49156841	8.39010988
9.15289204	9.30306128	7.38238586
2.19954118	4.26034830	7.19599376
7.19076214	4.25006607	7.20057944
3.46422955	11.94442682	7.20233648
8.44948910	11.96356043	7.14710261
-0.33368127	6.75696996	6.30235740
4.66323798	6.73461198	6.26393602
1.76288917	1.62687728	6.16470793
6.72681886	1.61241437	6.11462406
2.17085804	8.28125780	5.58115759
7.15741642	8.26962201	5.57099016
9.20523012	3.13076974	5.28230217
4.20687173	3.13422865	5.28918712
4.67809076	10.78538420	4.25163304
-0.32642878	10.79759484	4.26771371
6.72497587	5.68905490	4.00893473
1.73211851	5.69293690	4.01084762
7.17827565	12.34591318	3.65519366
2.20333963	12.34323283	3.64963424
9.22770022	7.20040150	3.32814212
4.23607390	7.20227694	3.31910724
5.47292217	2.23055554	2.34193027
0.48302217	2.23055554	2.34193027
6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348
4.22357812	11.29064837	1.28800348

5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
7.27439542	0.44810633	9.14968653
6.20861742	10.83334969	8.53761275
6.56483621	7.26754467	9.54392132
4.72642420	2.48561288	9.40020398
1.61304986	7.19295833	9.57150233
9.70452409	2.45058796	9.39001353
2.51722693	10.26879974	7.16767154
0.01223855	10.91230229	6.89395874
3.17246024	7.74984921	7.12487180
8.16074955	7.77366522	7.12197363
0.68844565	12.41170633	4.89134630
7.57810995	0.28035907	7.24461463
3.86759905	5.16883413	7.01393393
8.85887749	5.17248272	7.01139839
3.21899960	2.72600097	6.91309034
8.21971689	2.73308742	6.90719994
0.69755443	8.32820699	6.94688216
5.68417175	8.26086580	6.90864180
4.99777662	10.89682199	7.07867376
7.54624514	10.32170646	7.32294358
1.38037709	5.90328400	6.81802673
6.37747317	5.87890207	6.78272284
0.70339826	3.28701456	6.73264748
5.69268842	3.27366402	6.72118105
0.03970225	0.90102283	6.66947076
5.00419498	0.89387393	6.68866339
3.26668448	11.74160844	5.19743830
8.22354347	11.74574601	5.20563903
8.87508926	9.24902438	5.15052697
3.89740251	9.24522727	5.14725880
7.51147062	4.22607315	5.03931541
2.51744721	4.23206822	5.04341277
8.20483364	6.75899765	4.90860356
3.20869989	6.76151403	4.90030502
5.68480388	12.39751363	4.94737419
2.54087047	0.07783529	7.04534423
3.24309649	1.45812262	4.84226525
8.23253458	1.45435682	4.84456124

1.40110094	9.89062436	4.82339888
6.38671311	9.91813813	4.89858850
5.01353966	4.85677375	4.74307118
0.02561082	4.85921342	4.74272316
0.72565455	7.28989994	4.70570247
5.72327480	7.28216780	4.67906797
5.74833503	2.18933695	4.49711250
0.76852924	2.18686420	4.50792009
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422
5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946

7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# H<sub>2</sub>O+O

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	40	6	80

Cart

7.51426996	0.03075953	9.98910296
8.27810513	1.40267791	9.67280513
1.24611123	11.31682472	7.95753200
4.19276145	9.27526561	7.37070214
4.60398147	2.61332845	8.22530927
2.00661117	7.33956825	8.46404922
9.59458102	2.73162601	8.20476477
6.76469579	7.54529585	8.39305476
9.15510229	9.31823494	7.36947935
2.19742080	4.26714728	7.20723001
7.18526803	4.24980509	7.18912444
3.44432108	11.94945053	7.17706314
8.49125496	11.98989002	7.13434262
-0.32852702	6.75441120	6.31663411
4.67165777	6.74666178	6.27194459
1.74731736	1.63901091	6.16485317
6.74657570	1.55286705	6.18282680
2.18037800	8.28699939	5.59087496
7.16623061	8.27180668	5.56375845
9.19684873	3.12794692	5.27617494
4.20970460	3.13689480	5.29764806
4.67671760	10.78935499	4.25268654
-0.31971875	10.80249966	4.27053699
6.72541161	5.69256851	4.00805017
1.73464842	5.69771990	4.01191093
7.17871035	12.34467829	3.65319406
2.20051627	12.34630210	3.64023277
9.23013973	7.20059391	3.33244008
4.23760740	7.20208934	3.32198302
5.47292217	2.23055554	2.34193027

0.48302217	2.23055554	2.34193027
6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348
4.22357812	11.29064837	1.28800348
5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
7.53184360	0.80883774	9.40272777
6.21594370	11.16629335	8.31205423
6.59601239	7.31547507	9.55129512
4.69535637	2.42897048	9.40115820
1.65445899	7.18576409	9.58904261
9.60828191	2.55344071	9.40229018
2.51877709	10.26669022	7.16598730
0.02859236	10.91823853	6.87546127
3.18972446	7.76110370	7.13417017
8.17193618	7.78509759	7.11811492
0.68893894	12.42569110	4.88192191
7.53472349	0.15826711	7.37317915
3.86968312	5.17484185	7.01350868
8.85912806	5.16458596	7.01120732
3.20786279	2.72961417	6.91563588
8.19399165	2.71636170	6.88756221
0.70408936	8.33930886	6.94561817
5.69886402	8.28429428	6.91397535
4.96930858	10.91209609	7.02313786
7.55327803	10.35006548	7.28169038
1.39092900	5.91535727	6.83084177
6.38068947	5.88777763	6.78837048
0.69235473	3.30079545	6.75051688
5.68511662	3.26600454	6.73915907
0.02156274	0.92553606	6.65125916
4.98625179	0.90338407	6.67455977
3.26078832	11.75229487	5.18459574
8.23666464	11.75842236	5.19677816
8.88115322	9.25144567	5.14592693
3.90411168	9.24881045	5.14615194
7.51096142	4.23429099	5.03930437

2.51879456	4.24004285	5.04691227
8.20861714	6.75831983	4.91193677
3.21266330	6.76748639	4.90511907
5.68573913	12.40051624	4.95140834
2.52877497	0.09166029	7.04372081
3.24039073	1.46903009	4.84199940
8.21938185	1.45032577	4.83889702
1.40752151	9.89150710	4.81675607
6.39303746	9.91728789	4.88389082
5.01602109	4.85582071	4.74470064
0.02931549	4.86028667	4.74981089
0.72957961	7.29307828	4.71041803
5.72414864	7.28309409	4.68415761
5.76071672	2.18775509	4.51836390
0.76649282	2.19843292	4.51369261
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422
5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367

3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946
7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# CO+O (state1)

1.000000000000

9.97980022	0.00000000	0.00000000	
-0.76395801	12.66177369	0.00000000	
0.00000004	0.00000004	19.64039993	
H	C	O	Fe
1	41	6	80

Cart

1.22498414	11.39373418	7.89332442
4.18636061	9.30687325	7.34716863
2.41178374	0.78607635	8.91711172
8.93130413	2.35542887	8.55453064
2.12838061	7.39453918	8.57395673
6.72680256	7.54920426	8.39577419
4.67453120	2.97837778	8.27085361
9.13541201	9.32450333	7.40988060
2.20739799	4.28791918	7.17103334
7.20324272	4.26938067	7.15851626
3.39687951	11.97287379	7.17273127
8.50138357	11.98819248	7.11887903
1.76370907	1.57780382	6.14983422
4.66293938	6.77844363	6.27922381
-0.34126321	6.78263389	6.32198273
6.71759331	1.62586916	6.14526122
2.16442489	8.28815635	5.59545772
7.15645223	8.27918815	5.57501425
9.20871624	3.12784823	5.28442453
4.20720770	3.12619066	5.28839794
4.67014308	10.78397086	4.25029692
-0.31440169	10.81862562	4.28140502
6.72480406	5.67971610	4.01660035



1.73340867	5.69626301	4.01374235
7.17656094	12.35583479	3.63895990
2.19792770	12.35447640	3.64745007
9.22732124	7.20088925	3.33309401
4.23814919	7.20236320	3.32580601
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.21240796	11.38921387	8.23618288
4.75789549	2.93838979	9.45812385
2.31250379	1.14929386	10.01691373
1.68284811	7.22636866	9.65401062
6.57629973	7.28117123	9.54795581
9.37532258	2.20508923	9.62725121
2.49108105	10.27265150	7.13120756
-0.00401314	10.89023698	6.82182828
3.17093325	7.77802680	7.15570064
8.16182936	7.80382284	7.12802956
0.69505387	12.43070407	4.90016321
7.54245768	0.16639770	7.13617151
3.88020882	5.19440123	7.00976183
8.87589882	5.16809208	6.97538533
3.20897043	2.74052887	6.94686169
8.20512522	2.71011057	6.97317449
0.67786744	8.36439561	6.92422113
5.69556279	8.30397851	6.92425386
4.94400930	10.95103842	7.00585622
7.52640134	10.35615249	7.29436526
1.38269284	5.91929107	6.78737473
6.38176501	5.90319063	6.76245212
0.71445491	3.32246064	6.65768962
5.67440859	3.32159412	6.70519155
0.00112894	0.93351470	6.62196865

4.98720105	0.90729150	6.63577129
3.24584129	11.75535215	5.19362192
8.22989960	11.77792857	5.17577815
8.86831653	9.24851581	5.12149095
3.89439804	9.24519579	5.15537628
7.51508012	4.18720223	5.05597191
2.52788202	4.22634729	5.05226304
8.19992030	6.75349703	4.91811172
3.21251916	6.76838754	4.91368904
5.67690569	12.40186391	4.91954025
2.54503635	0.18077529	7.25401159
3.25226022	1.46097252	4.86102547
8.20109665	1.49741162	4.83595567
1.40577928	9.88771837	4.79464821
6.38926775	9.91878733	4.88153075
5.01463847	4.85944109	4.73470151
0.02181436	4.86108320	4.70951103
0.72541266	7.29207856	4.70568938
5.72229615	7.28514958	4.68829150
5.75402484	2.19414185	4.49954661
0.77262069	2.20285975	4.49125962
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233

3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CO+O (state2)

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
1	41	6	80

Cart

1.20663246	11.31999815	7.95411387
4.17940657	9.29616732	7.36537716
4.61726378	2.80114819	8.24901817
9.73174696	3.16059701	8.30256662
1.79160206	7.50809112	8.41046117
7.72888099	1.13097376	8.85252100
6.72231550	7.51842701	8.39032412
9.13235896	9.33245250	7.36887938
2.21223014	4.29639240	7.15186658
7.17965075	4.26047354	7.19249172
3.42509358	11.96357055	7.18658677
8.48006970	12.00456323	7.12983409
-0.35653879	6.77973378	6.31826087
4.64849589	6.77055297	6.28630069
1.75584291	1.66165111	6.17108493
6.74598243	1.54357232	6.17116928
2.16131234	8.28395528	5.59353996

7.14394326	8.27403243	5.57934459
9.19748974	3.11076621	5.31280668
4.21106888	3.12265582	5.29000489
4.66895608	10.79974875	4.25356070
-0.32162628	10.79353561	4.26408362
6.72175532	5.67544928	4.01656397
1.72809487	5.69890997	4.01397550
7.17826164	12.36051796	3.65489721
2.19583891	12.34812903	3.63461045
9.22541240	7.20021751	3.33580520
4.23648391	7.20114012	3.32458172
5.47292217	2.23055554	2.34193027
0.48302217	2.23055554	2.34193027
6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348
4.22357812	11.29064837	1.28800348
5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
6.21161278	11.29537628	8.25468250
6.55453564	7.25196261	9.54073400
4.65586037	2.71884547	9.43727678
1.55994191	7.27652783	9.55716114
7.71956369	1.51125948	9.95273144
-0.11325313	3.22740566	9.48115425
2.50700211	10.28408084	7.17890638
0.00420051	10.91754612	6.86869492
3.15888912	7.78656684	7.13306496
8.14417135	7.80867706	7.12821771
0.68496725	12.41263390	4.87539266
7.57705940	0.19705719	7.33546015
3.87795381	5.17851030	6.99969519
8.85571945	5.16127986	6.99875466
3.21759475	2.74434151	6.91088684
8.20849276	2.72513347	7.00168969
0.68352210	8.34125832	6.95441807
5.67158085	8.29347852	6.92585744
4.96755945	10.94141096	6.99377685

7.50111767	10.37469557	7.24017932
1.37311817	5.93104709	6.78164132
6.36326292	5.89252056	6.77789708
0.70179911	3.34330459	6.69968927
5.68387763	3.28036643	6.72377201
0.04174560	0.91733332	6.61568458
4.98287666	0.90657576	6.67046280
3.24371431	11.75957337	5.18601837
8.23446689	11.76070118	5.18184920
8.85763913	9.24072867	5.11285297
3.88770052	9.25456615	5.13353688
7.51116872	4.19094805	5.05880488
2.51850026	4.23102660	5.03015114
8.19404272	6.74947702	4.92078277
3.20472044	6.76867247	4.90875282
5.67502062	12.39163539	4.93649029
2.51253131	0.10013899	7.04482293
3.23172693	1.46744766	4.84183326
8.21760986	1.46496261	4.87725780
1.39854958	9.88765591	4.82132327
6.38105642	9.91198390	4.87982635
5.01144185	4.84976549	4.73692700
0.01588123	4.85173767	4.72760198
0.71471036	7.29101157	4.70761275
5.71572671	7.27757865	4.69044695
5.75635508	2.18420987	4.50819841
0.76273110	2.18881011	4.50124840
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422
5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906

2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946
7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# TS for CO+O->CO<sub>2</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
1	41	6	80

Cart

1.23217291	11.33985421	7.96500605
4.17726359	9.28867435	7.36550391
4.62668587	2.73406252	8.23367277
9.65257680	2.74773042	8.23944456
1.78426149	7.53058072	8.41421151
7.16077165	0.02027207	8.91917758
6.73780862	7.57761337	8.40706502
9.16875346	9.31485289	7.38432234
2.20297671	4.28453478	7.18352793
7.19402763	4.27410687	7.19509825
3.43158518	11.97306592	7.19282343

8.45533630	11.99530887	7.16869159
-0.34009131	6.79039938	6.30321147
4.65124714	6.77695483	6.28778583
1.75601272	1.64817444	6.16451230
6.74202140	1.64351178	6.13474515
2.16682590	8.29654109	5.58802080
7.15108430	8.28340414	5.58391603
9.20045995	3.14107106	5.29380506
4.20975983	3.14182677	5.28757087
4.67157517	10.80198952	4.25431200
-0.32332400	10.80973672	4.26781840
6.72438194	5.69794274	4.01250177
1.73245491	5.70597520	4.01266210
7.17607220	12.35381988	3.65272198
2.19702655	12.34768667	3.64730188
9.22678653	7.20063349	3.32919870
4.23546034	7.20066993	3.32282698
5.47292217	2.23055554	2.34193027
0.48302217	2.23055554	2.34193027
6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348
4.22357812	11.29064837	1.28800348
5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
6.21325535	11.13253870	8.47285159
6.57068911	7.32427147	9.55897417
4.72502576	2.61760751	9.41489201
1.57736313	7.28730691	9.56249949
6.98797833	0.32538823	10.04416673
9.76871915	2.58451440	9.41349034
2.50968864	10.29330093	7.18034203
0.00666632	10.93212022	6.89683294
3.16208501	7.78753565	7.13115360
8.15368249	7.79886436	7.13023124
0.68132081	12.42628860	4.89077703
7.55740383	0.22325563	7.11408013
3.87149129	5.18430848	6.99213870

8.85829705	5.19084662	6.99158211
3.22145203	2.74672271	6.91304401
8.21591449	2.74402637	6.93026712
0.70111254	8.33406621	6.95004503
5.68140637	8.29798518	6.92196412
4.97138998	10.93829969	7.01607060
7.55270435	10.32265727	7.30603497
1.37495898	5.91760085	6.78567954
6.36976443	5.90056375	6.76798281
0.70505423	3.31158455	6.71994732
5.69329024	3.30388041	6.71810668
0.02612381	0.92776607	6.66944662
5.02469313	0.90978725	6.71287357
3.25459196	11.76663045	5.19296065
8.21623020	11.75365091	5.20162557
8.87029691	9.25593025	5.13139877
3.89561144	9.26413200	5.14499074
7.50992739	4.22818131	5.04066552
2.51865478	4.24072738	5.03530359
8.19681503	6.76934149	4.91294774
3.20455665	6.77481472	4.90849098
5.66621291	12.40912095	4.92071578
2.52360357	0.10755418	7.05292867
3.23817843	1.47300692	4.84428839
8.23297070	1.47017486	4.84463609
1.40044441	9.90268958	4.82396664
6.38681789	9.91974170	4.88203874
5.01113585	4.86234296	4.72628935
0.02184415	4.86329412	4.72678413
0.72090764	7.30196576	4.70203804
5.71397754	7.29356276	4.68618083
5.74924276	2.19393672	4.50376743
0.76416299	2.19654160	4.50549674
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328
3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422



3.24625357	5.59719332	2.75910422
5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946
7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# CO<sub>2</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
1	41	6	80

Cart

1.23403015	11.32982048	7.95541527
4.18785267	9.28549605	7.35933880
4.62478700	2.75551048	8.24224745
9.61435787	2.59930497	8.21824241
1.79995956	7.52917906	8.41532139

6.27459402	12.15754540	8.84894844
6.75040007	7.54267880	8.40015604
9.16193323	9.30976501	7.37449278
2.19584213	4.27642051	7.18718645
7.19395891	4.26448417	7.19856749
3.44776660	11.96262639	7.19879912
8.44369244	11.98692487	7.19876332
-0.33658417	6.78267935	6.30241525
4.65354733	6.76461825	6.28598689
1.75295640	1.63230251	6.17024892
6.73259280	1.63256539	6.14950720
2.16847898	8.29445798	5.58918724
7.15654536	8.28389490	5.58142600
9.20009081	3.14495561	5.29571605
4.20738928	3.13935838	5.28872786
4.67779813	10.80700187	4.25668625
-0.32324249	10.81242292	4.26867726
6.72427346	5.70085812	4.01165149
1.73220016	5.70488732	4.01223103
7.17973328	12.35430078	3.65437811
2.19743307	12.34535373	3.65011189
9.22772207	7.20165299	3.32975771
4.23542656	7.20184441	3.32524972
5.47292217	2.23055554	2.34193027
0.48302217	2.23055554	2.34193027
6.73540357	9.72874639	2.00704745
1.74550357	9.72874639	2.00704745
7.98876734	3.77819959	1.47019894
2.99886734	3.77819959	1.47019894
9.21347812	11.29064837	1.28800348
4.22357812	11.29064837	1.28800348
5.52626486	6.13002817	0.45987182
0.53636486	6.13002817	0.45987182
7.45328915	1.12937154	0.40848067
2.46338915	1.12937154	0.40848067
4.75647854	8.73880611	0.18583303
-0.23342146	8.73880611	0.18583303
6.21494646	10.81271017	8.78202726
6.56873405	7.27934747	9.54755214
4.69457008	2.65148217	9.42612721
1.58104650	7.30674514	9.56463292
6.86841955	0.19841161	9.81928031
9.77930336	2.40496748	9.38215091
2.53756577	10.28987655	7.19128223

-0.00957572	10.92531006	6.90831164
3.16713034	7.78589569	7.12739732
8.15704474	7.79117913	7.12825510
0.68138060	12.42115418	4.89693353
7.54631884	0.16004791	7.07453156
3.86688206	5.17856499	6.99456355
8.85732832	5.18134500	6.98988714
3.21590398	2.74116819	6.91257295
8.21114899	2.73635485	6.91637821
0.70321864	8.33255780	6.95047911
5.68275344	8.29365980	6.91535735
5.03101406	10.94725047	7.01673122
7.51819282	10.31403813	7.30532261
1.37361272	5.91275188	6.79455640
6.37350044	5.89444189	6.76957965
0.70213714	3.29250638	6.72842479
5.69005125	3.29660630	6.72515864
0.02726693	0.91299006	6.68464781
5.01000527	0.90277166	6.70510435
3.25820642	11.76350736	5.19581398
8.22247269	11.75943874	5.20701505
8.87545288	9.25484869	5.12180969
3.89509577	9.25395949	5.12418601
7.50545346	4.23200442	5.03321148
2.51743828	4.23843607	5.03652729
8.19998603	6.76743479	4.91172073
3.20561768	6.76815072	4.90989887
5.67770569	12.40984532	4.92109124
2.53140726	0.09218367	7.05295647
3.23855529	1.46724926	4.84656900
8.21923944	1.48804154	4.82398222
1.40352023	9.90306327	4.83048670
6.38945947	9.91839586	4.87981444
5.01125069	4.86131078	4.73260583
0.02324071	4.86161989	4.73214287
0.72378035	7.30084338	4.70229069
5.71651193	7.29387549	4.68478650
5.74624802	2.18967404	4.50826379
0.76536803	2.19611547	4.51005627
8.92724451	3.16928099	3.13275412
3.93734451	3.16928099	3.13275412
9.65447774	0.51179240	2.92767386
4.66457774	0.51179240	2.92767386
8.19081638	10.75315178	2.92137328

3.20091637	10.75315178	2.92137328
7.52427827	8.16568472	2.89047266
2.53437827	8.16568472	2.89047266
6.46140326	3.88992115	2.81003309
1.47150326	3.88992115	2.81003309
8.23615357	5.59719332	2.75910422
3.24625357	5.59719332	2.75910422
5.72548353	11.29866287	2.69921895
0.73558353	11.29866287	2.69921895
5.02271343	8.84247544	2.64073298
0.03281343	8.84247544	2.64073298
7.16234573	1.15467185	2.58495906
2.17244573	1.15467185	2.58495906
5.69094282	6.28061655	2.47308962
0.70104282	6.28061655	2.47308962
4.72644856	4.52631212	0.98044427
-0.26345145	4.52631212	0.98044427
8.98416265	2.08401219	0.94984236
3.99426265	2.08401219	0.94984236
7.49692293	12.16127468	0.88189072
2.50702293	12.16127468	0.88189072
8.92881242	7.14167817	0.77916237
3.93891242	7.14167817	0.77916237
8.23179647	9.65808525	0.74752367
3.24189647	9.65808525	0.74752367
6.50168782	2.71004334	0.73384591
1.51178782	2.71004334	0.73384591
5.78449336	0.24636792	0.66762456
0.79459336	0.24636792	0.66762456
6.40908241	7.83185195	0.60482946
1.41918241	7.83185195	0.60482946
7.18588982	5.31081574	0.60368013
2.19598981	5.31081574	0.60368013
5.68450729	10.28863881	0.50651002
0.69460729	10.28863881	0.50651002

# CO+OH (state1)

1.000000000000

9.97980022	0.00000000	0.00000000	
-0.76395801	12.66177369	0.00000000	
0.00000004	0.00000004	19.64039993	
H	C	O	Fe
2	41	6	80

Cart

4.32016727	6.67456447	9.28565410
1.20174563	11.33648932	7.96371084
3.42226985	11.96313710	7.19616037
7.18147014	7.45967704	8.59422868
9.29462125	2.38911829	8.34828153
5.96905815	11.26349213	8.49455383
4.62511801	2.66071793	8.22263839
1.19667923	8.14666531	8.70226138
9.15637016	9.33481800	7.26875385
2.23832329	4.29226692	7.12839517
7.18128250	4.26742173	7.19146040
8.44907529	11.96899866	7.15072049
7.16886107	8.27768292	5.53021043
-0.32543463	6.79814856	6.29696560
4.69227490	6.69719588	6.22021599
1.75113145	1.62663731	6.18140694
4.21756071	3.13908787	5.28249173
2.16137206	8.28992847	5.67675063
4.15816377	9.30545991	7.32830339
9.20105788	3.14501673	5.29634455
6.71789187	1.63959803	6.15735247
4.66669995	10.77494396	4.26256392
-0.31719165	10.80396586	4.27413781
6.71659233	5.67043045	4.00874217
1.73888515	5.71128609	4.03677987
7.17427426	12.35309771	3.63660084
2.19878945	12.34585429	3.63399973
9.22705445	7.20080811	3.31883057
4.22296947	7.20188181	3.30736495
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304

3.53758689	6.45708632	8.74160993
1.30395244	8.07097383	9.86272973
6.68187493	7.32219807	9.65736587
9.76075774	2.27813868	9.43162923
6.23941333	11.34494934	9.64978397
4.76669516	2.48832259	9.39652827
2.51179400	10.28239939	7.16849939
0.71836174	8.34041746	6.99855682
3.27239595	7.70377031	7.19514565
8.15824477	7.78601266	7.13542491
0.68705311	12.43258688	4.87907369
5.66976599	12.40593414	4.91870286
3.21309908	2.73514767	6.91213455
8.85263626	5.19465512	6.96344788
3.89718294	5.22869296	7.24864143
8.20540872	2.72931949	6.95251106
0.01178562	10.95395027	6.84338485
5.70445911	8.35753618	6.86216405
4.99056601	10.94466381	7.01622627
7.52355423	10.31883702	7.17452350
1.36747398	5.87519647	6.63602629
6.41612402	5.91114145	6.73276487
0.71148228	3.31539088	6.70188567
5.68263827	3.28817559	6.72248636
4.98920216	0.89660393	6.67941873
8.21747883	1.48718285	4.84495142
2.50837026	0.09112794	7.06526548
8.23183199	11.77753350	5.17014590
8.89151232	9.23384600	5.14921339
3.88510355	9.23487291	5.19277225
7.51479967	4.20345072	5.03815425
2.54195188	4.22912199	5.03468559
8.20953938	6.74681499	4.91405427
3.19019271	6.79850452	4.91917584
5.75036764	2.19026415	4.50499314
3.24309565	11.75409471	5.19048755
0.01599478	0.91400065	6.68993175
7.53619258	0.14014621	7.08102630
1.40609340	9.88656158	4.82424416
6.39486260	9.92422755	4.85877283
5.00239367	4.88468787	4.77647548
0.01840606	4.85182596	4.69156685
0.71559545	7.32843769	4.69747976
5.71956283	7.29143372	4.66868560

0.76889225	2.20001124	4.51373118
3.23822155	1.47239747	4.84401970
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CO+OH (state2)

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
2	41	6	80

Cart

-0.05137516	5.83602786	9.60389210
6.22970401	11.34794856	7.96137995
4.19453832	9.31762949	7.35030374
9.13066370	2.22062886	8.39880749
6.73869776	7.83412036	8.46893073
1.76065785	7.73224818	8.43434308
0.97700923	11.36089074	8.43221595
4.58999276	2.56268294	8.21412085
9.18254837	9.28667301	7.35574171
4.20590208	3.13659923	5.29639265
7.25251312	4.30228789	7.11725607
-0.31615591	10.79806821	4.26729747
8.42576226	11.92908698	7.15528969
-0.37205924	6.70806778	6.28964804
4.64718089	6.80178382	6.30917201
1.74080590	1.59934823	6.20400275
6.72103759	1.62771809	6.15317295
2.16716020	8.27268233	5.56946958
7.16164101	8.27590621	5.58163850
9.20578250	3.13813510	5.27723525
2.21969381	4.27914890	7.19600977
4.23674200	7.20003493	3.33026080
7.18292918	12.34741525	3.63142242
6.72681590	5.67975581	4.02602405
1.71797068	5.67312364	4.01336655
3.47193697	11.96918366	7.16607859
2.19021907	12.35169368	3.64121623
9.22212075	7.19950860	3.33138089
4.67639766	10.81057288	4.26497160
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344



4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
9.23880565	5.30962127	9.15415795
4.79708297	2.39877617	9.37768975
9.66661542	2.01416794	9.42818782
6.61574293	7.69899543	9.64167004
1.62539121	7.55441590	9.60821856
1.15429244	11.42678448	9.60727953
2.54968907	10.29939141	7.20976578
0.69938514	8.29960761	6.91512784
3.16217722	7.81645119	7.12572238
8.14889396	7.79446827	7.13665765
2.54844510	0.08745420	7.09661381
8.22533766	1.48425094	4.84036850
3.87935595	5.18643784	6.98183738
8.89094649	5.27434790	7.40562036
3.19933802	2.72536179	6.92260193
8.20867005	2.71402376	6.94155648
0.00878915	10.91798690	6.94656867
5.70134188	8.34285422	6.92656860
5.01363840	10.93776452	6.88234202
7.51691398	10.27855901	7.19860548
1.37792934	5.90383050	6.77502901
6.34194731	5.88496583	6.72226735
-0.00155483	0.88601566	6.68961428
5.69138102	3.31019476	6.73935890
0.68741628	12.41221937	4.91352766
5.00536234	0.91798511	6.69293076
0.71949293	3.30608523	6.68096929
3.24761135	11.77200859	5.18111287
5.70607356	7.29258794	4.69178658
1.40581379	9.90753570	4.85800643
7.54084116	4.21930613	5.07278265
2.52202842	4.22211274	5.04049704
8.18642840	6.75701452	4.91414162
3.20722760	6.74421985	4.92120670
5.67697005	12.43430491	4.89215636
7.52824998	0.12400955	7.07281569
3.22967116	1.47106140	4.85003574

8.23673479	11.76737536	5.17815830
8.88237406	9.23529749	5.11946885
6.39932709	9.89938352	4.82970907
5.01885208	4.84366778	4.72349934
0.00288767	4.87847112	4.78009471
0.72056377	7.27190076	4.69622178
3.88367424	9.24823408	5.10408779
5.75984333	2.21388928	4.51722174
0.76757598	2.18904922	4.51937233
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943

1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CO+OH->COOH

1.000000000000

9.97980022	0.00000000	0.00000000	
-0.76395801	12.66177369	0.00000000	
0.00000004	0.00000004	19.64039993	
H	C	O	Fe
2	41	6	80

Cart

0.09435164	4.77861486	9.47002762
6.22982574	11.33148355	7.97577846
4.18038318	9.30973463	7.38909528
9.29104355	2.82288993	8.54946445
6.78838561	7.57055434	8.42364105
1.75844120	7.51434120	8.39364144
0.97489250	11.35250575	8.45383745
4.59737851	2.58503346	8.21338130
9.17015510	9.29018569	7.37214923
4.21469997	3.13854263	5.28524127
7.22084935	4.29128698	7.12134927
-0.31785046	10.80234858	4.26403520
8.42482534	11.94870848	7.17114045
-0.34722593	6.73911331	6.25890583
4.64504179	6.79793011	6.30257607
1.74882852	1.60755482	6.18926224
6.74590331	1.64158095	6.17614867
2.16790036	8.29144269	5.58266261
7.15601078	8.29004791	5.58171652
9.20779657	3.13494522	5.27978023
2.22013987	4.28442530	7.16781337
4.23773969	7.20025198	3.32707984
7.18368949	12.35099165	3.63835291
6.72688075	5.69013293	4.01910886
1.72648888	5.69346471	4.01370474
3.46487876	11.96794328	7.16764886
2.19340436	12.34806308	3.63970766
9.22198329	7.20066804	3.32028416
4.67376262	10.80893018	4.26281313

5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
9.24694573	4.54500823	8.99526229
4.76954431	2.42157965	9.38338596
-0.05104600	2.20496806	9.34702683
6.57561748	7.33431937	9.57070150
1.57298644	7.23288930	9.54128835
1.17777489	11.46422709	9.62159145
2.53807122	10.30052092	7.20895352
0.69439600	8.30013753	6.93270225
3.16452059	7.80111642	7.13191256
8.15138074	7.79010240	7.12395411
2.54435116	0.09499619	7.08744288
8.22477472	1.48606202	4.85230906
3.88907417	5.18169425	6.98141985
8.88245099	5.26493896	7.22017863
3.21031724	2.72964802	6.90891670
8.24333407	2.73914438	6.94870582
0.00301451	10.92391824	6.97522570
5.69309324	8.33217695	6.94575240
5.00113502	10.92234807	6.90824867
7.50993550	10.28591704	7.18211774
1.39088233	5.91560169	6.75682788
6.34478798	5.90389862	6.77535305
-0.00663655	0.88505262	6.63254397
5.69666907	3.29452370	6.73284727
0.68990619	12.41153572	4.90895922
5.01878840	0.90923560	6.69447608
0.73224062	3.29539195	6.64664750
3.24848325	11.76749552	5.18472689
5.70802051	7.29698297	4.69846477
1.40373765	9.91258088	4.85379777

7.53684617	4.23550114	5.07121189
2.52970445	4.23492991	5.03461149
8.19035992	6.76868813	4.90344883
3.20809565	6.76524069	4.91499946
5.67579029	12.42688385	4.89575322
7.51629930	0.10709779	7.06750011
3.23812392	1.46594383	4.84630379
8.23394866	11.76327833	5.18027662
8.88237929	9.24495972	5.12089518
6.39256848	9.90022034	4.82747807
5.02440415	4.85400321	4.72866737
0.00993144	4.87913900	4.75384687
0.72571553	7.29961166	4.68700898
3.88558095	9.25518662	5.12155551
5.76253308	2.20286869	4.51536136
0.77512547	2.19016946	4.49791015
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235

8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# COOH (state1)

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
2	41	6	80

Cart

0.03164937	4.28188808	9.72804657
6.22812813	11.32928654	7.98286961
4.18379521	9.30962225	7.39309415
9.29962163	2.89917869	8.50411795
6.80531765	7.55501449	8.42432933
1.77434337	7.49407609	8.39390871
0.97457927	11.37826352	8.45550192
4.58748678	2.59440203	8.20682387
9.17377154	9.29517324	7.38301271
4.21221064	3.14073405	5.27620388
7.20107648	4.28226304	7.13647945
-0.31639290	10.81052198	4.26802360
8.42193366	11.94556147	7.17261003
-0.33909199	6.75476375	6.27646776
4.65351887	6.79150970	6.30452848
1.75300657	1.59498261	6.17707019
6.74056315	1.63152277	6.16287858
2.17136055	8.29807777	5.58810318
7.15951786	8.29655518	5.58532545
9.19581886	3.13728770	5.25949184
2.22362835	4.28561939	7.15641028
4.23863111	7.20096321	3.32812411

7.18450449	12.34976093	3.64187641
6.72696391	5.70431548	4.01301934
1.73061055	5.70512604	4.01332591
3.46792276	11.96777659	7.16994953
2.19076329	12.34578184	3.64402908
9.22433162	7.20113045	3.32186320
4.67492685	10.80959146	4.26359089
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
9.24639356	4.19215862	9.10989308
4.75564114	2.43269893	9.37741264
0.06271443	2.05170386	9.02610561
6.58564656	7.33918538	9.57708407
1.57272654	7.21157097	9.53786843
1.16513805	11.47316415	9.62696173
2.53923493	10.29994861	7.20771784
0.70101821	8.30611751	6.94092797
3.17227175	7.79870688	7.13426128
8.16003392	7.79312902	7.12715474
2.54838281	0.09122291	7.09791675
8.22858821	1.47665394	4.84712569
3.89540738	5.17940440	6.98683454
8.88190144	5.22560272	7.14463775
3.20751743	2.72705253	6.89495856
8.21813472	2.74555675	6.91076458
0.00298095	10.92401455	6.97722167
5.69696598	8.33105725	6.94945671
5.00406356	10.92155383	6.90810241
7.50990246	10.28603318	7.18229200
1.39201426	5.91413600	6.76001105
6.36253973	5.91376408	6.79389477
-0.00089790	0.90259939	6.71916745

5.68765541	3.29239931	6.72668419
0.68866452	12.42213106	4.91916600
5.01569107	0.90813228	6.68911408
0.72733897	3.30505017	6.62635919
3.25010302	11.76675147	5.18582797
5.71257314	7.30040629	4.70098606
1.40428636	9.91681798	4.85303297
7.52816829	4.25409229	5.05952509
2.53100920	4.24545283	5.03094135
8.19643222	6.77569820	4.90661649
3.21036151	6.77341198	4.91481652
5.67397496	12.43061895	4.89508588
7.51141556	0.10371449	7.07166239
3.23993952	1.46250911	4.83862942
8.23995570	11.77497676	5.18913328
8.88513231	9.25175029	5.12450085
6.39634174	9.90520824	4.82858029
5.02460584	4.86249335	4.73289560
0.01002180	4.88295810	4.73988425
0.72580242	7.30715785	4.69113316
3.89086294	9.25626956	5.12492151
5.75946072	2.20349867	4.50971943
0.76826921	2.18341880	4.50036375
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425



-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# COOH (state2)

1.000000000000

9.97980022	0.00000000	0.00000000	
-0.76395801	12.66177369	0.00000000	
0.00000004	0.00000004	19.64039993	
H	C	O	Fe
2	41	6	80

Cart

5.38342663	11.35914282	10.76637434
1.22123881	11.35135590	7.97233576
4.20459131	9.32691293	7.40844379
5.53567763	11.51789412	8.88066098
1.78307931	7.67653853	8.44106124
6.76260199	7.69196010	8.44636596
4.62863442	2.62605353	8.21551666
9.58326589	2.58171284	8.21626906
9.18392068	9.30678885	7.37891399
2.19286863	4.27733642	7.20782367
7.18449682	4.26608192	7.20593680
2.20023439	12.34730666	3.64211695
8.42054084	11.94195183	7.13954559
-0.32791892	6.78054023	6.31252129
4.65608493	6.79407065	6.31080064

1.74440210	1.63737341	6.17879520
4.20915085	3.14307205	5.29247042
2.17922583	8.29562184	5.59229306
7.16200802	8.29819226	5.60015419
6.73707623	1.61501982	6.15660722
9.19533363	3.14436986	5.29678506
4.67503650	10.81033266	4.25722499
-0.31142187	10.81731462	4.26560138
6.72244142	5.70410124	4.01253548
1.73568853	5.70364104	4.01141935
7.17383405	12.35110731	3.64573728
3.43756780	11.98004329	7.20743814
9.22919206	7.20389565	3.34005639
4.23955900	7.20106606	3.33355117
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
5.06622227	10.88533873	9.96121208
9.73995122	2.39470894	9.38567980
6.24801641	12.55492984	9.05964484
1.62309266	7.48393884	9.60594931
6.62732573	7.52981408	9.61824428
4.74495425	2.43525212	9.38845760
2.51640675	10.29852292	7.20126329
0.00558955	10.92451062	6.88861750
3.17972789	7.82001050	7.13843176
8.16900189	7.80037237	7.13493167
5.75021311	2.18694041	4.50771436
7.52273774	0.12784385	7.13687519
3.86410598	5.18989497	6.98992774
8.84855657	5.18344741	6.98934379
3.21060935	2.74458778	6.91799033
8.20359259	2.73915130	6.90941109

0.71330453	8.33615546	6.94285499
5.69879931	8.33085836	6.94673763
4.99577389	10.97070637	7.11772830
7.52631100	10.25669089	7.06042287
1.38644313	5.91648942	6.79469199
6.36479925	5.90409084	6.78945009
0.70107895	3.28471219	6.73963484
5.68675408	3.28973854	6.72782758
0.69697185	12.42335908	4.89287785
4.98267108	0.92150164	6.65784118
3.25673177	11.75679740	5.20910841
8.24557174	11.78550449	5.17115300
8.89152185	9.22513996	5.06024005
3.90305277	9.25844906	5.12914644
7.50333833	4.23743691	5.03537384
2.51589485	4.23925922	5.03898933
8.19611564	6.76133500	4.92093710
3.21156431	6.77061705	4.91912028
5.69107275	12.39837257	4.94335510
3.23239812	1.47309575	4.84624689
0.76002195	2.19305126	4.51613863
0.01497620	0.89400399	6.68397248
1.40689740	9.89689803	4.82455934
6.39216407	9.90291645	4.82853664
5.01216550	4.86083059	4.73118282
0.02622546	4.86007057	4.73826587
0.72793021	7.29492454	4.70400677
5.71677634	7.29714834	4.70333361
8.21960639	1.47488083	4.84146909
2.51649714	0.09827927	7.06572168
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899

5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for COOH+C<sub>Cv</sub>->CO<sub>2</sub>+CH<sub>Cv</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
2	41	6	80

Cart

4.43344423	9.73153197	8.93232744
1.25895986	11.31710919	7.95190700
4.20257204	9.31011953	7.73078348
5.49827132	11.39184779	8.83124216
1.69909035	7.67022765	8.43535574
6.82953685	7.61832858	8.44988626
4.63396854	2.66254540	8.22238225
9.58193716	2.56134181	8.21537030
9.19105311	9.30877472	7.37612582

2.20017604	4.27820002	7.20231391
7.18924738	4.27007841	7.19893927
2.19152344	12.35072487	3.63582297
8.40819986	11.94606957	7.14264039
-0.32794801	6.78453487	6.30132068
4.64874168	6.82487332	6.33756285
1.74339463	1.62775439	6.18427127
4.21172159	3.14361777	5.29372957
2.18247452	8.33089539	5.62944092
7.15863571	8.30434068	5.61582763
6.74219583	1.60287661	6.15518597
9.19923183	3.15190052	5.29905171
4.68753332	10.83319237	4.28519572
-0.31908544	10.82220044	4.26955512
6.72276487	5.70948248	4.01615621
1.73851982	5.71168093	4.01477516
7.18100217	12.35191657	3.63597218
3.46202236	11.95551465	7.13666869
9.23025843	7.20256532	3.34060984
4.24028294	7.20558755	3.35348731
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
4.99981902	10.66058246	9.73899444
9.74723372	2.37547999	9.38246543
6.18716318	12.44838696	9.03691749
1.66080053	7.45204449	9.60551582
6.61146091	7.41819722	9.60202845
4.73874624	2.49693829	9.39844211
2.54917880	10.27818884	7.14276452
0.00196369	10.93482142	6.89092731
3.19995598	7.85879091	7.16371062
8.17191248	7.79533083	7.13568291

5.75372330	2.19884741	4.50507570
7.49571621	0.11077747	7.17162173
3.87875931	5.18566383	6.97788941
8.85592769	5.18186339	6.98185522
3.21274033	2.74375222	6.91706127
8.20246057	2.73537290	6.91121741
0.71928761	8.33224075	6.95216040
5.68022717	8.36267441	6.98073878
5.03264154	10.94754906	6.92283401
7.52583285	10.25195597	7.08193575
1.38199121	5.90891025	6.79137541
6.36376502	5.90852236	6.79161278
0.70308348	3.28426931	6.74014213
5.68933152	3.29335812	6.72623860
0.68436208	12.43190241	4.89066065
4.98104911	0.92215659	6.64324643
3.24977984	11.76909916	5.17141864
8.23059909	11.77908249	5.17715435
8.89154343	9.22893672	5.07431182
3.88040707	9.22733223	5.02387583
7.50539905	4.24178675	5.03607823
2.51922946	4.24191423	5.03952138
8.19402648	6.76749507	4.92053869
3.20044004	6.77281684	4.94472839
5.69574870	12.43534984	4.91258199
3.22693151	1.48235615	4.84289673
0.76307309	2.19896085	4.51811146
0.01428439	0.89158048	6.69313664
1.40314186	9.90180595	4.79784714
6.39265696	9.89591152	4.81151420
5.01301158	4.86096402	4.72191908
0.02867740	4.86499201	4.73389486
0.73034596	7.30933428	4.70231285
5.70832155	7.29882849	4.72252471
8.23140834	1.47984142	4.84343759
2.53057327	0.08200067	7.05180513
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265

6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CO<sub>2</sub>+CH<sub>Cv</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
2	41	6	80

Cart

4.18715622	9.34713978	9.09705605
1.26961172	11.28820701	7.91935646

4.20606355	9.23568690	7.99803973
5.44148155	11.56848796	9.08151341
1.84816453	7.59541305	8.44810347
6.72731911	7.76901035	8.48167737
4.63845585	2.61086334	8.21416250
9.57236782	2.57331017	8.21558535
9.19175696	9.29581640	7.37645014
2.20263995	4.27064001	7.19567027
7.18154423	4.25595758	7.19916622
2.20341085	12.34673625	3.64807325
8.41242243	11.92132695	7.13709214
-0.32046737	6.77382490	6.33272911
4.65355730	6.82657515	6.31838643
1.74868554	1.61282559	6.19101139
4.21254966	3.13824463	5.28948291
2.20108784	8.33546372	5.64788372
7.15541366	8.29305110	5.62496524
6.74329759	1.58466124	6.15435210
9.19753365	3.13974780	5.29457192
4.68778059	10.80773925	4.26220641
-0.31371738	10.80897992	4.26826591
6.72476884	5.70476563	4.01695328
1.73600401	5.70698966	4.01490977
7.17713353	12.34814220	3.64532375
3.46570460	11.90684058	7.17972049
9.23364131	7.20283230	3.35655073
4.24319900	7.21008013	3.35475508
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
4.97446273	11.03328002	10.06330014
9.73603348	2.40312963	9.38384486
6.15939310	12.63939054	8.97922889



1.64046784	7.39224303	9.60269934
6.67540307	7.57406040	9.65383273
4.72414597	2.41839775	9.38689026
2.57484728	10.21691704	7.15751003
0.00611153	10.90839554	6.87901372
3.21600342	7.82603099	7.15316000
8.16299657	7.79478114	7.14874625
5.75307350	2.18097260	4.50811736
7.50689496	0.08758422	7.16380926
3.88340286	5.18465536	6.98256349
8.84924003	5.17278006	6.98862180
3.21494690	2.73267790	6.91375300
8.20214534	2.72621882	6.90443074
0.72887654	8.32107164	6.96153872
5.66508223	8.37178496	6.99465967
5.01540254	10.86164583	7.10773481
7.51822010	10.23597962	7.09228560
1.39941386	5.91643224	6.80472184
6.36096570	5.89789544	6.78448456
0.70652763	3.27328466	6.73709840
5.68790738	3.26669619	6.72503378
0.69450783	12.42006321	4.89232412
4.99268603	0.87629494	6.67011599
3.26116989	11.72493087	5.19948538
8.24160434	11.76699825	5.17250490
8.89053078	9.21547608	5.06791635
3.88679382	9.20166412	4.99405471
7.50495665	4.23513954	5.03700159
2.51779283	4.23540595	5.04152032
8.19644772	6.76003649	4.93366272
3.20228144	6.75744330	4.92946525
5.69031525	12.39544512	4.94066052
3.23896424	1.46131734	4.85023677
0.76620566	2.18936293	4.51878237
0.01868092	0.87439498	6.69002543
1.40474854	9.88286833	4.78268102
6.38974086	9.88836265	4.82709166
5.01540754	4.85568347	4.72589407
0.02995881	4.86102812	4.74277425
0.73391501	7.30751471	4.71473074
5.71682896	7.29454929	4.72321730
8.22777251	1.46007982	4.84529265
2.54501465	0.05833612	7.04594007
8.92724419	3.16928101	3.13275409

3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# COOH (state3)

1.000000000000

9.97980000

0.00000000

0.00000000

-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
2	41	6	80

Cart

9.66699867	2.49752041	10.23942988
1.22884604	11.30068476	7.98578563
4.17511132	9.27854628	7.37947720
-0.07589258	3.28451499	8.51398194
1.79655845	7.53772025	8.42455317
6.79921467	7.47833274	8.41730062
4.58278852	2.57949209	8.22441545
5.98540487	11.34007432	8.43080480
9.16837021	9.26881689	7.39107294
2.19652826	4.25697285	7.15686702
7.19168919	4.26141158	7.13701929
2.19644173	12.34480142	3.63459561
8.44919719	11.93628669	7.15773430
-0.35590244	6.70317372	6.28455058
4.64911577	6.75352456	6.29707032
1.72918042	1.61662898	6.18636435
4.20307855	3.12819050	5.29955560
2.16454465	8.26594627	5.58712421
7.15720430	8.27570011	5.59220127
6.70448183	1.58436614	6.16838390
9.21272488	3.10326388	5.28066390
4.67001124	10.78621735	4.26335566
-0.31703973	10.77682446	4.25665755
6.72703726	5.68030984	4.01688356
1.72192032	5.67363680	4.01577595
7.18198657	12.33896292	3.63742716
3.42789232	11.93040773	7.17613431
9.22121546	7.20022542	3.33061217
4.23651955	7.20022000	3.33190863
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183

7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
0.03419304	2.22899144	9.35664438
6.18916651	11.42338977	9.60262295
9.46587901	4.38063254	9.00101595
1.60878633	7.31127360	9.58071344
6.58420073	7.27316632	9.57235169
4.71843834	2.40955189	9.40056938
2.51125527	10.26411529	7.19107406
0.00870472	10.88622438	6.90697925
3.16691816	7.77267391	7.12988172
8.15944102	7.76082702	7.12978279
5.75108558	2.18699522	4.51358045
7.53073381	0.07015974	7.06760951
3.86402073	5.16076095	7.00671136
8.87275535	5.19876385	7.22134599
3.20170764	2.70604416	6.91628020
8.18427930	2.67355092	6.89503107
0.69699384	8.28969009	6.94789440
5.68930802	8.29193379	6.95125238
4.98723410	10.90278712	6.96582040
7.52856927	10.26588201	7.19344727
1.39251110	5.90500874	6.76594095
6.34516150	5.88752431	6.81525965
0.68105124	3.27625892	6.73081825
5.68185859	3.25886624	6.73806513
0.68450641	12.39736648	4.88639481
4.97716622	0.87954201	6.69135233
3.23962531	11.74693582	5.18545870
8.23269452	11.73649842	5.17313500
8.87527351	9.22701752	5.12302591
3.89102193	9.22527709	5.11996686
7.52724373	4.22667210	5.08530162
2.50893683	4.20954525	5.04248254
8.18742448	6.75335210	4.90927978
3.20376558	6.74390364	4.91323246
5.66870793	12.40467133	4.90866625
3.22721370	1.46041515	4.84218047
0.77212169	2.18311572	4.50369314
0.00315339	0.85859350	6.61044670
1.40346447	9.87844362	4.83610287
6.38826199	9.88933575	4.84442064

5.02556891	4.84419671	4.75026553
0.01134072	4.85795646	4.79107418
0.71734611	7.27970753	4.69816030
5.71006301	7.28344926	4.70075046
8.22117032	1.45066578	4.83814894
2.50690301	0.06535402	7.05625192
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013

5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for COOH->CO<sub>2</sub>+H

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
2	41	6	80

Cart

8.88765844	1.40234346	8.05905881
1.23211253	11.31666517	7.97254853
4.18085684	9.30414785	7.36526530
9.69938442	3.36002647	8.46207644
1.79065940	7.58447928	8.42584290
6.79607692	7.49938344	8.40938255
4.61133088	2.61794775	8.21830350
5.97764501	11.29100580	8.46940917
9.17558472	9.27867926	7.37933031
2.20255366	4.26567227	7.16546798
7.19509273	4.29086580	7.10172255
2.19709375	12.34705608	3.63401932
8.46916562	11.92029416	7.14249721
-0.35572870	6.71685262	6.28334445
4.65120973	6.78222069	6.29881165
1.72759126	1.62824992	6.18537483
4.20470810	3.13713545	5.28995603
2.16833265	8.27841187	5.57924192
7.16166570	8.28568146	5.58455765
6.71020499	1.60826327	6.14910469
9.21156683	3.11585955	5.28511228
4.67397575	10.80383781	4.26435020
-0.31420405	10.78972761	4.25993989
6.73172701	5.68166456	4.02062323
1.72451348	5.68313488	4.01354844
7.18203953	12.34538810	3.64071268
3.43886465	11.95557171	7.18487884
9.22190158	7.20036093	3.32725996
4.23768087	7.20002961	3.32730191
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742

1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
9.23566199	2.31409684	9.09892829
6.22197033	11.38658707	9.62766713
9.58958144	4.54503290	8.96493035
1.61490611	7.35948153	9.58043392
6.56520366	7.27824265	9.55637624
4.76696819	2.45837236	9.39050950
2.52292688	10.28767186	7.18703107
0.02794403	10.88727041	6.88204113
3.16926794	7.79640079	7.12582994
8.16253123	7.77442893	7.12707471
5.75186724	2.19247999	4.50644862
7.58328486	0.14201443	7.10630689
3.86774145	5.17806939	6.98648202
8.88461932	5.21846432	7.23621724
3.20416495	2.72247277	6.92106489
8.20163823	2.68775819	6.93915120
0.70361033	8.30301412	6.93830811
5.69335917	8.31674417	6.94006610
5.00618986	10.93759827	6.98717703
7.53816434	10.27559713	7.18457984
1.40137085	5.91477652	6.76052617
6.34493498	5.90905020	6.78896666
0.68980083	3.28657181	6.72402453
5.67972749	3.28508717	6.71539998
0.68899260	12.40895163	4.88419079
4.99092917	0.89964734	6.68985123
3.24553407	11.76199587	5.18843813
8.24019290	11.74935040	5.17099193
8.87654366	9.23537679	5.11521849
3.89570904	9.24427680	5.12194963
7.53780791	4.22914209	5.08962424
2.52043495	4.22316811	5.03542656
8.19078022	6.76062306	4.90733219

3.20699822	6.75468215	4.91312488
5.67984378	12.41535466	4.92262987
3.22903113	1.47030388	4.84636017
0.76399858	2.18330623	4.50649405
0.01841158	0.86500732	6.64461643
1.40851809	9.88817226	4.82635265
6.39246308	9.90486103	4.84592804
5.02510678	4.85171926	4.72863903
0.01491055	4.86518865	4.77969980
0.71996169	7.28616548	4.69565993
5.71227234	7.29324826	4.69576031
8.22498608	1.46544913	4.84722857
2.51775693	0.08519379	7.05789382
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589



1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CO<sub>2</sub>+H

1.000000000000

9.97980000	0.00000000	0.00000000
-0.76395804	12.66177393	0.00000000
0.00000004	0.00000004	19.64040000

H	C	O	Fe
2	41	6	80

Cart

8.59901612	1.37456055	7.84334952
1.21326793	11.30609906	7.97464498
4.17636586	9.29697228	7.37927821
0.02890240	3.55670682	8.77111188
1.77459772	7.57059547	8.41810213
6.79510654	7.45637551	8.39759111
4.60568820	2.63033479	8.21185906
5.96200280	11.34694191	8.46802208
9.17007501	9.27032279	7.37851092
2.20559667	4.27671653	7.18185386
7.19328468	4.26367793	7.10802842
2.19328600	12.34658154	3.63851717
8.45377880	11.89860958	7.12792004
-0.35602393	6.70382966	6.27697310
4.64668234	6.77589550	6.28848675
1.72016990	1.61189503	6.19592909
4.19627197	3.14006471	5.27530121
2.16618634	8.28257718	5.57856228
7.15951060	8.28846652	5.58693957
6.67699200	1.56495949	6.13365160
9.19818544	3.12880774	5.29697527
4.66974140	10.80622070	4.26708043
-0.31280275	10.79797428	4.26257787
6.72554420	5.69168329	4.01657182
1.72200238	5.68562911	4.01180215
7.17544830	12.33980915	3.63424941

3.42508166	11.94964012	7.19318732
9.22066330	7.20119155	3.32292497
4.23523046	7.20041927	3.32179810
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
0.47158542	2.62834379	9.42262619
6.18799829	11.42560813	9.63214107
9.42097068	4.65306201	9.02558374
1.59753596	7.34170153	9.57230844
6.55605143	7.23958646	9.54547867
4.74977688	2.47829728	9.38552170
2.51487824	10.27940052	7.19621841
0.01926575	10.87855518	6.87451311
3.16244197	7.79210960	7.12479183
8.15773830	7.76677912	7.12189697
5.74433008	2.19530219	4.50093060
7.57352386	0.11836602	7.12804302
3.86665688	5.18123351	6.99505088
8.87319567	5.17816670	7.18593977
3.19675541	2.72890705	6.91025890
8.13233696	2.66043786	6.87295743
0.69656780	8.29841206	6.93291314
5.68404484	8.30702969	6.94074025
4.99123797	10.93012240	6.98931637
7.52286239	10.25892004	7.17141727
1.39902206	5.91603132	6.75741931
6.34281159	5.89714190	6.78836663
0.68421955	3.28890499	6.77699765
5.66052466	3.28452724	6.70469763
0.68495907	12.42192244	4.89321265
4.95905590	0.89928298	6.68878528
3.23780201	11.75964126	5.19397977

8.23710678	11.75950067	5.16976987
8.87389780	9.23443405	5.10096204
3.89343928	9.24349683	5.12040282
7.52651210	4.23814496	5.06899304
2.50639989	4.22514504	5.04297518
8.18965831	6.76238226	4.90404311
3.20339603	6.75853554	4.90848824
5.67273736	12.41312237	4.92654994
3.21854977	1.47075927	4.84398250
0.75054167	2.18844242	4.53186323
-0.00867734	0.87650560	6.69921181
1.40523741	9.89222960	4.82625551
6.38837956	9.90646098	4.84820605
5.01227270	4.86212572	4.73163592
0.00929159	4.86713437	4.77987314
0.71936318	7.29245189	4.69043850
5.71083338	7.30034676	4.69222816
8.21599708	1.45636070	4.81836721
2.50174995	0.07883338	7.07540176
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071

2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# C<sub>Cv</sub>+CH<sub>2</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	41	4	80

Cart

1.09144800	10.61388373	9.33561119
1.28865803	12.31859452	8.90737584
6.23838558	11.33134896	7.96057078
1.18039521	11.27673069	8.45835435
4.60349101	2.61814770	8.22288996
9.59901900	2.59386510	8.21285600
4.17177203	9.31077546	7.39627184
6.82364527	7.57502667	8.43670546
1.74816888	7.62572243	8.40734586
9.19421045	9.29935189	7.36585338
2.19246154	4.25978008	7.21096567
7.17840645	4.26622411	7.20682077
3.47897297	11.95833219	7.16784026
8.44981191	11.95978402	7.19107489
-0.33180838	6.76296842	6.28763366
4.65155989	6.77923250	6.31402910
1.74967927	1.61021877	6.16825055
6.73068585	1.62317223	6.17642252
2.17147350	8.28558061	5.56994845

7.16235518	8.28354008	5.59637304
9.19488278	3.14073502	5.29339633
4.20249452	3.13632844	5.29456114
4.67342109	10.80342895	4.26611574
-0.31666066	10.79759695	4.25899182
6.72218921	5.70026992	4.01217118
1.73350742	5.69493947	4.00947284
7.18229078	12.34705978	3.63858802
2.19324268	12.34571971	3.64177982
9.22707015	7.20174316	3.32675250
4.23984592	7.20101786	3.33569732
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.60361897	7.42048474	9.57553981
4.72668979	2.44489956	9.39907285
9.72436838	2.39497053	9.38390831
6.59446257	7.38838668	9.59023056
2.52397304	10.33125893	7.30326362
0.01414593	10.93483115	6.97025437
3.16712976	7.80994927	7.12150424
8.16785700	7.78880112	7.13162234
0.68598693	12.40962897	4.90717088
7.52784839	0.08927183	7.05580348
3.85990747	5.17864497	6.99858614
8.84716926	5.17888943	7.00240783
3.20653376	2.72929316	6.91664048
8.19485181	2.73126861	6.91524622
0.70342051	8.30469551	6.92013356
5.69533056	8.33056044	6.96008730
5.00540799	10.90640924	6.90373793
7.52957708	10.28806859	7.19167261
1.37702212	5.89374151	6.79387026

6.36537870	5.90757456	6.80725104
0.69415571	3.28107093	6.73650763
5.68343369	3.28257237	6.73899447
0.00922496	0.90407081	6.67394380
5.00587614	0.90242356	6.69527284
3.24356903	11.75515746	5.19287713
8.23567568	11.76115155	5.18701590
8.88552645	9.24264841	5.12319571
3.89143918	9.24489766	5.10981597
7.50363125	4.23754887	5.04218033
2.51490322	4.23263151	5.04142025
8.19775261	6.76532155	4.90999733
3.20922217	6.75852699	4.91602005
5.67431276	12.41619290	4.89653330
2.52770950	0.07605989	7.07719933
3.23514225	1.46191763	4.84651467
8.22000356	1.47133905	4.84372681
1.40244404	9.91854665	4.87145402
6.39582374	9.89232719	4.83111848
5.01386911	4.85618356	4.74119048
0.02242623	4.85983357	4.74231715
0.72756292	7.28878681	4.68956031
5.71343289	7.29113823	4.71014763
5.74860331	2.18989295	4.51682238
0.76118260	2.19067702	4.51370867
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970

0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for  $C_{cv}+CH_2 \rightarrow CCH_2_{cv}$

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	41	4	80

Cart

0.39059981	10.79044388	8.80388866
1.06989406	9.26310089	9.30874347
6.23586445	11.30221672	7.97190111
0.87102559	9.85308914	8.40428152
4.59507110	2.60284073	8.22807918
9.60211249	2.61611956	8.21096844
4.16864007	9.27806950	7.41755503
6.77101071	7.61288323	8.43675611
2.06555143	7.04894633	8.40585405
9.21989283	9.31969101	7.55870281
2.18459033	4.26265601	7.17599875
7.18514551	4.26267454	7.20479422
3.38821936	11.90755166	7.22238814

8.42262424	11.96668830	7.14562110
-0.31688751	6.78036400	6.32266970
4.67986432	6.75302909	6.28457915
1.73077071	1.64515781	6.14232588
6.71773004	1.60899512	6.18579613
2.17757282	8.28704838	5.60592270
7.17876414	8.31488344	5.62628127
9.18854256	3.13834158	5.28856457
4.20822487	3.14869287	5.30162024
4.66478264	10.79651778	4.26546467
-0.31246798	10.83019524	4.27534645
6.72976337	5.71072349	4.01464586
1.73528112	5.70352304	4.01564884
7.17242245	12.34728569	3.64026554
2.19806718	12.34859066	3.64029759
9.23275540	7.20627952	3.35076123
4.24104221	7.20288681	3.33275589
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.73728583	6.93935166	9.54887373
4.72686985	2.43242842	9.40404808
9.73016474	2.43711487	9.38686551
6.64377651	7.40960635	9.60614398
2.49554605	10.23332745	7.23250321
0.00249016	10.95895871	6.82898504
3.22234487	7.74079095	7.13184901
8.20099751	7.83081172	7.16211844
0.68803045	12.43998574	4.87774847
7.49456516	0.07131691	7.06751919
3.87068970	5.17539585	7.01859343
8.86205649	5.17737134	6.99256404
3.20764554	2.72940890	6.91729107



8.18885199	2.72637072	6.91481122
0.70405723	8.36548880	6.94953895
5.71393960	8.32422131	6.96799174
4.96001140	10.90699697	6.93859951
7.52688826	10.27368234	7.16231421
1.40598458	5.92049160	6.81991682
6.39420804	5.90924566	6.79800230
0.68393334	3.28617183	6.72442821
5.68501336	3.26875637	6.74611606
0.00981734	0.90479524	6.67433055
4.98723043	0.86153942	6.72317020
3.22891933	11.74100791	5.20212455
8.22806668	11.77707889	5.16834416
8.88847337	9.23497902	5.06427832
3.88680181	9.24197053	5.13014425
7.50615969	4.24240472	5.04227176
2.51557666	4.23692906	5.04202053
8.19788428	6.77241368	4.93815539
3.21197029	6.76740128	4.90702885
5.65513791	12.41834157	4.90500040
2.52354920	0.11638350	7.01660054
3.24067697	1.48221428	4.83536372
8.20770257	1.47360931	4.84169126
1.40157757	9.90050733	4.81569000
6.39523199	9.90253564	4.83017523
5.01978530	4.86682664	4.75070261
0.02183584	4.85902823	4.72827098
0.73037396	7.28604318	4.72152092
5.72605627	7.31355403	4.70388338
5.74600571	2.19104486	4.52167544
0.75367134	2.19789234	4.50339737
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899

0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# C<sub>v</sub>+CH<sub>3</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	41	4	80

Cart

1.98439235	10.66705522	9.19559418
1.49281042	12.37214519	9.12288747
6.23885777	11.29956068	7.95583242
0.27425784	11.09396426	9.24997880
1.22426902	11.35101169	8.75580851
4.62353252	2.61109397	8.22421598
9.62266067	2.62585489	8.22639216

4.18200819	9.29396190	7.37753711
1.78659685	7.48821451	8.39471036
6.77807817	7.55343344	8.41287025
9.17989773	9.28765865	7.36329320
2.20244041	4.25439671	7.19970814
7.19206577	4.25824909	7.20502255
3.45725910	11.95564807	7.15130417
8.44138562	11.95704750	7.18481531
-0.33363629	6.75822061	6.29592736
4.65961799	6.76324250	6.30261791
1.75176638	1.59795991	6.17217394
6.74081834	1.61676443	6.17575582
2.17326311	8.27890486	5.59182720
7.16334704	8.28555908	5.58542201
9.20211317	3.13219709	5.30176764
4.21051762	3.13101141	5.29999785
4.67105370	10.80565139	4.26712224
-0.31238647	10.79130295	4.25080503
6.72315252	5.69183371	4.01242442
1.73343076	5.69230814	4.01151158
7.18781826	12.34530206	3.64247328
2.19151803	12.34822774	3.64124090
9.22785057	7.20171628	3.33187539
4.23833882	7.20223349	3.33485302
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.58873208	7.33031574	9.56945976
4.75012516	2.43443468	9.39913942
9.76362585	2.45927688	9.40050531
1.59407395	7.23165954	9.54484160
2.52321484	10.28738346	7.20979371
0.04420778	10.93108381	6.99753840

3.17858673	7.77842004	7.12899691
8.16247455	7.78031946	7.12505148
0.68854661	12.40123283	4.91187970
7.51823091	0.07889436	7.05728881
3.87059937	5.16336068	6.99188418
8.86025357	5.16407927	6.99472805
3.21556560	2.71815191	6.91955880
8.20908025	2.72239610	6.92412803
0.70656864	8.29956604	6.94270019
5.69792674	8.31601354	6.94214126
4.99610919	10.90665007	6.89653085
7.53238263	10.28407389	7.17348643
1.38310617	5.88930920	6.78632394
6.37143669	5.89406244	6.79422410
0.70721990	3.27392243	6.73519500
5.69469048	3.27758587	6.74306003
0.01303144	0.89514837	6.68286654
5.00839101	0.89780501	6.68786169
3.23772544	11.75668302	5.18768089
8.24785866	11.75238896	5.18829852
8.88996583	9.23900264	5.11529451
3.89178390	9.23299519	5.09541891
7.51062085	4.22527556	5.03839565
2.52031087	4.22412583	5.03568356
8.19910627	6.75605136	4.91239813
3.21107134	6.75442763	4.91440982
5.67841156	12.41622093	4.89532459
2.51105742	0.07103585	7.10145109
3.23623185	1.46235077	4.84638166
8.22899654	1.46530683	4.84629874
1.40866576	9.89932033	4.85646424
6.39667549	9.89287513	4.82322016
5.01743356	4.84924774	4.74118186
0.02687546	4.85072230	4.74092760
0.72834758	7.28671421	4.69784773
5.71766778	7.28838462	4.70097153
5.75454260	2.18807739	4.51684992
0.76599577	2.18427482	4.51382606
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337

7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for  $C_{cv}+CH_3 \rightarrow CCH_3_{cv}$

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	41	4	80

Cart

0.45790337	9.57404061	9.63032027
0.37899729	11.36143719	9.40787164
6.22737419	11.30692222	7.97396415
8.84865665	10.43054803	9.67970344
-0.13235971	10.40427463	9.23637298
4.60875865	2.59768575	8.22614352
9.60434695	2.59886823	8.22042045
4.18527403	9.27659862	7.40607748
1.79532395	7.52013777	8.40439032
6.83095144	7.63118519	8.46981165
9.24566021	9.28658488	7.59765420
2.20098825	4.24625062	7.20445012
7.18440362	4.25116948	7.20507737
3.40428852	11.91265736	7.20395150
8.42597041	11.93428388	7.16524645
-0.33482318	6.77327016	6.30837840
4.67012994	6.75446155	6.31151790
1.73723607	1.62162079	6.16298809
6.72846141	1.60130608	6.18343973
2.17716031	8.29155108	5.59869303
7.18349327	8.31278952	5.64026881
9.19538162	3.13242405	5.29659488
4.20969384	3.13601081	5.30106206
4.67408987	10.80471762	4.26232343
-0.30984696	10.80339054	4.24923590
6.72823334	5.70367019	4.01679561
1.73530272	5.69443852	4.01380126
7.18381116	12.34516316	3.64494674
2.19251374	12.34728729	3.64510441
9.22889484	7.20381477	3.34486019
4.24198687	7.20271502	3.34441530
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304

-0.23342146	8.73880577	0.18583304
6.63395691	7.46462034	9.63389426
4.73982331	2.42272039	9.40138808
9.73735888	2.42251975	9.39559114
1.61370702	7.29279716	9.56484784
2.52600630	10.23031777	7.10465765
-0.02431317	10.87470667	7.08837670
3.18689027	7.76820387	7.12964958
8.19736741	7.81753614	7.17283384
0.68741189	12.40225373	4.91713411
7.50556903	0.05915009	7.06381299
3.87280983	5.15738877	6.99574346
8.85950880	5.16483639	6.99492426
3.21312589	2.71389300	6.91852631
8.19724125	2.71625905	6.91952938
0.71300782	8.28393109	6.94328501
5.70645644	8.31120244	6.97230594
4.97955397	10.90046913	6.92475944
7.47598626	10.24438846	7.10211061
1.37813539	5.87547647	6.79243758
6.39147769	5.90030854	6.79482216
0.69622054	3.26848494	6.73669441
5.69083633	3.25806874	6.74147226
0.01783474	0.87581233	6.70208137
4.99408468	0.85894110	6.70742096
3.25366196	11.76254841	5.18547272
8.25391166	11.75401826	5.18605489
8.89906295	9.23423319	5.07666737
3.90096541	9.22199113	5.07496274
7.50730844	4.22988675	5.04018538
2.51647364	4.22335296	5.03997309
8.19548182	6.76763160	4.93368934
3.21152509	6.75212875	4.91839075
5.67613676	12.41207117	4.90295325
2.51344066	0.07273575	7.02775538
3.22997459	1.47309015	4.83476473
8.22215403	1.46104103	4.84601658
1.39709956	9.89906529	4.84500953
6.39498943	9.88078183	4.80159092
5.02099318	4.85545316	4.74435040
0.02443895	4.85181313	4.73874645
0.72874846	7.28711123	4.70041705
5.72485462	7.30418234	4.71179649
5.74908520	2.18220478	4.51910659

0.75726987	2.18338610	4.51235519
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>Cv</sub>+CH



1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	41	4	80

Cart

1.05934162	11.19466199	9.32351560
6.25838523	11.24373464	7.91136503
9.24416028	9.39126112	9.04872934
1.13462488	11.23321282	8.22521145
4.62812149	2.64585587	8.22591214
9.61949403	2.62099468	8.23083683
4.16907229	9.31079313	7.38274624
1.74042184	7.59391666	8.41898596
6.89626585	7.38611326	8.41335242
9.19437859	9.26121015	7.95577759
2.19825613	4.25652136	7.18864492
7.19792461	4.26975147	7.18668574
3.50334207	11.96546461	7.13397048
8.44338207	11.87447818	7.13119600
-0.33633538	6.80380961	6.29706494
4.65310736	6.77101368	6.31757613
1.75143781	1.55763464	6.20820300
6.74552872	1.61521117	6.19237922
2.16717755	8.28535852	5.58512477
7.18960999	8.33884366	5.66234262
9.19999844	3.13990042	5.30288547
4.21256018	3.13444849	5.30004654
4.67442095	10.80466532	4.26783412
-0.30367571	10.81128844	4.27988141
6.72215404	5.70400768	4.01523372
1.73530859	5.69303809	4.01410726
7.18214448	12.35084858	3.63094339
2.19120492	12.34993781	3.63930196
9.22981456	7.21250941	3.34840602
4.24237847	7.20056034	3.34433288
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344

4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.61418716	7.12764340	9.54369439
4.75111116	2.48324948	9.40364702
9.75655337	2.46406671	9.40726419
1.59355767	7.34375173	9.57735021
2.51390455	10.32902609	7.25143692
-0.01743949	10.80484670	6.86850340
3.15385011	7.81040617	7.12960909
8.20852279	7.80487979	7.15217147
0.69751747	12.41476315	4.91769735
7.53396485	0.04873886	7.04162692
3.86878459	5.16801359	6.99711734
8.87643824	5.17356082	6.98528848
3.20483470	2.70380150	6.92231795
8.21067257	2.72504272	6.92718351
0.65426025	8.34523747	6.96096519
5.69877011	8.31944958	6.97662391
5.00542455	10.89215138	6.86609641
7.55689348	10.18531489	7.09089043
1.37332710	5.89738994	6.79876184
6.38142262	5.91357415	6.80732551
0.70690958	3.25622443	6.73675427
5.69200416	3.29150857	6.74088966
0.00623826	0.85882743	6.71094391
5.02008490	0.90594493	6.67064475
3.25143343	11.76103045	5.17383099
8.23844795	11.75757131	5.16229054
8.86754121	9.18722564	4.96937820
3.89432077	9.23513610	5.09724673
7.50873669	4.23243993	5.03948779
2.52257609	4.22777379	5.04242652
8.18683822	6.75343133	4.92321432
3.21313519	6.75947301	4.92419708
5.67863534	12.42622130	4.88545892
2.53362877	0.00046675	7.11830237
3.23136348	1.47183923	4.84184592
8.23303709	1.47221859	4.85419668
1.40343240	9.89005150	4.83291520

6.39271730	9.87888849	4.76939808
5.01826188	4.86255838	4.74741689
0.02975947	4.85076070	4.73613526
0.72972169	7.28317081	4.70528367
5.72419404	7.31840819	4.71448109
5.76136049	2.19530331	4.52124055
0.76780252	2.18274044	4.52441424
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013

2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CH<sub>Cv</sub>+CH->CHCH<sub>Cv</sub>

1.000000000000

9.97980000	0.00000000	0.00000000
-0.76395804	12.66177393	0.00000000
0.00000004	0.00000004	19.64040000

H	C	O	Fe
3	41	4	80

Cart

1.04986007	10.11635650	9.28070259
6.26058165	11.25999048	7.92998346
9.01218559	9.44693505	9.09626656
1.05114572	10.06389306	8.18603049
4.60332733	2.62150661	8.22550990
9.60501544	2.61343039	8.21983121
4.19045080	9.27644227	7.41668090
1.91780885	7.22713534	8.42358440
6.84767407	7.46226716	8.42121709
9.09838400	9.26942593	8.01335830
2.18325503	4.26445338	7.17775316
7.18703790	4.25594429	7.19027416
3.40796638	11.89618835	7.17569623
8.46171847	11.89012313	7.13904132
-0.33323948	6.81723091	6.33385056
4.66862729	6.74366794	6.30743890
1.73586672	1.60096062	6.17386624
6.72302623	1.59129628	6.19583380
2.16667085	8.29619439	5.64971819
7.18818746	8.33713149	5.65379387
9.19375101	3.13464086	5.29269722
4.20458328	3.13913750	5.30001652
4.67163735	10.79860251	4.26633788
-0.31087301	10.81827842	4.27763718
6.72608925	5.70363901	4.01484924
1.73295806	5.70580466	4.01996917
7.17448439	12.34979125	3.62890673
2.19103970	12.34844379	3.63627561
9.23582840	7.21281024	3.36312931
4.24092362	7.20411339	3.35159845
5.47292232	2.23055553	2.34193015

0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.62468069	7.22452634	9.56918148
4.72095656	2.46234906	9.40404068
9.72948185	2.44558499	9.39610604
1.65902834	7.06422284	9.57695622
2.54721032	10.21625434	7.10245535
-0.03209306	10.80533232	6.84615749
3.20445338	7.75032301	7.15248990
8.20588038	7.81469204	7.15613522
0.68796556	12.41495657	4.89880450
7.52817682	0.04127529	7.05275795
3.86756620	5.15715520	7.01151543
8.86805755	5.17347374	6.98316825
3.19935871	2.71398330	6.91720213
8.19376186	2.71584890	6.91782838
0.66368580	8.40506161	7.05425125
5.70809476	8.30183330	6.97422071
4.98673461	10.89043835	6.90105036
7.52433933	10.20789021	7.06585321
1.37335920	5.92485172	6.84077783
6.39258706	5.90467137	6.80111827
0.68760777	3.26794525	6.73024791
5.68657398	3.26138705	6.74037142
0.00518863	0.86699515	6.68887492
4.99135828	0.85455386	6.71914312
3.24310954	11.75176774	5.17599077
8.22542138	11.76305295	5.15779383
8.88408990	9.19341971	4.98598397
3.89368692	9.21391986	5.07810221
7.50524168	4.23047787	5.04032750
2.51367390	4.23649420	5.04693735
8.18946862	6.75755923	4.93034329

3.20278254	6.76296739	4.92506184
5.66863741	12.41887117	4.89792196
2.49096908	0.03241398	7.03773453
3.23226952	1.47124084	4.84308306
8.21465723	1.46960866	4.84639283
1.39901530	9.87489180	4.79860342
6.39297108	9.87698389	4.76613373
5.01718890	4.86298951	4.75071862
0.02656301	4.85650712	4.73386334
0.72825117	7.29544680	4.74779356
5.72574889	7.31453849	4.71129451
5.74746019	2.18353338	4.52351046
0.76024041	2.18592296	4.51269933
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589

1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CHCH<sub>Cv</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	41	4	80

Cart

1.07028240	10.06374182	9.27502450
6.22576073	11.25425070	7.95052994
8.84246673	9.21147553	9.13062211
0.70282997	9.84041709	8.26473873
4.59820567	2.64236132	8.23774602
9.60845125	2.64727024	8.22386562
4.16599139	9.25286236	7.40463831
1.89623540	7.16336585	8.38298844
6.74918733	7.49653165	8.39139251
9.35144112	9.27735589	8.15275637
2.19397366	4.23577873	7.17409584
7.18261289	4.25242142	7.19590678
3.35919291	11.88668181	7.20636556
8.43767082	11.89819996	7.12488956
-0.33447211	6.79487046	6.32946266
4.67868768	6.71560077	6.28742607
1.72970433	1.60931348	6.14892235
6.71328727	1.58295051	6.20425292
2.17781432	8.27041661	5.63628362
7.18542746	8.34862893	5.66149570
9.18557560	3.12734600	5.29142835
4.20654508	3.13551647	5.30593441
4.65865810	10.79288380	4.26465878
-0.31153506	10.83300123	4.30704328
6.72276979	5.70777377	4.01310649

1.73366257	5.69537283	4.01958953
7.16257802	12.35095102	3.62756623
2.19591330	12.34795845	3.64072098
9.23123235	7.21144345	3.36641432
4.23820190	7.20246515	3.33938324
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.68738825	7.24102455	9.55897102
4.71991934	2.50930552	9.41845821
9.72020389	2.49831231	9.40432608
1.67792579	6.89418320	9.52862864
2.44511351	10.18912976	7.17327262
-0.05040022	10.83512695	6.75701875
3.22183290	7.70736067	7.14595119
8.23951122	7.86078872	7.16384563
0.68481313	12.43454793	4.87838876
7.50218704	0.03416157	7.06328170
3.87317656	5.13435850	7.00303481
8.87053833	5.15439294	6.97501463
3.20270469	2.69727655	6.91848832
8.18450753	2.71103234	6.91936606
0.76002608	8.25669191	7.02780349
5.70576768	8.30090887	6.98296428
4.92971261	10.88201744	6.93833220
7.47344146	10.22599143	7.05621376
1.37117439	5.86521666	6.77968722
6.40553475	5.90857585	6.80484629
0.68245713	3.26303459	6.72815251
5.68706422	3.25290123	6.74518241
-0.00414366	0.86816743	6.67694154
4.97584403	0.83765558	6.72862787
3.22231822	11.72965814	5.19903646



8.21117580	11.77857465	5.15093766
8.87408151	9.19448704	4.96399543
3.88099007	9.22448702	5.11167130
7.50084740	4.23026797	5.03565622
2.51689310	4.21576267	5.03242558
8.17920345	6.76125202	4.95315157
3.21137992	6.75828813	4.91173990
5.65054690	12.40677492	4.90863630
2.46822600	0.04485925	7.02007474
3.24040487	1.46640223	4.83684400
8.20203615	1.46672133	4.84608816
1.39436836	9.85487592	4.78758738
6.38673449	9.88634957	4.78646130
5.02107740	4.86310130	4.76203963
0.01994761	4.84853607	4.72961357
0.72695718	7.28309767	4.72665567
5.72820472	7.32315078	4.70895236
5.74493743	2.17878297	4.52608656
0.75465368	2.19134679	4.50523722
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071

2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>Cv</sub>+CH<sub>2</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	41	4	80

Cart

1.31867304	12.26127629	8.85989171
1.11446805	10.58484155	9.35459734
6.26142493	11.25250949	7.91806457
9.19920162	9.34240848	9.08001248
1.18014407	11.20118180	8.43954560
4.60495194	2.64169457	8.22660407
9.61086008	2.59186834	8.21378175
4.15155117	9.28703914	7.35783042
2.17297968	7.36164805	8.59253883
6.90364965	7.41712515	8.42887172
9.15593594	9.25191408	7.97747602
2.18742329	4.24462595	7.19160580
7.18621555	4.26037587	7.19107035
3.46866328	11.93217013	7.16561647
8.44941093	11.88900438	7.15817493
-0.34461250	6.77072564	6.30381432
4.67441143	6.74741677	6.29306993
1.75400619	1.58088088	6.17086267
6.73123720	1.59824667	6.19921824

2.14851774	8.26820383	5.58540004
7.18909014	8.33067526	5.65666871
9.19355205	3.12785939	5.29225553
4.20446711	3.12899124	5.29272748
4.66369871	10.77711064	4.26549714
-0.30369829	10.79508604	4.26400883
6.72112834	5.70016351	4.01512583
1.73183299	5.68585473	4.00915089
7.18218061	12.34621864	3.64028827
2.19446847	12.34331889	3.63928210
9.22833613	7.21339207	3.34747336
4.24200914	7.20238595	3.34017545
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.58680100	7.21340090	9.55965635
4.71783214	2.49326521	9.40631677
9.72425322	2.40689685	9.38833358
1.70792539	7.20809319	9.66652875
2.49950092	10.29099131	7.24946121
0.00451439	10.84055246	6.96549823
3.15606882	7.75792221	7.14725174
8.20523626	7.79193427	7.14969374
0.68964167	12.39299157	4.91191627
7.53130653	0.03672169	7.04174303
3.85229957	5.18436921	7.02556006
8.87387359	5.15796294	7.01191281
3.20741485	2.71699400	6.91354825
8.19622361	2.71475868	6.91664537
0.61192735	8.38122439	6.94075950
5.70588946	8.31706196	6.97061315
4.99164455	10.88413888	6.90399843
7.56857343	10.19032258	7.11323699

1.37291258	5.88730835	6.80595145
6.39760368	5.91348738	6.80692058
0.69290444	3.25408900	6.73298486
5.68736453	3.27222242	6.73940812
0.01102869	0.85687424	6.67740593
5.00343702	0.88004318	6.70492493
3.24036372	11.73879611	5.19053556
8.23775766	11.73179485	5.17743392
8.86914898	9.18539911	4.98364327
3.88180833	9.21869506	5.14207893
7.50811274	4.23161483	5.04206234
2.51897509	4.23238867	5.04561273
8.18757902	6.74949858	4.92215195
3.21256055	6.75481892	4.91737290
5.67347309	12.39958451	4.89883066
2.51056699	0.03250691	7.07873815
3.23968120	1.44852284	4.84896558
8.21956480	1.45614124	4.84980362
1.39950228	9.89276393	4.84696347
6.38528103	9.87075373	4.77280757
5.01463279	4.86333374	4.76382928
0.02370413	4.85187789	4.74471668
0.72595733	7.27610074	4.71244705
5.72742944	7.31379245	4.71077029
5.75327118	2.17864463	4.52393788
0.76297859	2.17849278	4.51320709
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903

5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for  $\text{CH}_{\text{cv}} + \text{CH}_2 \rightarrow \text{CHCH}_2_{\text{cv}}$

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	41	4	80

Cart

0.51870205	10.89040773	8.84761586
1.26891356	9.37600895	9.31962168
6.24070373	11.25786093	7.94769821
8.84680653	9.43914580	9.14606396
0.88127029	9.90765156	8.44313183
4.59557969	2.63189800	8.23140889
9.60424094	2.62340951	8.21522822
4.16054519	9.27040118	7.38369855
2.35071972	7.06670465	8.58518766
6.91184502	7.42455983	8.42139607
9.16836356	9.27975841	8.10370378
2.18926821	4.25193241	7.17617555
7.18573773	4.26629781	7.18722863

3.38608262	11.89527302	7.21565796
8.42028544	11.91777766	7.14002780
-0.32382456	6.80850542	6.33313790
4.69477713	6.72887400	6.28376885
1.72920804	1.62965680	6.14565993
6.71953330	1.59980028	6.19733442
2.15230617	8.28184453	5.64513914
7.19920277	8.35204518	5.66708118
9.18931408	3.13592990	5.28643327
4.20764060	3.14278146	5.29800287
4.65810217	10.77669635	4.26588452
-0.30597797	10.82769129	4.27814792
6.72787535	5.71305819	4.01557890
1.73537854	5.70317558	4.01715264
7.17275794	12.34800344	3.64096254
2.19555173	12.34568891	3.64120518
9.23347111	7.21298413	3.35969828
4.24130456	7.20373622	3.34060282
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.63312407	7.21879525	9.56441346
4.72255500	2.47995524	9.40963114
9.71925625	2.45402919	9.39313841
1.90568522	6.85503649	9.65867139
2.48650738	10.22094889	7.18907037
-0.01546164	10.89258857	6.83144857
3.22338838	7.71375129	7.15729784
8.24301446	7.83146743	7.16331578
0.68494945	12.42563891	4.88630953
7.49725933	0.04277855	7.05761782
3.86721222	5.17387555	7.03576814
8.88060309	5.17461176	6.99510703

3.20904266	2.72184843	6.91495205
8.18937044	2.72326265	6.91481667
0.63788106	8.43405368	6.96185144
5.72462671	8.31688257	6.97988584
4.95701618	10.89273146	6.93620708
7.53902499	10.21115700	7.09484562
1.39242282	5.90758244	6.79720204
6.42456351	5.92914500	6.80365789
0.68446503	3.27352216	6.72769296
5.68745495	3.26416876	6.74119377
0.00543830	0.87557791	6.68428529
4.98805885	0.85027432	6.72175318
3.23124665	11.73087936	5.19661354
8.22685078	11.76379581	5.16659423
8.87527297	9.20546987	4.97782759
3.88028239	9.21979331	5.16321757
7.50764478	4.24200339	5.04195071
2.51760018	4.23771202	5.04551785
8.19072184	6.76661441	4.93715976
3.20735687	6.76554551	4.91492691
5.65477805	12.41130472	4.90362937
2.51299774	0.09163328	7.01068814
3.23878325	1.47166636	4.83642205
8.20769939	1.46732215	4.84638100
1.39692486	9.87947628	4.79498340
6.38566974	9.88651823	4.78642967
5.01808636	4.87314885	4.76298605
0.02511286	4.85864841	4.73138133
0.72598313	7.29219076	4.73498663
5.73037737	7.32698669	4.70989040
5.74678288	2.18429798	4.52279135
0.75400034	2.19297806	4.50533627
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425

5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>v</sub>+CH<sub>3</sub> (state1)

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
5	41	4	80

Cart

0.24268527	11.33397898	9.23055419
1.93063505	10.78718734	9.30102144
6.26480603	11.24755886	7.91831001
9.24442522	9.35804107	9.08765178
1.55912309	12.50046976	9.08568373
1.23470765	11.47293042	8.77461281
4.61859669	2.62792690	8.21549171



9.61725515	2.68835882	8.23116739
4.14764367	9.31945247	7.37909104
1.71755546	7.66931515	8.43155826
7.06072819	7.36444238	8.49998256
9.20224640	9.22545961	7.99298670
2.19808629	4.26588945	7.19091881
7.18788105	4.27184371	7.17741198
3.44734204	11.96654916	7.15084493
8.43600899	11.90579010	7.15618801
-0.33402648	6.80441812	6.28418696
4.65260992	6.77865068	6.33176352
1.74243019	1.59991354	6.17035623
6.74406393	1.61290070	6.18768709
2.15743448	8.28243186	5.58760823
7.18740987	8.34455034	5.66800544
9.19822927	3.13309612	5.29392577
4.20908373	3.13620603	5.29291396
4.66379539	10.80882316	4.26959422
-0.30745820	10.79793109	4.25287830
6.72319698	5.71198790	4.01790960
1.73280352	5.69670152	4.01379385
7.18701044	12.34561515	3.64486916
2.18777219	12.34899385	3.64067035
9.22885870	7.21287386	3.34337583
4.24119052	7.19986319	3.34321440
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.63239970	7.16645728	9.58915714
4.74420875	2.45205951	9.39244837
9.72915952	2.55086431	9.41228015
1.61733842	7.42306016	9.59550675
2.48932334	10.30746743	7.24894338

0.03019084	10.86321265	7.00243611
3.14973304	7.80650983	7.13063844
8.21432973	7.79280167	7.16590346
0.68415172	12.39907466	4.91579105
7.52087393	0.05048923	7.04665118
3.87133732	5.17064223	6.98808614
8.86635361	5.18850089	6.99234582
3.20922651	2.72546182	6.91363581
8.20689179	2.73432091	6.91814106
0.65435418	8.35375690	6.96365385
5.68289784	8.34704807	6.95286691
4.97860611	10.91655818	6.90664295
7.58216111	10.19611746	7.12199438
1.37920751	5.90094591	6.77467947
6.38723590	5.92178599	6.79461481
0.70171353	3.27451756	6.73001463
5.68956280	3.28674226	6.73343854
0.00406199	0.86983816	6.68094397
5.00836139	0.90352404	6.68243584
3.22902428	11.75578286	5.18989634
8.24547713	11.73450720	5.18415588
8.86826928	9.20287756	5.00681695
3.88946711	9.24181926	5.11763673
7.50830654	4.23569387	5.03536059
2.51965548	4.23160032	5.03375785
8.18605844	6.76537341	4.92341557
3.21267036	6.76302886	4.92506675
5.67545972	12.41369487	4.89639682
2.50189262	0.07005616	7.09050121
3.23158477	1.46344444	4.84601129
8.22728776	1.46063742	4.84974184
1.39363636	9.90161110	4.86448810
6.38448278	9.88818426	4.78184144
5.01666492	4.86399377	4.73455113
0.02125704	4.85508461	4.73489326
0.72834791	7.28796833	4.70226180
5.71946546	7.32485023	4.71324562
5.75504432	2.18638757	4.51774529
0.76231133	2.18349402	4.51205880
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337

3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>Cv</sub>+CH<sub>3</sub> (state2)

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
5	41	4	80

Cart

6.36646065	6.22571354	8.91231815
7.67221873	7.41731280	9.10465125
6.26619536	11.23175088	7.92431495
9.23462510	9.35395003	9.04659803
5.97279768	7.94865758	9.07933487
6.68677863	7.24566201	8.59982562
4.61427272	2.60356657	8.21209204
9.59159976	2.62341901	8.22341507
4.16051070	9.30088342	7.33695707
1.74560194	7.55507363	8.40869761
0.97093565	11.30951284	8.38981269
9.18447928	9.26385376	7.94633149
2.19641286	4.25200006	7.18948199
7.19165266	4.26444297	7.17110745
3.46139523	11.95204733	7.16599423
8.43689152	11.88061878	7.13744126
-0.33175041	6.80876201	6.30268082
4.65990421	6.74610430	6.31923763
1.73086195	1.58680064	6.18450001
6.73920044	1.60615736	6.18281501
2.17216946	8.27567623	5.58358885
7.19723859	8.35034917	5.69124200
9.19433389	3.13726770	5.29093230
4.20669078	3.13764667	5.29040230
4.67059990	10.79707121	4.26485572
-0.30555616	10.78768714	4.26825078
6.72594139	5.71241377	4.01707320
1.73726464	5.69503822	4.01134832
7.18382540	12.34660769	3.63790784
2.19074892	12.34573433	3.64106311
9.23027937	7.21125014	3.34966646
4.24297364	7.19899860	3.34271304
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067

2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.12621218	11.37938499	9.57374775
4.75011747	2.42810930	9.38643714
9.72709059	2.46700320	9.39955044
1.58258633	7.29082738	9.56356668
2.52283662	10.28661137	7.19794690
-0.01240558	10.81684905	6.92758432
3.15685146	7.77380508	7.12591887
8.21067516	7.77344730	7.17668675
0.68695390	12.40116035	4.91549713
7.52326395	0.04185056	7.04860254
3.86941597	5.15463300	6.99018648
8.88206065	5.17002665	6.95297411
3.20357916	2.70327868	6.91284057
8.20020805	2.72175502	6.91240441
0.66419263	8.34461328	6.96048271
5.70960944	8.32574687	6.97679342
4.99505639	10.90857401	6.89259906
7.55460775	10.18495810	7.07731077
1.37638040	5.89413930	6.80137295
6.41599330	5.93370258	6.82414177
0.69869728	3.26037920	6.73083934
5.69014842	3.27715964	6.73236364
-0.00711636	0.86306962	6.69255865
5.01410885	0.89016001	6.69084202
3.24534710	11.75707563	5.18184194
8.24382242	11.74317080	5.16754570
8.88061642	9.18171685	5.01200740
3.90058814	9.24019254	5.14274238
7.50097881	4.23957731	5.03884869
2.51642993	4.23001952	5.04291903
8.17468120	6.76588009	4.93047135
3.21792658	6.75793536	4.91756529
5.67544185	12.41355363	4.89323246
2.52970022	0.06021219	7.09117484
3.23161223	1.45765546	4.84659146
8.22529950	1.46270135	4.84529782
1.40134273	9.89280417	4.85762087
6.39479109	9.87865115	4.76466469
5.01579534	4.86611157	4.73778410
0.02649173	4.85051166	4.72453957
0.72974492	7.27910676	4.70904440

5.72384253	7.32669761	4.72129868
5.75188163	2.18799132	4.51848897
0.76044915	2.17888129	4.51641932
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CH<sub>cv</sub>+CH<sub>3</sub>->CHCH<sub>3</sub><sub>cv</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
5	41	4	80

Cart

7.39166993	7.20857773	8.99667968
8.86179217	7.71360474	9.90800218
6.27159733	11.21058902	7.92620622
-0.52826701	9.68490414	9.01623552
7.44727342	8.84441778	9.71045117
8.05957807	8.06311211	9.25191665
4.60513666	2.60281822	8.21485698
9.59549829	2.61155786	8.22561570
4.13683251	9.31680414	7.42622929
1.74316456	7.59411589	8.43437507
1.03482410	11.35578326	8.35403730
9.11006079	9.17249209	8.11166727
2.19111194	4.24962152	7.18974138
7.18377651	4.27415610	7.18399991
3.46396489	11.96085514	7.15350640
8.43515427	11.86326961	7.13349430
-0.34103951	6.81124606	6.31539053
4.63490547	6.76154306	6.35453965
1.72694773	1.57942232	6.17812598
6.73985663	1.60268105	6.18636956
2.15187190	8.28259308	5.60248449
7.17613123	8.34320756	5.71200389
9.19725791	3.13385062	5.29880630
4.20620395	3.13516002	5.29300763
4.66942585	10.80376399	4.26582216
-0.31208156	10.79810940	4.27364973
6.72427014	5.70966224	4.02452174
1.73364340	5.69586880	4.01544773
7.18009433	12.34939325	3.63402543
2.18814538	12.34743304	3.63838830
9.22894965	7.21353775	3.36038550
4.23434743	7.19767086	3.34548789
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742

1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.07453053	11.35262894	9.55521498
4.74167767	2.43357604	9.38971231
9.72397815	2.44896398	9.40175615
1.55007506	7.32533664	9.58336833
2.51148868	10.30762377	7.21175308
0.01220336	10.84422285	6.86289204
3.14453543	7.80087727	7.14847399
8.24246370	7.80541819	7.16571715
0.68338607	12.40648057	4.90758767
7.52056929	0.02966870	7.04963555
3.87073457	5.14733770	6.99407868
8.86587032	5.16651719	6.96807669
3.19845750	2.69956798	6.91297634
8.19571041	2.72185482	6.91945396
0.66017854	8.36576681	6.98212442
5.61835194	8.35539583	6.87819445
4.98762534	10.90453119	6.90330086
7.54719225	10.18140842	7.06400948
1.37268567	5.89149052	6.79415350
6.39074176	5.90452506	6.69038788
0.69546389	3.25180155	6.73379658
5.68614274	3.27932465	6.73669849
-0.00885440	0.85300049	6.69761627
5.01237599	0.89576046	6.68494737
3.23821619	11.75769626	5.17858406
8.22885778	11.74562744	5.16171809
8.86382329	9.18695054	5.00578137
3.87141283	9.24249089	5.11796498
7.50932529	4.22077561	5.02507256
2.51493731	4.22895279	5.04344017
8.17247293	6.76541191	4.94468328
3.20456862	6.75674652	4.93333684
5.67259870	12.41590344	4.89408542



2.53188483	0.05704321	7.09207904
3.22933907	1.46356514	4.84087590
8.22405768	1.46573666	4.84859430
1.39120975	9.88320869	4.83185883
6.38443752	9.88030665	4.76165894
5.00957201	4.85717953	4.72353590
0.02369068	4.84936816	4.72863741
0.71823622	7.27998076	4.72148647
5.70688434	7.33110227	4.69670890
5.75350152	2.18784020	4.51903950
0.75869362	2.18181408	4.51520021
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453

0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>2</sub> cv+CH<sub>2</sub>

1.000000000000

9.97980000	0.00000000	0.00000000
-0.76395804	12.66177393	0.00000000
0.00000004	0.00000004	19.64040000

H	C	O	Fe
5	41	4	80

Cart

6.10063418	7.00196774	9.22801342
7.72847046	7.40188505	8.75450077
0.26605246	8.64969432	8.51063011
8.97875318	9.59174322	9.09502456
6.24780750	11.26542102	7.95332116
6.63974831	7.21539979	8.29363321
4.60484558	2.61166576	8.21185715
9.59399695	2.58367099	8.21631405
4.19717260	9.25728246	7.37024788
2.59664705	7.11048714	8.74197830
0.96867996	11.37576556	8.38430018
9.26378500	9.24111664	8.08734095
2.19467049	4.23595080	7.17335242
7.17676684	4.26598275	7.17900872
3.46086218	11.92319551	7.16130132
8.43177735	11.87807931	7.14264349
-0.33991650	6.79109546	6.31043622
4.67919557	6.70166288	6.25034881
1.73248043	1.57499714	6.17857146
6.73147408	1.60583525	6.18241579
2.13962126	8.25652446	5.65998081
7.18341045	8.36181779	5.64979855
9.19328439	3.12728996	5.29175986
4.20494375	3.13149632	5.28188136
4.66346142	10.76514706	4.26274384
-0.30624336	10.79075412	4.27005063
6.72456330	5.70382637	4.02089248

1.73067789	5.69302105	4.01499026
7.18040360	12.34635685	3.63763538
2.19499766	12.34041773	3.64160491
9.23010342	7.21006105	3.35270421
4.23587664	7.20300733	3.33602005
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.10981588	11.44041067	9.57142123
4.73075796	2.43996712	9.38840025
9.71716313	2.39615728	9.38933715
2.24629775	6.80175638	9.81956030
2.52579073	10.24319924	7.18227975
-0.02318775	10.82742576	6.93100966
3.21301423	7.71301508	7.18379812
8.20476132	7.79290285	7.18041215
0.68948549	12.39971956	4.91293250
7.51768797	0.04115786	7.04607899
3.86370210	5.16685475	7.03529128
8.87995208	5.17043497	7.00593425
3.20314004	2.69496606	6.90496363
8.19121816	2.71903741	6.91466842
0.64179419	8.40437076	6.89859832
5.72852370	8.28608241	6.96597741
5.00125381	10.88052224	6.91131783
7.51124922	10.19828173	7.05203156
1.37786811	5.88166239	6.77820118
6.42693209	5.92899042	6.82112350
0.69200195	3.24988421	6.73505796
5.68165610	3.27259819	6.73001679
-0.00786629	0.85771665	6.68995076
5.00976030	0.87063311	6.68949021
3.25059362	11.73774552	5.18082117

8.24307371	11.74515278	5.16731457
8.88169597	9.18615268	5.02265251
3.87297010	9.20814411	5.17249919
7.50804093	4.23194544	5.03969408
2.51674236	4.22692439	5.04265610
8.17551022	6.76889243	4.94165855
3.19948974	6.76186491	4.91715094
5.66465982	12.40884256	4.89049540
2.53537139	0.04323547	7.08373782
3.23583720	1.44751244	4.84196559
8.21928706	1.46042192	4.84466410
1.39729245	9.87790011	4.83583230
6.38526180	9.88454867	4.75528693
5.00398700	4.87147287	4.74870389
0.01999079	4.84664160	4.73736969
0.71741826	7.26972991	4.72236593
5.72471561	7.32341597	4.70153339
5.75238065	2.18693961	4.51579632
0.76095213	2.17698209	4.51592591
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071

2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for  $\text{CH}_2\text{Cv}+\text{CH}_2\rightarrow\text{CH}_2\text{CH}_2+\text{Cv}$

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9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
5	41	4	80

Cart

5.97711174	7.50664634	8.94242248
7.35686705	6.44988219	9.31135915
8.75979557	8.95281056	9.33014671
6.98960620	9.20937628	9.38131547
6.26686524	11.23965424	7.94783601
6.92596623	7.09933095	8.53615276
4.60860790	2.62096660	8.22490082
9.59817432	2.54148025	8.21066288
4.15722236	9.29297785	7.33547737
2.39248689	7.21916369	8.65891542
0.89390358	10.56747044	8.31610181
7.83335248	8.93407847	8.73662096
2.19102515	4.25805698	7.17312792
7.20680407	4.27407862	7.18031410
3.45412274	11.93525292	7.18650294
8.48698642	11.81989592	7.16266159
-0.34434637	6.92291907	6.42075934
4.68446454	6.69530445	6.27788199
1.73967342	1.61183842	6.15374938

6.74597018	1.59470827	6.19414395
2.14878622	8.28565627	5.60793737
7.19478315	8.34852131	5.64198407
9.19816032	3.14020347	5.29471491
4.21887162	3.14424487	5.29936275
4.67041244	10.79429916	4.27075837
-0.29643950	10.81846246	4.30470227
6.72924203	5.70445033	4.01590898
1.73779371	5.70273586	4.02089371
7.17970904	12.34774304	3.63726294
2.20054380	12.34936738	3.63349070
9.23028556	7.20731982	3.36284171
4.23723037	7.20220951	3.33312394
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
0.93949112	10.57611328	9.51279613
4.74824700	2.46934662	9.40298760
9.75664275	2.36363279	9.38271790
1.92859752	6.98168498	9.71346847
2.54236435	10.27791030	7.14444349
0.05611775	10.89917346	6.72749571
3.19170803	7.73532916	7.15301777
8.12181696	7.77462824	7.17655734
0.69514934	12.45080709	4.86983307
7.55905892	0.02468442	7.05575418
3.86478328	5.17475674	7.04604632
8.90908972	5.18999744	6.92991759
3.21635744	2.72132745	6.91644259
8.20543548	2.71834391	6.91809944
0.68613235	8.52106252	6.90376893
5.67324805	8.31553635	6.89316873
5.00464919	10.90287142	6.89520126

7.52831551	10.17492523	7.14660264
1.35934709	5.90361554	6.75760677
6.45489970	5.93156700	6.82682398
0.69795609	3.25672078	6.73119914
5.70281784	3.27300394	6.73911723
0.01837673	0.84086447	6.70751554
5.01430778	0.88267478	6.71011697
3.24472973	11.75458163	5.18325443
8.22903300	11.74135160	5.17100262
8.88597587	9.19818227	5.05965645
3.88270001	9.22484408	5.15199741
7.51275252	4.23983566	5.03741873
2.52527370	4.23417065	5.04607160
8.19430574	6.76628893	4.94342864
3.20628221	6.76489444	4.91294392
5.67857245	12.41561813	4.90254619
2.52842277	0.07350150	7.03449618
3.24930737	1.48127294	4.83783710
8.22955412	1.46448501	4.84864292
1.42340369	9.87946692	4.73219869
6.39207150	9.89218678	4.75706662
5.01265027	4.87605384	4.75979498
0.03361948	4.84275766	4.70092721
0.71391572	7.28624785	4.73133070
5.73220025	7.31905419	4.69713989
5.76017048	2.18926853	4.52179443
0.76000083	2.19448380	4.50958593
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903

2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>2</sub> C<sub>v</sub>+CH<sub>3</sub>

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9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
6	41	4	80

Cart

5.89410204	7.93102969	9.03498812
7.56777830	7.41892521	9.27321967
0.13678149	8.53819528	8.50655079
8.99316884	9.64362594	9.10471469
6.32240867	6.21801259	8.87574761
6.25310097	11.23297846	7.95853713
6.67781286	7.24846408	8.63499059
4.59747313	2.59062762	8.21188929
9.57575907	2.54560315	8.21919835
4.15865731	9.28217822	7.34633121
2.57729677	7.18539220	8.78337019



0.95763338	11.37696892	8.37925019
9.22121334	9.25206102	8.09775546
2.19326468	4.22882221	7.17853400
7.19716815	4.23939780	7.17533152
3.45480887	11.92889082	7.16168957
8.43135027	11.85704436	7.13047373
-0.33748640	6.79283321	6.32733150
4.67393449	6.72740988	6.30636275
1.73097939	1.56828974	6.17294940
6.73463264	1.58388539	6.17872566
2.12706687	8.25128729	5.66879809
7.20373201	8.34197772	5.70218652
9.19399592	3.12444758	5.29496661
4.20940403	3.12951490	5.28427519
4.66495081	10.75281103	4.26308969
-0.30176601	10.78324350	4.26758391
6.72364375	5.70102023	4.01989203
1.73534392	5.69390340	4.01561423
7.18231244	12.34379225	3.63673145
2.19674636	12.33954838	3.63863895
9.23237910	7.21366328	3.36507693
4.24110138	7.20084202	3.35328770
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.07637907	11.46334710	9.56756825
4.71038651	2.41510928	9.38864458
9.71216297	2.36919081	9.39447747
2.21805510	6.90709143	9.86484154
2.50967178	10.26059468	7.18050344
-0.02200350	10.80802555	6.92653382
3.19404231	7.71937491	7.19930121
8.20048138	7.76376886	7.19255402

0.69047883	12.39506352	4.90962888
7.51932111	0.01817727	7.04951798
3.86944477	5.15367374	7.01945855
8.89281956	5.14164062	6.95558581
3.20203637	2.68897954	6.90315913
8.19590319	2.69440513	6.91071021
0.62131503	8.39604870	6.90180722
5.72040150	8.32111281	6.98106289
4.99714584	10.88972459	6.91454840
7.52380469	10.16541895	7.04209199
1.37998566	5.87012073	6.76715527
6.42877678	5.90957689	6.82530199
0.69494077	3.23391808	6.73950018
5.68706446	3.25788994	6.73546514
-0.00437306	0.83996589	6.69226136
5.01028362	0.86778499	6.68934329
3.25204682	11.73553014	5.17831691
8.24617220	11.73570242	5.16241702
8.88428539	9.16945182	4.99659166
3.88009226	9.20299651	5.19755634
7.50046571	4.22551155	5.04137093
2.51858937	4.22235603	5.04178396
8.17483263	6.74850063	4.94416410
3.20681864	6.75803178	4.93218284
5.66831596	12.39841370	4.89370654
2.52970392	0.04121157	7.08052104
3.23750369	1.44621611	4.83951962
8.22185662	1.45236439	4.83964963
1.39882324	9.86929064	4.83904452
6.38931639	9.86316109	4.76645679
5.00972513	4.86483141	4.74945545
0.02658884	4.83172293	4.71787122
0.71918929	7.25643883	4.72824328
5.72255274	7.31696098	4.72857472
5.75325529	2.18171311	4.51692037
0.76084852	2.17392073	4.51523235
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265

6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>3</sub> cv+CH<sub>2</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
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H	C	O	Fe
6	41	4	80

Cart

5.89410204	7.93102969	9.03498812
7.56777830	7.41892521	9.27321967
0.13678149	8.53819528	8.50655079

8.99316884	9.64362594	9.10471469
6.32240867	6.21801259	8.87574761
6.25310097	11.23297846	7.95853713
6.67781286	7.24846408	8.63499059
4.59747313	2.59062762	8.21188929
9.57575907	2.54560315	8.21919835
4.15865731	9.28217822	7.34633121
2.57729677	7.18539220	8.78337019
0.95763338	11.37696892	8.37925019
9.22121334	9.25206102	8.09775546
2.19326468	4.22882221	7.17853400
7.19716815	4.23939780	7.17533152
3.45480887	11.92889082	7.16168957
8.43135027	11.85704436	7.13047373
-0.33748640	6.79283321	6.32733150
4.67393449	6.72740988	6.30636275
1.73097939	1.56828974	6.17294940
6.73463264	1.58388539	6.17872566
2.12706687	8.25128729	5.66879809
7.20373201	8.34197772	5.70218652
9.19399592	3.12444758	5.29496661
4.20940403	3.12951490	5.28427519
4.66495081	10.75281103	4.26308969
-0.30176601	10.78324350	4.26758391
6.72364375	5.70102023	4.01989203
1.73534392	5.69390340	4.01561423
7.18231244	12.34379225	3.63673145
2.19674636	12.33954838	3.63863895
9.23237910	7.21366328	3.36507693
4.24110138	7.20084202	3.35328770
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304

1.07637907	11.46334710	9.56756825
4.71038651	2.41510928	9.38864458
9.71216297	2.36919081	9.39447747
2.21805510	6.90709143	9.86484154
2.50967178	10.26059468	7.18050344
-0.02200350	10.80802555	6.92653382
3.19404231	7.71937491	7.19930121
8.20048138	7.76376886	7.19255402
0.69047883	12.39506352	4.90962888
7.51932111	0.01817727	7.04951798
3.86944477	5.15367374	7.01945855
8.89281956	5.14164062	6.95558581
3.20203637	2.68897954	6.90315913
8.19590319	2.69440513	6.91071021
0.62131503	8.39604870	6.90180722
5.72040150	8.32111281	6.98106289
4.99714584	10.88972459	6.91454840
7.52380469	10.16541895	7.04209199
1.37998566	5.87012073	6.76715527
6.42877678	5.90957689	6.82530199
0.69494077	3.23391808	6.73950018
5.68706446	3.25788994	6.73546514
-0.00437306	0.83996589	6.69226136
5.01028362	0.86778499	6.68934329
3.25204682	11.73553014	5.17831691
8.24617220	11.73570242	5.16241702
8.88428539	9.16945182	4.99659166
3.88009226	9.20299651	5.19755634
7.50046571	4.22551155	5.04137093
2.51858937	4.22235603	5.04178396
8.17483263	6.74850063	4.94416410
3.20681864	6.75803178	4.93218284
5.66831596	12.39841370	4.89370654
2.52970392	0.04121157	7.08052104
3.23750369	1.44621611	4.83951962
8.22185662	1.45236439	4.83964963
1.39882324	9.86929064	4.83904452
6.38931639	9.86316109	4.76645679
5.00972513	4.86483141	4.74945545
0.02658884	4.83172293	4.71787122
0.71918929	7.25643883	4.72824328
5.72255274	7.31696098	4.72857472
5.75325529	2.18171311	4.51692037
0.76084852	2.17392073	4.51523235

8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for  $\text{CH}_3\text{Cv} + \text{CH}_2 \rightarrow \text{CH}_2\text{CH}_3 + \text{Cv}$

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
6	41	4	80

Cart

7.02760071	8.26567634	9.77683640
8.40304629	7.10479825	9.95007146
-0.23753997	8.80065261	9.10298014
8.35753159	9.83062601	8.92299814
6.96845991	6.67296424	8.99940592
6.27108689	11.20169755	7.93267348
7.63854866	7.50591160	9.27647490
4.60527176	2.62564704	8.22024440
9.59834206	2.59959073	8.21876090
4.12750196	9.31296320	7.39096093
2.45367988	7.17086798	8.70761171
1.06033832	10.97769176	8.36906917
8.86616032	8.95680041	8.44290650
2.18617854	4.26048910	7.16882008
7.19537760	4.26472464	7.17523371
3.46335082	11.94500384	7.16244124
8.46227168	11.85478318	7.14575254
-0.35470054	6.83180072	6.35780678
4.65171401	6.75423096	6.30907883
1.73624105	1.60901218	6.16363409
6.74412356	1.59247475	6.18806680
2.10385209	8.29568135	5.66543488
7.19171576	8.34009798	5.72578540
9.19831431	3.13298784	5.29468612
4.21087363	3.14280036	5.29244451
4.66846186	10.78377035	4.27029357
-0.30344663	10.80910023	4.28636483
6.72532918	5.71035307	4.02687196
1.73366307	5.70969984	4.02108087
7.18028316	12.34854640	3.63574115
2.19578644	12.34733186	3.63465589
9.22800601	7.21283039	3.35958815
4.23323767	7.20029987	3.34213629
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899

2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
1.08078490	11.11416860	9.56114055
4.74450400	2.47717608	9.39885371
9.73413776	2.43798931	9.39588021
2.04659179	6.88482442	9.77303357
2.51314960	10.30666301	7.17968756
0.05087554	10.91929847	6.81142041
3.17312851	7.75720470	7.18657102
8.18347917	7.72677866	7.21960865
0.69457613	12.42544568	4.88674139
7.53803032	0.02114541	7.05152571
3.86571472	5.17701948	7.01824338
8.88077995	5.15827525	6.95486384
3.20833855	2.72214586	6.91354980
8.19929155	2.71301220	6.91585173
0.57801250	8.51077784	6.94470346
5.63956105	8.35023890	6.88348868
4.99611700	10.89266144	6.90285009
7.53013133	10.16534767	7.04403426
1.36786695	5.90211219	6.75019929
6.39584541	5.88106356	6.65915950
0.69376092	3.25772115	6.72924307
5.68962215	3.27489038	6.73187190
0.00826118	0.85226242	6.69325147
5.01300978	0.88794357	6.69854321
3.24467733	11.75148870	5.17842940
8.22907131	11.73913766	5.17019337
8.87029238	9.18827393	5.02663535
3.85468863	9.22389344	5.14703679
7.51320499	4.21905175	5.01856469
2.51797788	4.23574518	5.03925989
8.17785867	6.77103660	4.94858179
3.19030434	6.77721823	4.93011185
5.67330513	12.41293443	4.89667581
2.53353212	0.07741676	7.05429015
3.24201440	1.47098148	4.84239727



8.22597825	1.46016725	4.84651206
1.40270079	9.87533419	4.76587269
6.37985971	9.87144960	4.75824818
4.99826815	4.86768309	4.72622841
0.02345917	4.85008981	4.71421126
0.70624495	7.29039828	4.73764976
5.71197709	7.33613465	4.69338088
5.75452281	2.18421776	4.51906218
0.75945212	2.18628416	4.50906625
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943

1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CO+C<sub>Cv</sub>->CCO<sub>Cv</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
1	40	4	80

Cart

6.24098425	11.30620884	7.99107812
4.19113686	9.29768179	7.38262178
3.12752828	3.51116882	8.58029183
9.57290575	2.52656523	8.22891287
1.76274329	7.62758154	8.42683944
6.77287570	7.58666641	8.41966198
9.19895795	9.31060002	7.37430894
2.19865976	4.24608550	7.49715599
7.19866666	4.27268626	7.20898144
3.40895792	11.93893224	7.21001388
8.44534835	11.96084606	7.16736833
-0.32576587	6.77316585	6.31930916
4.65277885	6.77242672	6.31558468
1.72872674	1.63224043	6.12150618
6.71984208	1.60249591	6.21348923
2.17028961	8.29376587	5.59305138
7.16420506	8.28836753	5.59267182
9.19490894	3.13601160	5.31189019
4.21184069	3.14059022	5.30386766
4.66987241	10.81129096	4.26561236
-0.31699618	10.82311525	4.27369765
6.72619090	5.69671369	4.01393426
1.73198472	5.68698061	4.01178299
7.17703742	12.34847175	3.63833013
2.19324347	12.34831349	3.64011149
9.23220341	7.20115329	3.34410678
4.23800064	7.20101228	3.34237416
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015

6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.60059357	7.34385323	9.57323247
3.31557659	3.64875289	9.75075959
9.76978410	2.34361909	9.39325012
1.63948519	7.38246120	9.58533187
2.52472823	10.25458352	7.10992036
0.02835418	10.92955756	6.84215681
3.18412556	7.79008062	7.13110940
8.17332389	7.80404955	7.13371249
0.68423593	12.44341239	4.88960761
7.50556630	0.07440232	7.08136799
3.86602608	5.16513852	6.95977554
8.86995932	5.16559023	6.98541935
3.18267871	2.71116193	6.90563020
8.18381862	2.72101362	6.93495388
0.71904124	8.32397721	6.94715672
5.70348900	8.32223492	6.94700679
4.98204389	10.92749831	6.93237045
7.53442094	10.28952334	7.18964394
1.37627898	5.86408875	6.82800351
6.36967207	5.89331623	6.76973980
0.68720176	3.30196870	6.76703716
5.69867910	3.30273749	6.68256027
0.00715059	0.90385352	6.69525413
4.96829650	0.87879870	6.65456862
3.23890750	11.76230806	5.18542594
8.22861026	11.77597111	5.17536965
8.88037404	9.23786272	5.08907467
3.89697136	9.23268476	5.08652025
7.51349610	4.22520007	5.04342021
2.51623602	4.21229528	5.04838275
8.19822515	6.75450243	4.92468321
3.19901979	6.74823526	4.92272507

5.66882879	12.41962641	4.90009400
2.52502838	0.12215791	7.04744863
3.24185977	1.48450014	4.82705385
8.20741102	1.47976569	4.84908529
1.40035368	9.89328349	4.80426055
6.39627722	9.90246264	4.83840734
5.01302612	4.85271841	4.70007686
0.03342551	4.84683742	4.74336406
0.72541825	7.27379926	4.71487461
5.71289616	7.28909013	4.70694653
5.75899162	2.19345433	4.51377783
0.74994269	2.20719434	4.51647610
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589

5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CO+CH->CHCO

1.000000000000

9.97980000	0.00000000	0.00000000
-0.76395804	12.66177393	0.00000000
0.00000004	0.00000004	19.64040000

H	C	O	Fe
2	41	4	80

Cart

6.76405994	6.69090617	9.30656610
1.23892426	11.33112155	7.98381390
6.84402839	7.16355663	8.32065684
4.61805974	2.64140276	8.22433820
9.58451806	2.64125244	8.23322289
4.16452305	9.31765411	7.25139959
1.80755840	7.64251974	8.42735677
6.38639971	8.76704771	8.73336540
9.21100495	9.30038030	7.37063021
2.19847666	4.25657108	7.20464361
7.16461707	4.29349870	7.17479075
3.45096242	11.97195745	7.17306176
8.38742475	11.93272403	7.20833642
-0.31544830	6.76784909	6.29664081
4.65173759	6.72623360	6.28432951
1.73185436	1.61760699	6.18059039
6.72583915	1.65529201	6.15392605
2.17516312	8.27783923	5.56873526
7.17166803	8.29748031	5.60980984
9.19530692	3.14437837	5.30256579
4.20333924	3.14296520	5.29455455
4.67301415	10.82550804	4.27945363
-0.31914069	10.81240211	4.26259455
6.72166811	5.70290210	4.01829054
1.73207652	5.69035260	4.01071750
7.18533580	12.35081131	3.63572849

2.18317418	12.34967742	3.63526816
9.22435957	7.20325181	3.33418424
4.23792750	7.20550666	3.33299324
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.47862156	9.28229482	9.80420367
4.76326773	2.48595677	9.40099291
9.71733876	2.48477787	9.41093662
1.65251299	7.42969116	9.58934076
2.53306973	10.30734501	7.18448015
-0.00970460	10.94287620	6.92304224
3.18965328	7.78307863	7.10675203
8.22637749	7.76262007	7.14289592
0.67298005	12.42371306	4.90076304
7.50332776	0.10547353	7.01825183
3.86749763	5.16942477	7.01716234
8.86346377	5.18612304	7.00972820
3.20885876	2.72392588	6.92284412
8.19342214	2.74822461	6.92267325
0.73302087	8.32237371	6.94178748
5.75942875	8.35182003	7.08918201
5.00087082	10.94629051	6.79732465
7.52659921	10.24029717	7.11079893
1.38820551	5.88774691	6.77569040
6.39947803	5.96597390	6.83644029
0.69474781	3.27497141	6.74291488
5.68061750	3.29343833	6.72726431
-0.00395582	0.88140575	6.71282065
5.00602574	0.90647514	6.68632023
3.23192764	11.78425599	5.17073526
8.22696310	11.76419641	5.18836386
8.89187236	9.23630887	5.09575890

3.89945107	9.23705683	5.09882485
7.50322348	4.24011510	5.04162203
2.51694007	4.22846463	5.04191688
8.18396344	6.77188960	4.91922944
3.20550333	6.75460755	4.90714451
5.67223137	12.44764484	4.87276324
2.51771997	0.09326991	7.07241976
3.22251637	1.47962384	4.84232267
8.22324453	1.48884358	4.84012924
1.40753709	9.90669768	4.84568281
6.39422775	9.89262945	4.80957895
5.01122076	4.86746477	4.73732397
0.02277703	4.85602894	4.73984090
0.72107045	7.29161024	4.69594462
5.71474492	7.31606006	4.72822831
5.74387897	2.20180050	4.50729527
0.75710659	2.19166893	4.51836642
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235

3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CO+CH<sub>2</sub>->CH<sub>2</sub>CO

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
3	41	4	80

Cart

5.94507994	8.43163804	9.01748138
7.71328014	8.22125795	9.27015075
1.24604075	11.34918055	7.98855153
6.94892549	8.69796269	8.62353250
4.60851159	2.59893903	8.22178701
9.58038583	2.55463224	8.22798871
4.17187501	9.33432156	7.28111349
1.79408908	7.69567327	8.43180620
6.92520687	10.38283574	9.08688402
9.21528395	9.34026885	7.29056107
2.19581631	4.26603437	7.20861464
7.18563637	4.27007820	7.21187921
3.46175757	11.98234627	7.18495758
8.40851935	11.93451267	7.21044243
-0.33473154	6.79239173	6.31468490
4.66586805	6.77609307	6.33116839
1.73446981	1.62100415	6.17855529
6.72738869	1.63500037	6.15665348
2.17198777	8.27981623	5.56073213
7.15846574	8.27023116	5.51758422
9.19892441	3.13312890	5.30805654



4.20585895	3.13427960	5.30026187
4.66842609	10.81119095	4.26351019
-0.32613717	10.81323011	4.26909443
6.72010616	5.68513118	4.01459974
1.73138881	5.68900416	4.01149706
7.18758088	12.34572295	3.64940029
2.18335332	12.34937711	3.64164070
9.23002108	7.19815520	3.32774168
4.23825074	7.20153104	3.33698212
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.55778701	10.81953029	10.12701423
4.75687285	2.43251954	9.39661335
9.74064206	2.38795293	9.39997910
1.62979091	7.52673409	9.60178870
2.54043169	10.32102308	7.18677010
0.02070836	10.96511946	6.89869076
3.17998444	7.80789862	7.11767084
8.13824644	7.84516544	7.10348009
0.66569893	12.42020252	4.89870965
7.52015762	0.11316345	7.04161896
3.86676940	5.17807013	6.98654757
8.84475176	5.19694871	6.98799089
3.20852866	2.73107244	6.92405449
8.20087958	2.73269369	6.92579866
0.72655424	8.32942692	6.92787604
5.72114699	8.36390302	6.89482454
5.02193957	10.96180856	6.85720209
7.52081826	10.27097287	7.41806945
1.37655166	5.89599011	6.77536410
6.38753294	5.88857470	6.70568707
0.69885871	3.27171109	6.74687699

5.68804959	3.28592940	6.73816307
0.00923388	0.88276046	6.72489818
5.00032091	0.91552238	6.68570851
3.23777840	11.77550721	5.17992733
8.19783984	11.71937643	5.22289084
8.89401142	9.24756787	5.13052171
3.89083883	9.24329714	5.11340739
7.51274605	4.21531292	5.03036393
2.51421216	4.22458820	5.04070452
8.19974120	6.75304739	4.92183247
3.20612467	6.74735943	4.92240045
5.66897592	12.43015295	4.88715109
2.53112148	0.10532930	7.07352675
3.22328949	1.47529422	4.84484502
8.22892218	1.46960254	4.84289182
1.40510959	9.90984902	4.83570740
6.38709738	9.91819780	4.84503640
5.00729674	4.84180878	4.71772780
0.02349691	4.84375397	4.73257571
0.72192217	7.27933338	4.70142587
5.69641687	7.27208047	4.70290278
5.74856793	2.19624059	4.50984303
0.75923086	2.19162457	4.51860815
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425

-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CO+CH<sub>3</sub>

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	41	4	80

Cart

2.58654742	1.59347832	9.41989477
2.46746284	12.60457083	9.69630728
6.23474279	11.30305530	7.96631051
1.44365438	0.21981113	9.53892416
2.44377670	0.52719001	9.21010589
4.68796672	2.92138770	8.25755258
9.62993793	2.68734692	8.22176072
4.18680303	9.29280028	7.39558620
1.79340284	7.47517689	8.40092999
6.78637326	7.51612748	8.40626871
9.19659391	9.30972172	7.38877535
2.19795560	4.26605582	7.17865254
7.20078398	4.27080828	7.17767685
3.38860469	11.92960719	7.16358586
8.44621811	11.96317716	7.16745422

-0.33068320	6.77421093	6.30407226
4.66324839	6.76850511	6.30974415
1.76100414	1.58710835	6.15033857
6.73918557	1.61995448	6.18490824
2.17705021	8.30132097	5.60797364
7.16506112	8.29304184	5.59765797
9.20034557	3.13248831	5.29162829
4.21438241	3.12605217	5.30008092
4.67092890	10.81112726	4.26423868
-0.31408065	10.82270105	4.27124539
6.72448648	5.70011685	4.01356247
1.73505127	5.69711052	4.01573969
7.18070640	12.34758007	3.63906636
2.18807653	12.35234901	3.65184950
9.22903565	7.20074966	3.33552170
4.23875332	7.20411950	3.34077111
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.60166090	7.25460926	9.55593814
4.73882710	2.87220865	9.44788694
9.75086771	2.55391565	9.40259148
1.58672831	7.19996606	9.54321983
2.51957878	10.23591888	7.08839127
0.04057463	10.93284108	6.84008189
3.18588454	7.77669708	7.13698496
8.17577303	7.79941286	7.13365538
0.68401712	12.43529964	4.90662097
7.51121509	0.07855853	7.06497359
3.87524501	5.16712183	6.99515451
8.87015656	5.17187585	6.99284672
3.22848419	2.73390618	6.93457918
8.20939064	2.72858684	6.91723867

0.71359930	8.32609179	6.95545068
5.70110775	8.32086171	6.95604097
4.97498574	10.92032761	6.91290579
7.53915843	10.29101649	7.18771595
1.38126895	5.90404994	6.78265520
6.38283944	5.90862808	6.78039127
0.70399030	3.28516986	6.71639701
5.70138515	3.29302507	6.71640359
0.02170176	0.89977436	6.68744905
5.00681795	0.87257368	6.67457967
3.24552646	11.76812728	5.17945541
8.23410779	11.77533785	5.17533364
8.88132975	9.24467008	5.09503416
3.89960193	9.22450867	5.07042298
7.51098038	4.22983737	5.03395937
2.52275471	4.21949772	5.04213650
8.20004291	6.76259433	4.92046525
3.20752972	6.75673718	4.92087951
5.67403789	12.41716924	4.89875701
2.53310209	0.15481269	7.24088822
3.24760900	1.46614302	4.85767089
8.22202258	1.46779587	4.84544807
1.40648988	9.88982964	4.79409260
6.39714903	9.90341456	4.84297383
5.01747788	4.85461931	4.73738623
0.02683561	4.85595768	4.73267118
0.72924181	7.30017896	4.70475198
5.71728529	7.29275728	4.70594100
5.75667501	2.18331288	4.50751503
0.76519404	2.19090968	4.50645568
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899

5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for CO+CH<sub>3</sub>->CH<sub>3</sub>CO

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	41	4	80

Cart

2.62052863	2.16274747	10.04444046
3.70278612	0.79612985	9.55337760
6.24240900	11.29854182	7.98905289
2.11077502	1.08398657	8.76339819
3.00812169	1.56928318	9.20822647
4.27735491	2.70472485	8.61131076
9.62632429	2.61005409	8.21355544
4.20106658	9.27288527	7.40117132

1.79000649	7.54878545	8.41882801
6.77857600	7.59538883	8.42573553
9.20525951	9.30072049	7.39021770
2.18163612	4.25088326	7.20886527
7.21763135	4.27240244	7.18423935
3.41780120	11.89507778	7.17226986
8.45170691	11.95004989	7.17621794
-0.33040097	6.77259795	6.30714529
4.66225585	6.75160664	6.31134842
1.70419237	1.62927556	6.13267844
6.74714338	1.59861087	6.20562795
2.18111999	8.28349094	5.59979404
7.16603914	8.27703202	5.59243905
9.19350784	3.13084991	5.28478585
4.22214227	3.12191930	5.35808124
4.67600976	10.78930803	4.25622135
-0.31283295	10.80999844	4.26628070
6.72229578	5.68619740	4.01305616
1.74025587	5.65378946	4.02497743
7.18514248	12.34559453	3.63417228
2.19728764	12.35133291	3.63605171
9.23257603	7.20078711	3.34172040
4.23887406	7.20307479	3.34646193
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.63088152	7.36718770	9.58775066
5.07340148	2.97870651	9.46573045
9.75638778	2.42262403	9.38991874
1.62599687	7.30569176	9.57566797
2.53521971	10.21920909	7.09575699
0.03744027	10.91959806	6.85641995
3.19126108	7.76615022	7.13357430

8.17777440	7.79824647	7.13310246
0.68795545	12.43055021	4.87879975
7.51269537	0.05686578	7.06754844
3.86166029	5.14577229	6.98228186
8.88167289	5.16994282	7.00101441
3.23389384	2.67980481	7.15270268
8.20084689	2.71894614	6.91874160
0.72340191	8.31735938	6.95612856
5.70866649	8.30632390	6.95171817
4.99489954	10.90083405	6.92592938
7.54377838	10.27852932	7.19887507
1.37897154	5.88795116	6.79551766
6.37570101	5.89088931	6.78102787
0.69041479	3.27099472	6.72347232
5.70225463	3.28267397	6.72566059
0.00207845	0.88861612	6.67454435
5.00430345	0.83700797	6.63104515
3.24907404	11.74718847	5.16853122
8.23321308	11.76023927	5.17736553
8.88518558	9.22975300	5.08921145
3.90661772	9.20775640	5.07725963
7.50402264	4.21878059	5.04988635
2.52406406	4.15277897	5.10744959
8.20130111	6.74929175	4.92221058
3.20181598	6.72826835	4.92213888
5.67615836	12.40741226	4.89088633
2.53384408	0.08243459	6.99444714
3.23456637	1.50967135	4.88800636
8.21651201	1.46510338	4.84297577
1.40426848	9.88059926	4.80458864
6.40092018	9.89191206	4.84616632
5.01235163	4.83456867	4.73798624
0.03515854	4.84479751	4.73854649
0.73311917	7.27733297	4.70850597
5.71640848	7.27269141	4.70801555
5.75444440	2.18833588	4.52261798
0.75130112	2.19205754	4.50101992
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265



2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# H+CH<sub>Cv</sub>

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9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
2	40	4	80

Cart

4.28472379	9.44277776	9.03183489
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6.23278268	11.23305456	7.93940917
4.22725774	9.27584247	7.94343044
4.60924062	2.56618334	8.22637446
9.61363946	2.64105785	8.23156793
1.82819438	7.52117173	8.43818228
6.72899684	7.74514564	8.46896442
9.19453644	9.29788937	7.39749165
2.21044504	4.25932764	7.19134775
7.18649081	4.25069284	7.19250339
3.40962124	11.87389628	7.16674490
8.44098784	11.93730566	7.16859108
-0.33659989	6.77887544	6.32991031
4.64727677	6.82737578	6.33834219
1.73992399	1.61996367	6.16783246
6.72902005	1.58800991	6.18036851
2.19271656	8.33808870	5.66568518
7.15034705	8.29076522	5.61525937
9.20136079	3.13698173	5.30011155
4.20945396	3.13357012	5.30166680
4.67935440	10.82039559	4.28063171
-0.32098777	10.80523868	4.26690482
6.72378891	5.69440193	4.02073732
1.73466031	5.70400098	4.01998340
7.18172045	12.34673096	3.63861921
2.19029874	12.34722201	3.63759055
9.23168812	7.19873948	3.35294065
4.24064981	7.20977254	3.36442075
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.64575118	7.52395681	9.63707790
4.76869861	2.38537399	9.39663293
9.73409939	2.49620739	9.41153531

1.62785046	7.24612635	9.58018414
2.56519541	10.17693335	7.05159695
0.02990785	10.90976424	6.86837824
3.21643537	7.82091290	7.17134973
8.15238835	7.80351530	7.14855879
0.67826773	12.42823726	4.88946673
7.49858456	0.03719680	7.06300240
3.88929603	5.16807939	6.96572851
8.85991380	5.16401010	6.98285273
3.21993115	2.71957399	6.92307528
8.20069119	2.71193959	6.92381169
0.72035111	8.31519911	6.97828308
5.66569127	8.35418470	6.97638405
4.96684587	10.82741285	6.86494778
7.52887809	10.26799618	7.17867304
1.38662508	5.89584637	6.78475659
6.36086631	5.87821261	6.75697946
0.70289922	3.27642573	6.73650805
5.69181286	3.24641530	6.73789860
0.01716224	0.88094027	6.70187700
4.99378081	0.83798371	6.70575181
3.24024954	11.75489443	5.17290959
8.23215577	11.75953776	5.17483930
8.88002838	9.23035075	5.10267072
3.88477746	9.19522254	4.98051691
7.50747664	4.21966040	5.04048290
2.51552092	4.22462934	5.03813325
8.18966228	6.75943475	4.93357952
3.19241188	6.75390455	4.94029527
5.67070596	12.42723764	4.89679645
2.52445402	0.06488695	7.02591587
3.23249670	1.47489097	4.84051127
8.22443983	1.46851334	4.84688112
1.39377661	9.88431882	4.77838237
6.38970958	9.88045451	4.81072151
5.01411276	4.84053992	4.71553143
0.02541542	4.85479352	4.72887368
0.72559912	7.30859845	4.72025584
5.70663507	7.28219521	4.72006338
5.75181326	2.18603761	4.51419635
0.75953524	2.19060289	4.51454485
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382

4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for H+CH<sub>cv</sub>->CH<sub>2 cv</sub>

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9.97980000	0.00000000	0.00000000
-0.76395804	12.66177393	0.00000000
0.00000004	0.00000004	19.64040000

H	C	O	Fe
2	40	4	80

Cart

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5.17675882	10.33700085	8.30553514
4.31756441	9.31832696	8.04726850
4.61106301	2.56640798	8.22206999
9.60154606	2.61402612	8.22638165
1.83822511	7.55267422	8.43333894
6.73579522	7.69213484	8.46659636
9.19610368	9.28375128	7.41096759
2.20151676	4.26026710	7.19533103
7.18486479	4.24652987	7.20117634
3.43423233	11.86335395	7.16618017
8.39374902	11.91112770	7.19473439
-0.31672147	6.76309202	6.32770154
4.65773247	6.81963868	6.33218057
1.73172166	1.60923101	6.18439041
6.72634111	1.60178350	6.16717484
2.20728858	8.34197817	5.67259906
7.16391274	8.28572078	5.63054181
9.19815007	3.13902027	5.30303610
4.20481355	3.13580449	5.30224792
4.68630102	10.82090177	4.29356139
-0.31869309	10.80817228	4.26811422
6.72562210	5.69709908	4.01792754
1.73674250	5.70826507	4.01795218
7.18391617	12.34873467	3.64270435
2.18764060	12.34925200	3.63945976
9.23300478	7.20174595	3.35583257
4.24226386	7.21162469	3.36432432
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304

-0.23342146	8.73880577	0.18583304
6.67181718	7.47754662	9.63788476
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9.73034718	2.45344999	9.40376169
1.67473842	7.29201909	9.58603751
2.53845872	10.17910508	7.03479812
0.01012935	10.90744328	6.88650034
3.24911105	7.84863396	7.16801038
8.17498691	7.77925809	7.15271828
0.67793789	12.42111335	4.89855104
7.46714667	0.02584923	7.03466848
3.88781901	5.16856503	6.97548851
8.85810784	5.16023215	6.98837522
3.21008639	2.72038740	6.92347669
8.19709850	2.71148150	6.92003052
0.72860325	8.31764143	6.98507145
5.68546148	8.33337561	6.99107508
4.95442112	10.79563352	6.81493453
7.52047955	10.22162512	7.12034741
1.40910790	5.90971999	6.78986245
6.36597570	5.87921922	6.78099309
0.70079895	3.26405901	6.73939668
5.68557078	3.24825479	6.73952356
0.00367147	0.85553980	6.71853718
4.99656184	0.83576582	6.70998475
3.24549977	11.76035465	5.16940711
8.23084907	11.75487698	5.18455402
8.88527547	9.21779943	5.07806274
3.89226954	9.18552525	4.95635476
7.50550744	4.22325073	5.04032858
2.51411648	4.22825348	5.03838306
8.19818204	6.75416613	4.93328431
3.19565395	6.75727560	4.94476709
5.67632457	12.42447798	4.89785006
2.53339879	0.04953973	7.02545852
3.22285739	1.47700440	4.84259331
8.22148540	1.47310946	4.83931961
1.40151130	9.88304554	4.78015460
6.39296978	9.86857764	4.80558713
5.01679569	4.84535875	4.72934679
0.03121318	4.85886911	4.74355700
0.73584202	7.31568037	4.71888898
5.71687215	7.28393462	4.71940561
5.74459479	2.18430497	4.51425347

0.75591321	2.18465439	4.52076987
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>2</sub> cv

1.000000000000

9.97980000	0.00000000	0.00000000	
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0.00000004	0.00000004	19.64040000	
H	C	O	Fe
2	40	4	80

Cart

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5.42906466	9.62254259	8.09768918
4.14274106	9.25966188	8.07515900
4.61000578	2.57032363	8.21971034
9.59589459	2.60639315	8.22352403
1.86769630	7.52772742	8.44174997
6.77224900	7.57655877	8.46567307
9.20202153	9.28143471	7.42192079
2.19526104	4.25827588	7.19798793
7.18203747	4.25429086	7.20156278
3.41091665	11.87788991	7.16904423
8.39523606	11.90382161	7.19416628
-0.31384228	6.75819255	6.32878540
4.65506158	6.79778785	6.31503357
1.72925328	1.61206086	6.18242318
6.72235126	1.60901162	6.16919959
2.21038760	8.34452028	5.67230316
7.15262207	8.29076097	5.65918068
9.19219366	3.14141017	5.29966525
4.20269958	3.13866731	5.30042277
4.68188697	10.82043019	4.27514946
-0.31953762	10.80669503	4.26805396
6.72483426	5.70405855	4.01682851
1.73573051	5.70871750	4.01757735
7.18255970	12.34785470	3.64219267
2.18794084	12.34889245	3.63808047
9.23218592	7.20291744	3.36022696
4.24322625	7.21221389	3.36067209
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183



0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.69201480	7.38360731	9.63998689
4.74843477	2.39164797	9.39430300
9.72613695	2.43765831	9.39847632
1.63805312	7.31976716	9.59300197
2.57838323	10.17273977	7.03997490
0.01301738	10.90426052	6.88294218
3.24002419	7.81223906	7.17141851
8.18461344	7.77474140	7.15869338
0.67750620	12.42001881	4.89644945
7.48395000	0.04212973	7.02991996
3.88189228	5.16312580	6.98990000
8.85859981	5.16027296	6.99598221
3.20661128	2.72045416	6.92210873
8.19290965	2.71584003	6.91837364
0.72697581	8.31721245	6.97630551
5.67165181	8.33141637	7.04620925
4.97744783	10.86375924	6.84065328
7.52221540	10.21365408	7.11910642
1.41072957	5.91180275	6.79658015
6.36552078	5.89660684	6.81512385
0.69536188	3.26443589	6.73933268
5.68328034	3.25537524	6.73914342
0.00341072	0.85348827	6.71870553
4.99942829	0.84142470	6.72096524
3.24297520	11.76246444	5.16891908
8.23106076	11.75442549	5.18339761
8.87657939	9.21560707	5.07019988
3.89068077	9.19408092	4.96814119
7.50183919	4.23483053	5.04478930
2.51285701	4.23129909	5.04011214
8.19394363	6.75794333	4.93679498
3.19571997	6.75838487	4.93533049
5.67391869	12.41707080	4.89676072
2.51925033	0.05312577	7.02380052
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6.38448871	9.86417395	4.81236205
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0.73463817	7.31762849	4.71720995
5.71570137	7.29301941	4.73660493
5.74249708	2.18381606	4.51679331
0.75241267	2.18414345	4.52149408
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
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8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
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5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002

0.69460732 10.28863907 0.50651002

# H+CH<sub>2</sub> cv

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9.97980000	0.00000000	0.00000000
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H C	O Fe	
3 40	4 80	

Cart

3.88658270	9.37714391	9.20179494
5.28766995	9.48120271	8.19989818
6.25472539	11.32662959	7.98261805
4.07803873	9.21885316	8.12595218
4.61059625	2.57608829	8.22114829
9.59802283	2.60447179	8.21719424
1.85563286	7.47590745	8.42867612
6.78338031	7.57141419	8.46855963
9.19648399	9.29729451	7.41295877
2.19712728	4.26210508	7.19774510
7.18267768	4.25153993	7.20168014
3.40342556	11.87757586	7.18377209
8.44936181	11.93860847	7.16002250
-0.32437650	6.76506862	6.32859959
4.64791142	6.78769097	6.30730931
1.73987093	1.62148988	6.17288201
6.72472186	1.59554032	6.18151400
2.20510131	8.34494007	5.66946788
7.13633819	8.28001968	5.65856884
9.19311528	3.13953383	5.29323103
4.20625554	3.13810660	5.29987764
4.68077016	10.80965756	4.26462552
-0.31954426	10.80222285	4.27099474
6.72367577	5.70402891	4.01626307
1.73393314	5.70845284	4.01809010
7.17937547	12.34753200	3.64086086
2.19560064	12.34838885	3.63965653
9.23114154	7.20165494	3.35899757
4.24225782	7.21249915	3.35794187
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742

7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.68387369	7.38002629	9.64225127
4.74120804	2.39021245	9.39499541
9.72909709	2.43392363	9.39313147
1.60922028	7.28372546	9.57950867
2.59388168	10.16519579	7.04694978
0.03256008	10.90193596	6.84654157
3.22211262	7.79026041	7.16704382
8.17203228	7.79226816	7.16162602
0.68409375	12.42548741	4.88583397
7.51034186	0.05430768	7.06017417
3.88234035	5.15994618	6.99658958
8.85530620	5.16610043	7.00038549
3.21059541	2.72280130	6.91959493
8.19426760	2.71513895	6.91519695
0.71657815	8.31661445	6.97087179
5.65448015	8.31413133	7.04304128
4.98639515	10.87986435	6.91485601
7.53255363	10.27271565	7.18535062
1.39889850	5.91133229	6.80483560
6.36391670	5.89109210	6.81271890
0.69576197	3.27810536	6.73624214
5.68606407	3.25182756	6.74046442
0.01803793	0.88316595	6.69349717
4.99526358	0.84151159	6.71419060
3.24667915	11.74632927	5.18044514
8.23328481	11.75972841	5.17407513
8.86485426	9.22370762	5.09061510
3.89359054	9.19497888	4.98502269
7.50324109	4.23624341	5.04537026
2.51408909	4.23215049	5.04068672
8.19191585	6.76151785	4.93850819
3.19197603	6.75888887	4.92925170
5.67345812	12.40640279	4.90870417
2.52261448	0.05712673	7.02050307

3.23219156	1.47457825	4.84244970
8.21669030	1.46649316	4.84322588
1.39506834	9.87581953	4.76510760
6.37950702	9.87371133	4.85671722
5.01642508	4.85417195	4.74158606
0.02508415	4.86460272	4.74447269
0.73076189	7.31777290	4.71675509
5.71107248	7.28757304	4.73649099
5.74761263	2.18212019	4.51830103
0.75642663	2.18945704	4.51737222
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453

6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for H+CH<sub>2</sub> cv->CH<sub>3</sub> cv

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9.97980000	0.00000000	0.00000000
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H	C	O	Fe
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Cart

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5.14788866	8.56900265	8.57181407
5.29303891	10.45646879	8.31977497
4.38180675	9.38782070	8.19964209
4.60802377	2.57855484	8.22414784
9.60198807	2.60890479	8.22545421
1.86672541	7.79465788	8.47676131
7.35940055	7.29440936	8.68428199
9.18444346	9.28694520	7.36701470
2.20058178	4.26891152	7.20524032
7.18508218	4.24939054	7.18769358
3.43029839	11.86945288	7.17621842
8.38805622	11.91621259	7.19307504
-0.29844306	6.75580227	6.30327318
4.65324547	6.82480411	6.34400480
1.73176225	1.62194440	6.18339303
6.72843631	1.60708022	6.16757928
2.20782881	8.33913855	5.64748128
7.14120188	8.27770147	5.64635985
9.19989577	3.14088193	5.30191691
4.20442808	3.13509694	5.30202911
4.68960135	10.82764811	4.29371501
-0.32119241	10.79324449	4.26804306
6.72495972	5.69929682	4.01794439
1.73613503	5.70444929	4.01698509
7.18412902	12.34817500	3.64142027
2.18728182	12.35087948	3.64041957
9.23223866	7.20412831	3.34899056

4.24397043	7.21159189	3.36409408
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
6.91671328	7.08591709	9.75492338
4.75166324	2.40228856	9.39866678
9.73015740	2.44032680	9.40235216
1.72977580	7.66501702	9.65469082
2.48573126	10.21133156	6.99974085
0.00876497	10.92156019	6.88840053
3.24528214	7.89211085	7.14958262
8.19820305	7.74511867	7.17808888
0.67680388	12.41886240	4.89715079
7.46479050	0.03121326	7.03743619
3.88982295	5.17549805	6.97699389
8.85960318	5.18176265	7.01880926
3.20981915	2.72903977	6.92492986
8.20014849	2.71872102	6.91954038
0.73832167	8.34083144	6.97104579
5.66844996	8.41944909	6.90553998
4.94711264	10.81265583	6.82282226
7.51586637	10.22497845	7.08757551
1.43441132	5.92282453	6.76922223
6.36860551	5.88704680	6.77472775
0.70264532	3.27009329	6.74324820
5.68368077	3.25291372	6.73840668
0.00529932	0.85991537	6.72134991
4.99675553	0.84085028	6.71012673
3.24792712	11.76620183	5.17034668
8.23682683	11.76144948	5.17859093
8.87652777	9.20748947	5.11931352
3.90253867	9.19346989	4.95802039
7.50943772	4.22871122	5.04287526

2.51772601	4.23042704	5.03770490
8.20095072	6.75672241	4.92894097
3.19855489	6.75604210	4.95077190
5.67897596	12.42550759	4.90085020
2.53136230	0.06425771	7.02907821
3.22142805	1.47898260	4.84403611
8.22066305	1.47666461	4.83982333
1.40377420	9.88500409	4.76829716
6.39732177	9.87249535	4.78445801
5.01836400	4.84237563	4.72619630
0.02857801	4.86363855	4.75284373
0.73995311	7.31473658	4.71133132
5.70965433	7.27203621	4.73086913
5.74477300	2.18376653	4.51427276
0.75534298	2.18591677	4.52202663
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367



3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# CH<sub>3</sub> cv

1.000000000000

9.97980000	0.00000000	0.00000000	
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H	C	O	Fe
3	40	4	80

Cart

3.76000046	8.70923077	8.93413324
5.50073431	8.73166882	9.28009911
4.62773437	10.22153669	8.88933235
4.75016343	9.15459196	8.59173718
4.60893925	2.57521191	8.22219636
9.60746214	2.64218208	8.22898212
1.73299882	7.55879834	8.42487694
7.49763767	7.09806093	8.66852244
9.17594385	9.27597397	7.37133987
2.21673041	4.26885119	7.19872912
7.17731491	4.25079599	7.16649345
3.38916373	11.82295561	7.18820573
8.37898836	11.91077470	7.19413477
-0.29906576	6.73876759	6.26817360
4.64189876	6.85371678	6.36677356
1.73299289	1.62897145	6.17369134
6.72055082	1.60451768	6.16351734
2.19407108	8.36996282	5.68544070
7.14830019	8.29680843	5.61986352
9.19999274	3.13980681	5.29923938
4.20335182	3.14156574	5.29227793
4.68454006	10.81835435	4.26860288
-0.32297873	10.80193775	4.27398974

6.72481788	5.69840933	4.01944717
1.73859455	5.71779322	4.01949653
7.17889734	12.34801891	3.64315529
2.19208394	12.35135853	3.64176611
9.23066772	7.20468259	3.33721700
4.23924782	7.21040349	3.37473423
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
7.07755528	6.79765723	9.72562543
4.75926158	2.40850929	9.39586080
9.73295048	2.49584030	9.40788560
1.58784650	7.29409985	9.58367083
2.35506202	10.25285057	6.86394890
-0.01228822	10.91974678	6.87939761
3.24943782	7.92661891	7.22370543
8.20112521	7.72337885	7.15902167
0.68811685	12.41969298	4.90105872
7.47637485	0.04142875	7.02848398
3.91077433	5.17151472	6.97531289
8.85440045	5.18358455	7.01912365
3.21509171	2.72629287	6.91938046
8.19900501	2.72045509	6.91950551
0.72167244	8.32678000	6.97739393
5.66052187	8.43617803	6.92367498
4.96525095	10.79719321	6.86152672
7.52295848	10.20972667	7.07190086
1.43070861	5.91852140	6.79591637
6.36065217	5.89092649	6.73249036
0.70585771	3.27665066	6.74052671
5.68262568	3.24374438	6.72991251
0.00678840	0.86052219	6.72233196
5.00034773	0.79980459	6.74407856

3.26275852	11.77125518	5.16541363
8.23936628	11.76638929	5.17504562
8.87360653	9.20341694	5.11882183
3.90284568	9.20574188	5.00491883
7.51103453	4.22526572	5.03622804
2.52075605	4.24579231	5.03651051
8.19519270	6.76206526	4.91102515
3.19944422	6.78002575	4.99087844
5.68181958	12.41198270	4.91097803
2.52028664	0.07615802	7.03711751
3.23089536	1.47523066	4.84427159
8.21818801	1.47760542	4.83950851
1.39487118	9.86467433	4.69102593
6.39765726	9.88336956	4.76283946
5.01225451	4.85177125	4.71643983
0.02809377	4.87249351	4.76749994
0.74934599	7.32358974	4.70960305
5.70935374	7.29639115	4.72637180
5.74308821	2.17936404	4.51388486
0.75595214	2.18704280	4.52079472
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233

7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# H+CH<sub>3</sub> cv

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	40	4	80

Cart

4.03162849	7.39796891	9.51673514
5.46211026	8.19913887	8.97860826
4.05450131	9.19118922	9.38244833
5.99643991	10.02559102	7.82145650
4.33868587	8.24969402	8.89751682
4.60063221	2.57318114	8.22459220
9.60327495	2.60940878	8.22638629
1.73721881	7.53585069	8.45613592
7.68188356	6.98143653	8.72185977
9.17953853	9.26064837	7.35790306
2.20925098	4.24006294	7.20669214
7.17553409	4.24287996	7.16732583
3.45651647	11.78668072	7.16566321
8.40320542	11.89266095	7.19393762
-0.30267804	6.72109221	6.26535959
4.63613697	6.81896179	6.36079330
1.74102808	1.59357350	6.17618825
6.72207557	1.59439220	6.15580948

2.20603400	8.36267472	5.67901336
7.11272322	8.29017975	5.71337301
9.20263992	3.14222985	5.29921550
4.20327818	3.14056894	5.29943640
4.69557650	10.83017205	4.30835301
-0.32185398	10.78455181	4.28014960
6.72379217	5.70495507	4.02303298
1.73640939	5.70984181	4.01910935
7.19218557	12.34951580	3.63343060
2.18421855	12.35094972	3.63065403
9.22841783	7.20439618	3.34486526
4.23688024	7.21212667	3.36787370
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
7.35595312	6.61760732	9.78883801
4.75532029	2.42138441	9.39965250
9.72939131	2.47071585	9.40561369
1.42360478	7.27660780	9.57845267
2.46400788	10.16886479	6.93528598
0.00605477	10.89397629	6.86482626
3.18080212	7.75833356	7.22909015
8.22231900	7.69443042	7.17873192
0.68336342	12.41465569	4.89852256
7.51013789	0.05595600	7.03141131
3.89218800	5.14703848	6.96712909
8.85285655	5.17174856	7.02995142
3.21128955	2.70298558	6.92043264
8.19874336	2.71163392	6.91935278
0.72223846	8.31278987	6.95054852
5.59630711	8.44770627	7.01904946
5.04636283	10.90166388	6.65717436
7.52622903	10.21045304	7.10381513

1.41553772	5.88035373	6.77557115
6.36114002	5.88721931	6.73366614
0.70517370	3.25495943	6.73945193
5.68315925	3.23791665	6.73222098
0.02258207	0.84563676	6.73231980
4.99782881	0.81104597	6.72252626
3.24100555	11.77384660	5.15377135
8.23112609	11.74987876	5.17713048
8.85575691	9.19357285	5.13799966
3.90804124	9.19022278	5.01582003
7.51040791	4.22467770	5.03779040
2.51778234	4.23294252	5.03431035
8.17859653	6.76522166	4.91893435
3.19349576	6.77104210	4.95571990
5.68535342	12.45823655	4.86220253
2.55535030	0.02771048	7.02754580
3.23003406	1.47571577	4.83916676
8.23782201	1.47571958	4.84306452
1.39909186	9.86422281	4.71972615
6.41394493	9.84203275	4.72365881
5.01574303	4.85448552	4.72391536
0.02037449	4.87138465	4.76487772
0.74007684	7.32067697	4.70417608
5.70391967	7.30793552	4.75008964
5.74540728	2.19277728	4.51015570
0.75962705	2.18283725	4.52057393
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425
5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903

5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

# TS for  $H+CH_3 \text{ cv} \rightarrow CH_4(g)$

1.000000000000

9.97980000	0.00000000	0.00000000	
-0.76395804	12.66177393	0.00000000	
0.00000004	0.00000004	19.64040000	
H	C	O	Fe
4	40	4	80

Cart

4.30975048	7.85896189	9.02215812
5.74073114	8.59940962	9.72546605
4.32315898	9.62252273	9.33564404
5.69763592	9.67091321	8.06604140
4.93666552	8.77977208	8.99720565
4.59276800	2.54550504	8.22349733
9.58950465	2.58820739	8.22692522
1.70364226	7.90873378	8.49863763
7.67767345	6.97758464	8.70820288
9.17204295	9.27104333	7.36442780
2.20967852	4.24664156	7.20800722
7.17376329	4.24496891	7.16606153

3.43379090	11.79353972	7.17556346
8.38322310	11.89696496	7.20604174
-0.29998698	6.73314577	6.27345880
4.65546066	6.84950389	6.40692692
1.73269276	1.59987588	6.17652852
6.71278205	1.60103824	6.15507936
2.18236804	8.34583454	5.65085549
7.12037882	8.27476015	5.70493824
9.20002705	3.13743089	5.30153677
4.20167066	3.13400271	5.29960067
4.68787582	10.82426983	4.29748697
-0.33057127	10.79051215	4.27523115
6.72184586	5.70241752	4.02437213
1.73425433	5.70065238	4.02089651
7.18762363	12.34911149	3.63431224
2.18025863	12.35068814	3.63233913
9.22759930	7.20472348	3.34428955
4.24194350	7.20975064	3.37879978
5.47292232	2.23055553	2.34193015
0.48302215	2.23055553	2.34193015
6.73540354	9.72874641	2.00704742
1.74550355	9.72874641	2.00704742
7.98876715	3.77819967	1.47019899
2.99886727	3.77819967	1.47019899
9.21347809	11.29064846	1.28800344
4.22357798	11.29064846	1.28800344
5.52626467	6.13002825	0.45987183
0.53636485	6.13002825	0.45987183
7.45328903	1.12937152	0.40848067
2.46338916	1.12937152	0.40848067
4.75647831	8.73880577	0.18583304
-0.23342146	8.73880577	0.18583304
7.35432483	6.61746258	9.77798654
4.75549645	2.38498519	9.39697758
9.73008569	2.42952778	9.40277939
1.67146358	7.83092091	9.68884570
2.42808946	10.20314158	6.90318646
-0.01033572	10.91038088	6.88056266
3.18585875	7.82737922	7.18820132
8.23474542	7.70102500	7.17616322
0.67417318	12.41265246	4.90168202
7.49535662	0.06194916	7.03151913
3.88885778	5.16860414	6.96242200
8.85631175	5.17181214	7.02811916



3.20906000	2.70704466	6.92273059
8.19534630	2.71140257	6.92082457
0.72647095	8.34234712	6.95434443
5.61987631	8.52027755	6.93465546
5.02959808	10.90283667	6.67522977
7.50846986	10.20627654	7.10074767
1.42177077	5.87949005	6.74945993
6.36185752	5.89574606	6.75016983
0.70156960	3.25352063	6.74300637
5.67923403	3.23731409	6.73431428
0.01199388	0.84375481	6.73527117
4.99223772	0.80694193	6.73263962
3.23515032	11.77190134	5.15285919
8.22303371	11.75166621	5.18165808
8.86228072	9.19212314	5.13302526
3.89529132	9.19234353	5.01031906
7.50596695	4.22216145	5.04131307
2.51777331	4.22399259	5.03526011
8.18135311	6.76012742	4.91947530
3.19792526	6.75587071	4.97489030
5.67861603	12.44771168	4.86755504
2.53990824	0.04521791	7.03709927
3.22256937	1.47317785	4.84087106
8.22805242	1.47607498	4.84250441
1.38594516	9.87167826	4.71231010
6.40446739	9.84343580	4.73578054
5.01255154	4.84302683	4.71695722
0.01806106	4.86161033	4.75601540
0.73642667	7.30359915	4.70301121
5.69703650	7.28852262	4.75691609
5.74053349	2.18676354	4.51103844
0.75629910	2.18286131	4.52039068
8.92724419	3.16928101	3.13275409
3.93734455	3.16928101	3.13275409
9.65447807	0.51179242	2.92767382
4.66457796	0.51179242	2.92767382
8.19081593	10.75315189	2.92137337
3.20091629	10.75315189	2.92137337
7.52427816	8.16568470	2.89047265
2.53437829	8.16568470	2.89047265
6.46140337	3.88992119	2.81003308
1.47150326	3.88992119	2.81003308
8.23615360	5.59719324	2.75910425
3.24625349	5.59719324	2.75910425

5.72548342	11.29866314	2.69921899
0.73558354	11.29866314	2.69921899
5.02271366	8.84247589	2.64073300
0.03281343	8.84247589	2.64073300
7.16234589	1.15467191	2.58495903
2.17244577	1.15467191	2.58495903
5.69094276	6.28061676	2.47308970
0.70104283	6.28061676	2.47308970
4.72644854	4.52631235	0.98044425
-0.26345146	4.52631235	0.98044425
8.98416233	2.08401227	0.94984233
3.99426270	2.08401227	0.94984233
7.49692297	12.16127491	0.88189071
2.50702286	12.16127491	0.88189071
8.92881203	7.14167833	0.77916235
3.93891239	7.14167833	0.77916235
8.23179626	9.65808487	0.74752367
3.24189639	9.65808487	0.74752367
6.50168800	2.71004343	0.73384589
1.51178777	2.71004343	0.73384589
5.78449345	0.24636792	0.66762453
0.79459333	0.24636792	0.66762453
6.40908241	7.83185196	0.60482943
1.41918242	7.83185196	0.60482943
7.18588972	5.31081581	0.60368013
2.19598985	5.31081581	0.60368013
5.68450737	10.28863907	0.50651002
0.69460732	10.28863907	0.50651002

#### 4. Interface

# Fe<sub>5</sub>C<sub>2</sub>(100)//Fe<sub>2</sub>C(011)

1.000000000000

4.60093331	0.00000000	0.00000000
0.00027824	5.04220787	0.00000000
0.03925410	2.48268598	21.00283815

C	Fe
16	36

Cart

4.22491450	4.05994622	0.03578439
4.53244306	2.75794632	2.94010372
4.51106351	1.21182544	5.32247724
4.51240452	4.73756546	7.72460120
2.47889701	1.54108675	0.05831227

2.19162597	5.28114006	2.94291799
2.21274068	3.73228820	5.32255084
2.20979517	2.21684974	7.72472658
2.49888166	6.10488724	18.53396491
0.19338396	1.88745010	13.00799920
2.23060725	5.71007122	10.10438672
0.19523907	4.84483122	15.51964458
4.49027898	3.19047652	10.10630664
1.95438309	2.32448863	15.51688021
4.25801247	3.58479304	18.52905233
1.93946263	4.40688619	12.99178332
3.00267530	5.08988617	1.23041557
2.91855228	3.60792235	3.53245617
2.91020694	2.07512124	5.93803129
2.91596042	5.60619753	8.32549712
1.42470003	3.27113276	0.03205651
1.47820927	1.85481874	2.23972940
1.50679256	5.38515922	4.72186407
1.51235549	3.87410101	7.10916493
3.71780461	2.57378073	1.22853664
3.80621734	1.08653440	3.53231066
3.81352788	4.59627713	5.93729243
3.80589134	3.08517104	8.32668897
0.67799298	0.74962497	0.03500611
0.64456245	4.37649610	2.24803588
0.61654735	2.86400570	4.71993801
0.60900963	1.35304703	7.10973566
3.77723280	1.57209031	10.80027463
2.99855020	4.04023089	15.24745620
1.46344749	5.83825871	16.66334600
0.61592445	4.86234527	9.51467858
3.76432701	5.11335223	17.38536788
2.99354780	2.67644028	13.01435164
1.41856396	5.89975124	11.81680182
0.70372797	6.91133694	18.80913876
2.98889882	2.59092924	17.38694665
3.74032123	5.19778533	13.01273066
0.70317848	3.37482983	11.81824329
1.45511284	4.38886751	18.80173690
2.94350343	4.09364265	10.80631319
3.75019092	6.56067442	15.24170691
0.68806454	3.31599538	16.66419487
1.50367195	2.34110715	9.51457402
1.37065661	5.88289707	14.23867967

3.67842822	5.06539569	19.80891176
0.77609671	3.36415306	14.24056709
3.08386445	2.54749885	19.81164478

# Fe<sub>5</sub>C<sub>2</sub>(100)//Fe<sub>3</sub>C(010)

1.000000000000

4.50700941	0.00000000	0.00000000
0.00003648	5.00213582	0.00000000
-0.00518574	-1.57565321	24.84239252

C	Fe
16	44

Cart

1.69984310	0.72346702	1.22594793
3.95788478	-0.05786225	6.93201873
1.70435792	3.66846824	3.81359488
3.95372395	2.89300996	9.51854858
3.39687762	1.16747157	3.80954674
1.13662994	0.39178735	9.52558295
3.39068876	3.22466282	1.21959280
1.14347346	2.44331020	6.93607418
3.92725246	2.89884342	16.12991076
3.93249722	2.88139341	22.84808816
1.68314019	4.17042410	12.74277485
1.67250778	-0.83996519	19.45718637
3.38596228	1.66938346	12.75411056
3.37536756	1.66072340	19.45488426
1.12353350	0.39811109	16.13497902
1.12873710	0.38031948	22.83881232
2.92868468	4.66305686	4.97053203
2.17016765	2.09796059	9.36837457
0.66718604	3.88570479	10.67981703
4.42750986	2.87615732	3.62253103
2.92161510	4.73581321	0.06587344
2.17413589	0.73441241	7.12322913
0.67507751	3.94891811	5.77492117
4.42332982	1.51789225	1.37770580
2.16184111	2.23367157	0.06846051
2.92676565	3.23634870	7.12488007
4.42945835	1.44849740	5.77428180
0.66798443	4.01879274	1.37502082
2.17594984	2.16138690	4.97098734
2.92078669	-0.40279838	9.37123531
4.41580035	1.38554079	10.67692543

0.67311340	0.37444419	3.62092175
0.60768113	3.91870906	8.22967444
2.86081621	4.69644787	2.51597723
4.48925200	1.41603681	8.22831809
2.23594823	2.19680610	2.51736447
2.16124100	0.67589197	11.53078014
2.14618931	0.67021787	18.23914885
4.40012258	1.39032614	17.34974453
4.40972159	1.37053086	24.05882731
0.64771610	3.89598920	14.90973610
0.64522191	-1.12054581	21.60849007
2.90234262	3.17407734	13.98226016
2.89847713	3.16299269	20.67985975
0.64719300	3.89029699	17.35057708
0.65955780	-1.12836874	24.05698697
2.91695455	3.17451633	11.53310982
2.90053282	3.17142081	18.23913288
2.15848785	0.66989840	13.97999095
2.15206351	0.66271239	20.68139800
4.40767597	1.39327740	14.90739588
4.40925487	1.38302973	21.61010689
2.92070357	-0.39682312	16.11302377
2.93069627	-0.40994819	22.79815969
0.68086707	2.45968991	12.79117424
0.66514697	2.45578686	19.47731566
4.38814218	-0.04117990	12.78822664
4.38257058	-0.04499446	19.47821345
2.13004011	2.10406680	16.11126928
2.13069155	2.09112280	22.80046966

# Fe<sub>5</sub>C<sub>2</sub>(100)//Fe<sub>7</sub>C<sub>3</sub>(010)

1.000000000000

4.53060611	0.00000000	0.00000000
-0.00003921	4.97248625	0.00000000
0.00836638	-1.55175089	27.70370231

C	Fe
20	48

Cart

2.79300511	2.76254185	14.02466396
0.52020137	4.01740021	0.83412800
2.23430734	1.53236283	5.90288929
4.49899538	0.27397207	8.95550529
2.22921480	1.53138471	0.83364295

4.50222671	0.27637445	14.02370577
2.78920289	2.76037148	8.95584419
0.52427488	4.01881471	5.90310483
2.81416472	-0.15510205	11.48823814
0.54599953	1.96159997	3.37405645
2.20865996	4.44786920	3.36978968
4.47717256	2.33117386	11.48543277
0.53081318	-0.94542609	17.11817506
2.79795462	3.24983710	22.85063300
0.53139955	1.98283822	19.71032161
2.79703049	1.20335050	25.44269502
2.23541685	-0.50348308	19.70921868
4.50120456	-1.28285830	25.44319421
2.23461711	1.54091542	17.11827608
4.50183662	0.76353154	22.85098366
4.02690821	3.73994565	7.80788858
3.27310742	4.81086289	1.07520161
1.08230753	0.51215472	2.13495548
1.76174141	3.03900697	7.05033655
1.01527788	1.96927920	13.78246089
3.35411663	1.29499105	12.72351443
1.76726182	1.48603675	27.39264747
1.74519230	4.45372597	9.22144398
3.93640307	3.77973018	10.25585207
4.03210477	3.74300437	15.16869428
4.01072786	2.32568214	5.63542354
1.67133672	2.99964981	4.60220587
0.99621455	0.55305045	7.05046168
1.74905251	-0.51719331	13.78161226
3.93999422	3.78087772	12.72318743
3.26156524	1.25395819	7.80797361
4.00723910	2.32432328	1.07392955
1.66800403	2.99801842	2.13453035
3.26396140	1.25658148	15.16888635
3.27835828	-0.16074634	5.63646641
1.08719721	0.51295192	4.60259338
0.99895152	-1.00033717	27.39286073
1.01256449	1.96728641	9.22222783
3.35214867	1.29318344	10.25614127
1.72345144	3.12033065	11.50172160
3.98549415	3.65838624	3.35452648
3.29971638	1.17224276	3.35508114
1.03732279	0.63415099	11.50236573
1.76474443	2.96675456	20.87019416

1.00610333	0.41802492	25.24787239
4.02925107	2.18608389	26.60502489
3.27076116	1.19714131	19.54368677
1.76329044	3.04350714	15.95573933
1.00676260	-0.93699289	23.01701543
4.03023424	2.26606719	21.69035419
3.27031280	-0.16003533	17.31327328
1.00226771	0.55720227	15.95582372
1.76231446	1.54938246	23.01707187
3.26909083	-0.21995549	21.69045973
4.02577482	2.32619367	17.31299780
1.00361733	0.48044324	20.87033529
1.76170933	2.90441014	25.24822222
3.26783009	-0.30033713	26.60485879
4.02646270	3.68329421	19.54358313
3.96077642	2.22692984	24.14629318
1.69411434	3.00471797	18.41447654
3.33842062	-0.25933841	24.14622510
1.07146810	0.51858300	18.41457025

# Fe<sub>3</sub>C(010)//Fe<sub>2</sub>C(011)

1.000000000000

4.57444910	0.00000000	0.00000000
-0.00006049	5.08101721	0.00000000
0.00028594	1.08187725	34.27178684

C	Fe
24	60

Cart

3.10176062	4.88758811	0.30632832
3.09169497	3.33452696	2.68979301
3.09309712	1.80579502	5.08904300
3.09337850	0.27606896	7.48719231
3.09339896	3.82762543	9.88645299
3.08111133	2.27388213	12.27053873
0.79494016	2.34836641	0.30812479
0.80752243	0.79372009	2.69011395
0.80669666	4.34625709	5.08919688
0.80535865	2.81653968	7.48728726
0.80320167	1.28677424	9.88662576
0.81277861	4.81553565	12.27209587
1.04453371	4.77099574	18.44777847
1.02839460	4.75857237	25.07293671
1.05770346	4.74903009	31.61802827

3.34480596	0.95802488	15.23550244
3.31629259	0.94621009	21.78481067
3.33123727	0.93580133	28.40901801
0.53585667	3.49927439	15.24554112
0.51185720	3.48595402	21.79399005
0.52527078	3.47626442	28.39562626
2.81244829	2.23041356	18.46035549
2.79862767	2.21886607	25.06461677
2.82457816	2.20766556	31.60714087
1.50531517	0.67048416	0.90008143
1.49936787	4.20922948	3.30326000
1.49970344	2.68063400	5.69939949
1.49935052	1.15054958	8.09739619
1.50146010	4.70407940	10.49008782
1.53244778	3.18678911	12.93775547
0.07543588	5.05793200	33.90751710
0.10889085	2.45779777	2.08877397
0.11239372	0.93119571	4.47912349
0.11226558	4.48216410	6.87708525
0.11158473	2.95262281	9.27311302
0.10384187	1.41104480	11.67706664
2.39262614	3.21066394	0.90013824
2.40004948	1.66868514	3.30306096
2.39988077	5.22120159	5.69919887
2.39888696	3.69115191	8.09722771
2.39477830	2.16357380	10.48873844
2.36085003	0.64642672	12.94244657
3.82113525	2.51758072	33.91260328
3.79006565	4.99825971	2.08727575
3.78726070	3.47172442	4.47903873
3.78666158	1.94167404	6.87713111
3.78546713	0.41206924	9.27313944
3.79123076	3.95125786	11.67720070
3.86948624	2.46279498	14.00197102
3.82360921	2.48390559	20.57695054
3.82943976	2.46732904	27.18660403
1.54318058	3.23878927	19.66961076
1.53516643	3.22130642	26.28048500
1.58385759	3.24294466	32.84946094
2.31839579	0.69951159	17.24721849
2.29630651	5.76523284	23.86209454
2.32341023	5.75226453	30.43967560
0.03526061	5.03571776	16.41335191
0.00932807	5.02036791	22.99597121



0.03183707	5.00792175	29.60781010
2.30310499	0.69451306	19.67352587
2.29936904	5.76490568	26.27726661
2.30824383	5.78674875	32.84867731
0.01991382	5.00018070	14.00281204
0.01247915	5.02116503	20.58006003
0.01542727	5.01182306	27.18270328
3.83777766	2.49218444	16.41087994
3.81302563	2.47823117	22.99498949
3.83498688	2.47068917	29.61084490
1.54819924	3.23694360	17.24425986
1.52566898	3.22609086	23.86292425
1.55046551	3.21496943	30.44226859
0.04511727	1.41634207	18.49690337
0.02741382	1.40095599	25.08692411
0.05146900	1.40075974	31.72844854
2.33720259	4.30659950	15.12439654
2.31490558	4.30408355	21.77098782
2.33274418	4.28991829	28.35804397
1.54480713	1.76694401	15.12153614
1.51321016	1.76412305	21.76813940
1.52303162	1.74887651	28.36307943
3.81128718	3.95720930	18.49214034
3.79958671	3.94102847	25.08956957
3.83235806	3.94022924	31.73160726

# Fe<sub>3</sub>C(010)//Fe<sub>7</sub>C<sub>3</sub>(010)

1.000000000000

4.51844427	0.00000000	0.00000000
0.00022955	4.98500070	0.00000000
-0.03779112	-0.02877869	29.68525143

C	Fe
20	52

Cart

2.66804548	4.35027547	14.21245342
0.43636401	0.63580666	1.02578563
2.11968036	3.12667459	6.09536412
4.37679431	1.86135217	9.14685633
2.13513379	3.12787964	1.03055278
4.36586438	1.85751331	14.21424305
2.67357577	4.35354965	9.14546147
0.41600580	0.63369108	6.09226967
2.69406940	1.42582602	11.66928993

0.45010311	3.56130254	3.55971697
2.10398800	1.06881688	3.57504090
4.34739041	3.91837642	11.67688251
2.66012266	4.34015648	20.80562264
2.65648785	4.32902926	27.51920554
0.40215100	0.62719192	17.40663492
0.39925231	0.61488935	24.12255616
2.11106986	3.11970162	17.40865420
2.10876985	3.10745363	24.12482145
4.36922673	1.84766902	20.80763045
4.36554726	1.83647669	27.52304114
3.14772300	2.84758902	7.99581970
3.17854898	1.43155354	1.23729697
0.98988852	2.10501725	2.32667081
0.88868251	2.13938127	7.24343352
0.89220812	3.55350256	14.00168135
3.22413971	2.87983875	12.91303356
1.63335686	4.60842019	29.57068746
1.63001257	1.06476423	9.42108227
3.81695305	0.38764663	10.44627617
3.89931854	0.34776344	15.35775629
3.89238075	3.92203501	5.82289084
1.56224714	4.59822544	4.79541505
1.64459663	4.63269438	7.24450700
1.62352589	1.06142879	14.00392442
3.81089503	0.38844366	12.91392021
3.90336874	0.35582394	7.99625035
3.91054027	3.92500325	1.24200395
1.57762357	4.59980827	2.32861825
3.13337933	2.84071200	15.35702020
3.16304943	1.43063672	5.81771253
0.97677225	2.10773789	4.79354465
0.86673637	2.11683880	29.56898229
0.90108998	3.55768108	9.41829239
3.23181929	2.88116275	10.44543134
1.60297482	4.71225229	11.71182165
3.87777128	0.27513522	3.53131465
3.19460338	2.76747759	3.52811649
0.92019236	2.21972984	11.71044766
0.87776409	2.13360085	16.18925390
0.87582908	2.12175407	22.90689598
3.13539892	2.83380008	22.02237023
3.13046327	2.82378409	28.73877540
3.8886799	0.34785335	19.58172459

3.88377061	0.34053642	26.28627543
1.62791828	4.61614197	18.64330206
1.62777300	4.60838502	25.34868138
3.89282714	0.34065842	22.02299039
3.88911435	0.32998899	28.73944734
1.63635213	4.62538238	16.18952701
1.63344673	4.61359415	22.90762197
0.88452323	2.12295648	18.64287616
0.87931954	2.11508351	25.34780488
3.14112976	2.83969408	19.58114066
3.14023582	2.83186964	26.28558552
1.64946481	1.05510669	20.77843103
1.65288857	1.05025609	27.46482787
3.91664737	3.90613355	17.46448433
3.90765609	3.89984225	24.15197223
3.11504458	1.41363038	17.46394977
3.11893672	1.40736850	24.15117757
0.86133046	3.54766499	20.77781565
0.85073681	3.54282529	27.46377725

# Fe<sub>7</sub>C<sub>3</sub>(010)// Fe<sub>2</sub>C(011)

1.000000000000

4.60584827	0.00000000	0.00000000
-0.00004018	5.03218859	0.00000000
-0.00840895	1.05879511	30.60722138

C	Fe
24	52

Cart

3.15217237	4.96541853	0.39674740
3.12117030	3.42765217	2.77782370
3.12191973	1.91516404	5.18050609
3.12380663	0.40160915	7.58272869
3.12507577	3.92003513	9.98513539
3.09365215	2.37983415	12.36415192
0.79091070	2.45037982	0.39822302
0.82163617	0.91131779	2.77785083
0.82062711	4.43123838	5.18047590
0.81919182	2.91769380	7.58274228
0.81868900	1.40357958	9.98525785
0.84986729	4.89750163	12.36629070
1.08367559	4.81145747	28.14531177
3.39267401	1.08093795	15.22163077
0.51340687	3.57615315	20.19947854

2.81667182	2.31332905	23.17051735
0.53484955	3.59757248	15.24011262
2.83178450	2.29510976	28.13211453
1.05221773	4.83020283	23.17416501
3.35516047	1.05906167	20.19568272
1.08446785	1.87068765	25.65015161
3.38947601	4.02085701	17.71731088
0.50565379	1.50418366	17.73637290
2.80672745	4.38725986	25.63505699
1.52862550	0.78322351	0.98725032
1.51832932	4.28919631	3.39373534
1.51982250	2.77720731	5.79673939
1.51944926	1.26253897	8.19674207
1.52401271	4.78298495	10.59019740
1.55914965	3.28409872	13.09100889
0.07209548	5.12129771	30.27529848
0.11643632	2.56415303	2.17364992
0.12038406	1.05394203	4.56609038
0.11998236	4.57183762	6.96640299
0.12201130	3.05844930	9.36971206
0.11254794	1.53135489	11.77604619
2.41502041	3.29922902	0.98703869
2.42439212	1.77314029	3.39365155
2.42275878	0.26113282	5.79680669
2.42360082	3.77865857	8.19690068
2.41983889	2.26695365	10.58889037
2.38400394	0.76871757	13.09651201
3.85396049	2.60560751	30.27890028
3.82646543	5.08029272	2.17282629
3.82211587	3.57006782	4.56617484
3.82284622	2.05579018	6.96637243
3.82167212	0.54242152	9.36947874
3.83203398	4.04721886	11.77572811
1.54424346	3.30398331	22.02896929
1.59053934	1.87739682	15.31592153
3.97467096	2.55280622	16.48139713
3.84711332	2.58417551	21.34137747
3.88747876	4.01519999	28.05458136
1.66805530	3.33924214	26.88811296
0.02944326	5.08166322	14.07231458
-0.00535646	1.50093713	23.51200837
2.22504053	5.85364928	24.44724901
2.32370084	5.84217678	29.29780450
2.29760023	4.38814986	19.85943022

4.52837992	5.06902493	18.92296466
0.01790444	5.10066948	21.34353116
0.02746651	1.49827021	28.05020158
2.23624479	5.85227088	26.88573397
2.32111404	0.78792831	22.02690467
2.33608490	4.39435127	15.32170255
4.54278883	5.07310329	16.48444164
1.60173013	3.32359717	29.29970970
1.57323221	1.87460049	19.85362099
3.95090075	2.55462747	18.92002526
3.91224277	2.56895264	14.06963499
3.87643514	4.01487259	23.51687948
1.64861023	3.33613339	24.44970164
4.59008272	5.19187292	25.77929197
2.28918588	0.70029164	17.59324580
1.60684379	3.21511831	17.58514312
3.90788967	2.67671310	25.78552454