Thermodynamic Properties of Ketenes: Group Additivity values from Quantum Chemical Calculations

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Table A: The MP2/6-31G(d') optimized geometries of the ketenes.
The cartesian coordinates are given in angstroms

SET I ALKYLKETENES

Methylketene (1)			
H	-1.234	-0.839	-1.975
C	-1.281	-0.715	-0.886
C	0.106	-0.697	-0.279
C	0.570	0.341	0.405
O	0.974	1.265	1.010
H	0.776	-1.546	-0.386
H	-1.816	0.220	-0.680
H	-1.880	-1.538	-0.476

Ethylketene (2)			
C	-0.996	-0.511	-1.891
C	-1.026	-0.524	-0.357
C	0.365	-0.550	0.244
C	0.841	0.452	0.972
O	1.248	1.344	1.621
H	1.034	-1.388	0.062
H	-1.589	-1.401	-0.005
H	-1.570	0.357	0.011
H	-2.013	-0.523	-2.305
H	-0.482	0.384	-2.260
H	-0.464	-1.389	-2.278

iso-PropylKetene (3)			
C	-0.989	0.280	-1.241
C	-0.971	0.221	0.290
C	0.444	0.249	0.841
C	1.523	0.244	0.066
C	-1.714	-1.021	0.798
H	-0.491	1.184	-1.616
H	-0.481	-0.595	-1.669
H	-2.021	0.283	-1.613
H	-2.761	-1.015	0.462
H	-1.710	-1.067	1.895
H	-1.233	-1.933	0.420
H	0.620	0.237	1.915
O	2.476	0.245	-0.623
H	-1.495	1.113	0.670

Methylisopropyketene (7)			
C	0.229	-0.326	-2.062
C	0.262	-0.220	-0.551
C	1.432	-0.105	0.069
C	-1.031	-0.200	0.249
C	-0.790	-0.344	1.755
C	-1.846	1.068	-0.049
H	-1.622	-1.071	-0.086
H	1.235	-0.431	-2.486
H	-0.235	0.558	-2.522
H	-0.355	-1.207	-2.365
H	-2.057	1.175	-1.120
H	-2.808	1.044	0.481
H	-1.292	1.958	0.280
H	-0.207	0.505	2.140
H	-0.246	-1.268	1.988
H	-1.744	-0.363	2.297
O	2.473	-0.017	0.615

t-Butylketene (4)			
C	-0.064	-0.603	-1.934
C	-0.045	-0.615	-0.396
C	1.408	-0.620	0.097
C	-0.765	-1.873	0.117
C	-0.783	0.615	0.113
C	-0.217	1.539	0.879
O	0.293	2.354	1.558
H	-1.829	0.771	-0.148
H	0.431	-1.499	-2.335
H	-1.095	-0.587	-2.312
H	0.454	0.284	-2.321
H	-0.754	-1.905	1.214
H	-1.812	-1.887	-0.214
H	-0.277	-2.781	-0.264
H	1.930	-1.512	-0.277
H	1.953	0.264	-0.260
H	1.456	-0.637	1.194

Methylethylketene (6)			
C	0.494	-0.001	-1.284
C	0.518	0.000	0.231
C	1.848	0.001	0.954
C	-0.613	0.001	0.927
O	-1.612	0.002	1.552
C	-0.912	-0.002	-1.891
H	1.051	0.878	-1.645
H	1.051	-0.882	-1.643
H	2.437	0.888	0.679
H	1.728	0.002	2.044
H	2.437	-0.887	0.681
H	-0.861	-0.003	-2.987
H	-1.477	-0.890	-1.580
H	-1.477	0.887	-1.582

Dimeketene (5)			
H	-1.639	-0.621	-1.637
C	-1.574	-0.352	-0.573
C	-0.130	-0.292	-0.127
C	0.372	0.835	0.363
O	0.818	1.836	0.798
C	0.738	-1.525	-0.243
H	-2.090	0.606	-0.436
H	-2.124	-1.115	-0.003
H	0.799	-1.858	-1.289
H	1.760	-1.347	0.114
H	0.315	-2.352	0.345

Diethylketene (**9**)			
C	-0.257	0.000	-1.673
C	-0.265	0.000	-0.157
C	0.878	0.000	0.520
O	1.893	0.000	1.121
C	-1.591	0.000	0.579
C	-1.465	0.000	2.106
H	-2.171	0.880	0.257
H	-2.171	-0.880	0.257
H	-0.819	0.880	-2.027
C	1.141	0.000	-2.297
H	-0.819	-0.880	-2.027
H	-2.456	0.000	2.576
H	-0.925	-0.888	2.458
H	-0.925	0.888	2.458
H	1.077	0.000	-3.392
H	1.710	0.888	-1.993
H	1.710	-0.888	-1.993

Ethylt-butylketene (**11**)			
C	-0.290	0.196	-1.729
C	-0.277	0.048	-0.217
C	1.030	0.001	0.578
C	-1.435	-0.032	0.432
H	0.440	-0.507	-2.160
C	-1.661	-0.059	-2.364
H	0.056	1.204	-2.007
C	1.779	-1.306	0.266
C	1.907	1.202	0.184
C	0.753	0.064	2.087
H	0.135	-0.782	2.417
H	1.698	0.025	2.646
H	0.237	0.996	2.358
H	2.173	1.175	-0.881
H	2.842	1.194	0.761
H	1.385	2.147	0.385
H	1.176	-2.176	0.560
H	2.010	-1.395	-0.803
H	2.731	-1.343	0.816
O	-2.461	-0.106	1.009
H	-1.612	0.065	-3.453
H	-2.010	-1.078	-2.153
H	-2.413	0.644	-1.983

Methylt-butylketene (**8**)			
C	0.559	0.478	-1.910
C	0.540	0.526	-0.372
C	1.983	0.478	0.159
C	-0.242	-0.671	0.167
C	0.176	-2.101	-0.121
C	-1.325	-0.471	0.912
O	-2.286	-0.304	1.574
C	-0.110	1.843	0.076
H	1.115	1.337	-2.311
H	1.045	-0.434	-2.279
H	-0.463	0.509	-2.311
H	1.993	0.509	1.257
H	2.502	-0.434	-0.164
H	2.557	1.337	-0.217
H	-0.508	-2.819	0.350
H	0.177	-2.309	-1.200
H	1.184	-2.309	0.263
H	0.459	2.696	-0.316
H	-1.140	1.927	-0.297
H	-0.129	1.927	1.171

Ethylisopropylketene (**10**)			
C	-1.595	-0.382	-2.227
C	-1.561	-0.189	-0.707
C	-0.162	-0.139	-0.121
C	0.886	0.017	-0.925
C	0.043	-0.197	1.385
C	-0.557	1.039	2.073
C	1.517	-0.365	1.771
H	-0.505	-1.086	1.744
H	-2.112	0.728	-0.445
H	-2.101	-1.018	-0.221
H	-1.090	0.444	-2.744
H	-1.100	-1.317	-2.515
H	-2.630	-0.418	-2.590
H	-1.622	1.157	1.840
H	-0.033	1.946	1.741
H	-0.458	0.962	3.164
H	1.950	-1.267	1.319
H	2.108	0.502	1.443
H	1.622	-0.445	2.861
O	1.818	0.138	-1.636

Set II - Oxygenated Ketenes

Hydroxyketene (12)			
O	-0.677	-0.081	-1.497
C	-0.763	0.086	-0.115
C	0.341	-0.013	0.631
O	1.303	-0.091	1.301
H	-1.732	0.148	0.373
H	-0.741	0.794	-1.902

Dimethoxyketene (15)			
C	-0.010	-0.027	0.137
C	-0.106	-0.282	1.444
O	-0.190	-0.507	2.599
O	-1.094	-0.217	-0.681
O	1.172	0.426	-0.389
C	-0.913	-1.358	-1.535
C	1.082	1.808	-0.771
H	2.038	2.057	-1.243
H	0.262	1.959	-1.484
H	0.922	2.439	0.114
H	-1.786	-1.387	-2.195
H	0.003	-1.254	-2.129
H	-0.862	-2.278	-0.937

Methoxyhydroxyketene (16)			
H	-1.415	-0.138	-1.758
O	-1.455	-0.133	-0.789
C	-0.160	-0.140	-0.317
O	0.609	0.988	-0.411
C	0.154	2.019	0.481
C	0.322	-1.224	0.294
O	0.766	-2.185	0.814
H	0.785	2.891	0.287
H	-0.897	2.264	0.283
H	0.267	1.697	1.525

Ethylhydroxyketene (19)			
C	0.205	0.373	-1.236
C	0.327	-0.026	0.210
O	0.972	-1.221	0.545
C	-0.289	0.644	1.188
O	-0.841	1.252	2.033
H	1.925	-1.050	0.541
H	-0.310	1.342	-1.305
H	1.215	0.532	-1.650
C	-0.531	-0.689	-2.064
H	-0.541	-0.421	-3.128
H	-0.040	-1.662	-1.956
H	-1.567	-0.792	-1.721

Methoxyketene (13)

C	0.444	0.477	-0.275
C	0.455	0.510	1.061
O	0.466	0.567	2.235
O	-0.705	0.078	-0.939
H	1.315	0.810	-0.835
C	-0.542	-1.212	-1.530
H	-1.480	-1.430	-2.051
H	0.288	-1.215	-2.252
H	-0.353	-1.977	-0.763

Dihydroxyketene (14)			
C	0.015	0.030	-0.391
C	-0.037	-0.071	0.938
O	-0.083	-0.159	2.113
O	-1.078	-0.318	-1.150
O	1.162	0.480	-1.002
H	-0.864	-1.139	-1.620
H	0.981	1.362	-1.361

Methylhydroxyketene (17)			
C	-0.033	0.008	-0.370
C	-0.023	0.024	0.966
O	0.005	0.031	2.143
O	-0.903	0.890	-1.018
C	0.934	-0.810	-1.175
H	-1.645	0.372	-1.363
H	0.407	-1.525	-1.825
H	1.543	-0.158	-1.814
H	1.607	-1.384	-0.525

Methylmethoxyketene (18)			
C	-1.227	0.185	-1.675
O	-1.184	0.300	-0.251
C	0.121	0.272	0.235
C	0.550	-0.880	0.761
O	0.933	-1.888	1.236
C	0.941	1.530	0.255
H	-2.283	0.255	-1.954
H	-0.668	0.996	-2.163
H	-0.820	-0.782	-2.004
H	1.905	1.364	0.753
H	1.150	1.897	-0.760
H	0.405	2.321	0.797

Ethylmethoxyketene (22)			
C	-1.393	0.211	-1.933
C	-1.400	0.206	-0.401
C	-0.018	0.190	0.194
C	1.094	0.238	-0.547
O	2.075	0.280	-1.200
O	0.141	0.250	1.578
C	0.078	-1.044	2.179
H	-1.966	-0.667	-0.039
H	-1.928	1.095	-0.022
H	-2.418	0.230	-2.322
H	-0.869	1.093	-2.324
H	-0.899	-0.684	-2.331
H	0.155	-0.883	3.260
H	-0.874	-1.547	1.955
H	0.909	-1.679	1.840

isopropylmethoxyketene (23)			
C	-1.244	0.891	-1.615
C	-1.141	0.030	-0.352
C	0.277	-0.038	0.156
O	0.563	-0.766	1.312
C	0.391	0.021	2.492
C	1.321	0.452	-0.523
O	2.237	0.889	-1.121
C	-1.678	-1.388	-0.590
H	-1.758	0.503	0.432
H	-2.286	0.939	-1.957
H	-0.897	1.917	-1.438
H	-0.647	0.459	-2.430
H	0.584	-0.649	3.337
H	1.103	0.859	2.514
H	-0.632	0.416	2.568
H	-2.746	-1.362	-0.848
H	-1.132	-1.864	-1.415
H	-1.549	-2.006	0.305

isopropylhydroxyketene (20)			
C	0.218	-0.996	-1.868
C	0.220	-1.006	-0.333
C	1.647	-0.981	0.226
C	-0.605	0.140	0.194
C	-0.078	1.148	0.896
O	0.397	2.029	1.518
O	-1.945	0.263	-0.192
H	-2.466	-0.327	0.371
H	-0.263	-1.941	0.004
H	0.711	-1.894	-2.265
H	-0.807	-0.961	-2.254
H	0.753	-0.112	-2.240
H	2.218	-1.837	-0.154
H	2.171	-0.067	-0.086
H	1.656	-1.027	1.323

tbutylmethoxyketene (24)			
C	0.566	0.798	-1.924
C	0.594	0.808	-0.390
C	2.050	0.805	0.108
C	-0.124	2.062	0.134
C	-0.103	-0.419	0.154
O	-0.156	-0.583	1.540
C	-1.488	-0.524	2.053
C	-0.501	-1.432	-0.626
O	-0.910	-2.296	-1.316
H	1.079	1.689	-2.310
H	1.081	-0.084	-2.330
H	-0.463	0.808	-2.307
H	-1.396	-0.544	3.145
H	-1.996	0.398	1.738
H	-2.081	-1.391	1.725
H	0.397	2.969	-0.205
H	-1.159	2.103	-0.230
H	-0.136	2.070	1.231
H	2.569	1.720	-0.213
H	2.080	0.754	1.203
H	2.592	-0.062	-0.292

tbutylhydroxyketene (**21**)			
C	-0.714	0.144	-1.883
C	-0.739	0.189	-0.346
C	0.685	0.169	0.163
O	1.574	1.178	-0.232
C	-1.518	-1.013	0.201
C	1.191	-0.853	0.861
O	1.625	-1.754	1.485
H	1.475	1.916	0.386
C	-1.410	1.493	0.119
H	-1.731	0.239	-2.290
H	-0.101	0.962	-2.281
H	-0.286	-0.804	-2.233
H	-2.548	-0.993	-0.178
H	-1.064	-1.962	-0.118
H	-1.561	-0.999	1.298
H	-2.439	1.555	-0.263
H	-1.447	1.544	1.216
H	-0.865	2.369	-0.255

Set III Bisketenes

HC(CO)C(Me)CO (**40**)			
C	0.516	0.398	-1.293
C	0.607	0.466	0.037
C	1.944	0.543	0.741
C	-0.681	0.498	0.780
H	-1.089	1.402	1.231
C	-1.350	-0.646	0.939
O	-1.926	-1.660	1.057
O	0.427	0.329	-2.462
H	2.778	0.537	0.027
H	2.016	1.465	1.335
H	2.071	-0.307	1.424

(HCCO)2 (**39**)			
C	-0.189	1.418	-0.657
C	0.865	0.693	-0.276
H	1.802	0.835	-0.811
C	0.708	-0.248	0.862
H	1.048	-0.027	1.871
C	0.137	-1.433	0.638
O	-0.373	-2.467	0.429
O	-1.124	2.043	-0.986

(MeCCO)2 (**41**)

C	0.722	0.163	-1.456
C	0.784	0.201	-0.123
C	2.101	0.254	0.622
C	-0.529	0.233	0.580
C	-1.071	1.494	1.220
C	-1.176	-0.933	0.645
O	-1.735	-1.966	0.686
O	0.649	0.122	-2.628
H	2.955	0.259	-0.067
H	2.165	1.161	1.240
H	2.203	-0.614	1.287
H	-2.030	1.311	1.721
H	-0.370	1.885	1.970
H	-1.224	2.274	0.462

HOC(CO)C(H)CO (**42**)			
H	-1.660	-1.023	0.964
C	-1.037	-0.324	0.407
C	0.400	-0.130	0.658
O	0.889	0.446	1.829
C	-1.603	0.428	-0.544
O	-2.070	1.085	-1.393
C	1.278	-0.626	-0.225
O	2.027	-1.087	-1.005
H	0.659	1.387	1.808

HOC(CO)C(Me)CO (**43**)			
C	0.492	0.113	-2.158
C	0.486	0.167	-0.645
C	1.607	0.173	0.087
O	2.577	0.163	0.747
C	-0.759	0.265	0.135
C	-1.173	-0.811	0.819
O	-1.513	-1.778	1.395
O	-1.591	1.384	0.066
H	1.511	0.153	-2.563
H	0.013	-0.810	-2.512
H	-0.071	0.964	-2.562
H	-1.152	2.100	0.549

CH2(HCCO)2 (**25**)			
C	-0.898	-0.599	-2.085
C	-0.866	-0.527	-0.759
C	0.439	-0.544	0.013
C	0.680	0.758	0.754
C	0.724	0.813	2.080
O	0.766	0.845	3.254
O	-0.909	-0.667	-3.258
H	-1.814	-0.408	-0.241
H	1.273	-0.738	-0.676
H	0.436	-1.379	0.728
H	0.776	1.694	0.209

CMe2(HCCO)2 (**31**)			
C	-0.429	-0.936	1.619
O	-0.184	-1.816	2.357
C	-0.701	0.069	0.791
C	0.374	0.800	0.003
C	0.226	0.472	-1.479
C	-0.535	-0.537	-1.893
O	-1.218	-1.415	-2.269
H	-1.747	0.350	0.684
C	1.779	0.399	0.483
C	0.180	2.314	0.196
H	0.788	1.020	-2.233
H	2.541	0.922	-0.110
H	1.924	0.667	1.540
H	1.943	-0.679	0.362
H	0.309	2.584	1.253
H	0.914	2.875	-0.399
H	-0.824	2.620	-0.125

(HOCCO)2 (**44**)			
C	-0.107	-0.798	0.099
C	-0.115	-0.755	1.443
O	-0.108	-0.671	2.612
C	-0.309	0.460	-0.602
C	0.768	1.256	-0.729
O	1.720	1.940	-0.772
O	-1.533	0.890	-1.111
O	-0.127	-2.039	-0.547
H	-1.792	0.254	-1.794
H	0.752	-2.185	-0.927

CHMe(HCCO)2 (**28**)			
C	-0.426	-0.484	1.680
O	-0.209	-1.339	2.456
C	-0.667	0.496	0.815
C	0.424	1.118	-0.036
C	0.252	0.729	-1.496
C	-0.517	-0.297	-1.849
O	-1.210	-1.188	-2.173
H	-1.705	0.803	0.698
C	1.829	0.763	0.472
H	0.307	2.212	0.032
H	0.816	1.225	-2.284
H	2.594	1.227	-0.164
H	1.977	1.115	1.502
H	1.985	-0.323	0.441

CH2(HCCO)(MeCCO) (**26**)			
C	-0.625	0.161	-0.644
C	-0.584	0.150	0.874
C	0.765	0.221	-1.251
H	-1.221	1.011	-1.006
H	-1.140	-0.747	-0.996
C	-1.082	1.183	1.544
C	0.051	-1.016	1.595
C	1.280	-0.796	-1.934
H	1.395	1.095	-1.105
H	-0.483	-1.950	1.365
H	1.095	-1.139	1.275
H	0.041	-0.883	2.683
O	-1.531	2.101	2.129
O	1.717	-1.701	-2.543

CHMe(HCCO)(MeCCO) (29)			
C	0.689	0.161	0.182
C	0.683	0.140	1.718
H	1.740	0.154	-0.147
C	0.044	1.423	-0.371
C	-0.002	-1.072	-0.391
C	0.702	-1.882	-1.174
C	-1.455	-1.356	-0.084
C	-0.607	2.295	0.393
H	0.057	1.621	-1.441
O	-1.170	3.069	1.076
O	1.337	-2.588	-1.870
H	-1.603	-1.633	0.969
H	-2.058	-0.460	-0.286
H	-1.848	-2.173	-0.701
H	-0.341	0.171	2.112
H	1.160	-0.777	2.083
H	1.230	1.002	2.122

CH2(MeCCO)2 (27)			
C	-1.901	0.146	-0.864
C	-0.551	-0.517	-1.010
C	0.219	-0.922	0.236
C	0.605	0.289	1.068
C	1.555	1.312	0.490
C	-0.011	-0.723	-2.206
O	0.471	-0.918	-3.263
C	0.077	0.446	2.277
O	-0.389	0.572	3.352
H	-0.398	-1.614	0.832
H	1.130	-1.475	-0.041
H	-2.603	-0.520	-0.342
H	-1.813	1.068	-0.272
H	-2.341	0.404	-1.835
H	2.525	0.849	0.258
H	1.151	1.726	-0.443
H	1.737	2.143	1.182

CMe2(HCCO)(MeCCO) (32)			
C	1.742	-1.102	-0.661
C	1.077	0.228	-0.370
C	1.651	1.350	-0.791
C	-0.254	0.289	0.381
C	-0.100	-0.389	1.752
C	-0.703	1.744	0.591
C	-1.308	-0.425	-0.459
H	2.572	-0.993	-1.370
H	1.008	-1.791	-1.103
H	2.142	-1.568	0.250
H	0.195	-1.442	1.657
H	0.671	0.129	2.337
H	-1.046	-0.348	2.311
H	-0.845	2.259	-0.369
H	0.040	2.302	1.178
H	-1.658	1.764	1.129
H	-1.572	-0.034	-1.440
C	-1.932	-1.528	-0.058
O	2.165	2.341	-1.168
O	-2.483	-2.501	0.307

CHMe(MeCCO)2 (30)			
C	-0.336	-0.618	-1.925
C	-0.331	-0.592	-0.390
C	1.092	-0.602	0.161
C	2.040	0.536	-0.144
C	-1.091	0.595	0.184
C	-1.523	1.566	-0.615
O	-1.920	2.420	-1.322
C	1.470	-1.622	0.923
O	1.792	-2.534	1.597
H	-0.844	-1.504	-0.037
C	-1.303	0.685	1.679
H	2.315	0.562	-1.207
H	1.563	1.494	0.104
H	2.967	0.459	0.438
H	0.145	0.278	-2.340
H	0.212	-1.496	-2.289
H	-1.363	-0.663	-2.311
H	-1.870	1.580	1.962
H	-1.859	-0.193	2.040
H	-0.339	0.709	2.204

HC(CO)CH2OH (33)			
O	-0.927	-0.536	-1.857
C	-1.003	-0.566	-0.438
C	0.356	-0.582	0.222
H	-1.598	0.277	-0.047
H	-1.546	-1.488	-0.205
H	1.036	-1.416	0.074
C	0.783	0.448	0.947
H	-0.380	0.224	-2.093
O	1.136	1.361	1.593

MeC(CO)CH2OH (34)			
C	0.073	-0.286	-1.754
C	0.086	-0.267	-0.241
C	1.218	-0.345	0.451
O	2.211	-0.426	1.076
C	-1.215	-0.083	0.506
O	-1.828	1.171	0.226
H	-1.945	-0.830	0.167
H	-1.067	-0.229	1.589
H	-1.194	1.854	0.484
H	1.084	-0.301	-2.177
H	-0.464	-1.171	-2.124
H	-0.446	0.604	-2.130

MeC(CO)CH(CH3)OH (36)			
C	0.339	-1.042	-1.629
C	0.334	-1.026	-0.101
O	1.658	-1.148	0.422
C	-0.367	0.177	0.496
C	-0.574	0.232	1.995
C	-0.726	1.193	-0.282
O	-1.056	2.085	-0.975
H	-0.169	-1.932	0.268
H	2.122	-0.332	0.181
H	0.884	-1.925	-1.981
H	-0.680	-1.069	-2.034
H	0.845	-0.150	-2.027
H	-0.967	1.201	2.325
H	-1.279	-0.547	2.317
H	0.381	0.052	2.505

MeC(CO)C(CH3)2OH (38)			
C	0.504	0.588	-1.908
C	0.450	0.598	-0.381
O	1.824	0.675	0.024
C	-0.305	1.832	0.122
C	-0.156	-0.697	0.146
C	0.443	-2.031	-0.256
C	-1.189	-0.654	0.981
O	-2.104	-0.618	1.721
H	1.828	0.630	0.992
H	0.203	2.733	-0.240
H	-1.343	1.845	-0.234
H	-0.317	1.867	1.221
H	0.982	1.510	-2.262
H	1.097	-0.261	-2.265
H	-0.507	0.522	-2.327
H	1.536	-1.957	-0.206
H	0.124	-2.840	0.413
H	0.164	-2.313	-1.280

HC(CO)CH(CH3)OH (35)			
C	-0.689	0.259	-1.951
C	-0.694	0.164	-0.431
C	0.707	0.234	0.139
C	1.160	-0.694	0.975
O	1.539	-1.529	1.708
O	-1.492	1.254	0.023
H	-1.153	-0.795	-0.129
H	1.364	1.062	-0.117
H	-1.415	1.281	0.986
H	-0.214	1.197	-2.261
H	-0.140	-0.582	-2.389
H	-1.720	0.254	-2.327

HC(CO)C(CH3)2OH (37)			
C	-0.013	-0.602	-1.969
C	-0.005	-0.595	-0.442
C	1.428	-0.588	0.098
C	-0.807	0.586	0.077
C	-0.327	1.451	0.964
O	0.112	2.215	1.741
O	-0.657	-1.817	-0.075
H	-1.832	0.727	-0.258
H	-0.775	-1.791	0.886
H	1.951	-1.479	-0.268
H	1.980	0.304	-0.227
H	1.435	-0.618	1.197
H	0.503	-1.499	-2.335
H	-1.045	-0.625	-2.337
H	0.488	0.290	-2.361

Table B -Calculated Harmonic vibration frequencies (in cm^{-1}) and rotational constants (in GHz) at Hf/6-31G(d') level.

Methylketene (1)			
Frequencies	163.7	234.1	582.1
Frequencies	633.3	710.4	962.6
Frequencies	1153.4	1185.1	1248.0
Frequencies	1544.1	1563.7	1618.3
Frequencies	1649.5	2371.1	3190.6
Frequencies	3251.2	3270.7	3371.3
Rot.Consts	*39.521*	*4.544*	*4.181*

Ethylketene (2)			
Frequencies	78.0	198.8	289.5
Frequencies	364.0	597.2	660.6
Frequencies	689.7	833.1	950.2
Frequencies	1082.4	1179.1	1210.5
Frequencies	1254.1	1395.7	1468.7
Frequencies	1548.6	1574.8	1622.5
Frequencies	1630.1	1640.6	2366.8
Frequencies	3185.6	3195.1	3229.5
Frequencies	3255.0	3266.8	3365.0
Rot.Consts	*19.231*	*2.350*	*2.318*

isopropylketene (3)			
Frequencies	63.2	157.7	260.7
Frequencies	293.5	363.9	397.5
Frequencies	456.3	595.5	662.9
Frequencies	723.1	867.3	1003.0
Frequencies	1024.6	1039.5	1191.5
Frequencies	1212.8	1246.9	1302.7
Frequencies	1469.0	1476.2	1537.4
Frequencies	1552.5	1565.8	1624.7
Frequencies	1628.1	1639.6	1647.0
Frequencies	2362.9	3177.5	3182.1
Frequencies	3187.6	3249.7	3251.9
Frequencies	3259.1	3263.7	3359.3
Rot.Consts	*7.071*	*2.178*	*1.838*

tertbutylketene (4)			
Frequencies	58.6	158.6	255.1
Frequencies	312.8	314.9	336.8
Frequencies	338.5	419.8	426.4
Frequencies	453.9	597.6	665.1
Frequencies	691.8	830.2	983.1
Frequencies	1003.5	1018.3	1043.7
Frequencies	1142.8	1146.3	1232.1
Frequencies	1334.0	1345.2	1386.6
Frequencies	1535.8	1540.7	1550.1
Frequencies	1572.6	1618.0	1622.7
Frequencies	1625.8	1640.5	1644.2
Frequencies	1655.9	2360.9	3179.2
Frequencies	3181.7	3190.7	3243.4
Frequencies	3250.3	3252.1	3259.2
Frequencies	3261.5	3265.1	3355.4
Rot.Consts	*4.442*	*1.621*	*1.606*

Dimeketene (5)			
Frequencies	191.6	192.9	202.9
Frequencies	302.9	332.7	600.2
Frequencies	758.2	779.1	1075.4
Frequencies	1086.8	1121.6	1196.8
Frequencies	1320.0	1540.0	1547.1
Frequencies	1566.1	1608.5	1621.5
Frequencies	1633.4	1661.1	2363.6
Frequencies	3175.7	3179.4	3232.1
Frequencies	3232.6	3267.2	3268.5
Rot.Consts	*8.232*	*3.945*	*2.758*

Methylethylketene (6)			
Frequencies	78.3	157.8	189.8
Frequencies	243.7	271.5	328.2
Frequencies	430.2	598.0	756.1
Frequencies	763.6	851.3	1026.0
Frequencies	1110.5	1117.6	1166.5
Frequencies	1223.2	1287.9	1400.9
Frequencies	1486.0	1537.9	1556.2
Frequencies	1564.3	1615.6	1631.8
Frequencies	1636.2	1643.3	1652.4
Frequencies	2358.8	3170.9	3178.3
Frequencies	3190.3	3197.0	3232.4
Frequencies	3258.6	3265.6	3266.8
Rot.Consts	*4.003*	*3.292*	*1.868*

Diethylketene (9)			
Frequencies	60.1	82.1	153.9
Frequencies	182.5	223.5	281.6
Frequencies	340.2	398.3	432.6
Frequencies	596.2	749.8	765.0
Frequencies	834.0	870.2	1012.8
Frequencies	1059.1	1158.3	1161.6
Frequencies	1173.8	1235.0	1262.5
Frequencies	1392.6	1411.5	1476.1
Frequencies	1491.6	1537.9	1552.2
Frequencies	1574.3	1630.0	1636.3
Frequencies	1636.4	1638.6	1642.4
Frequencies	1648.1	2353.4	3168.3
Frequencies	3175.2	3190.0	3190.8
Frequencies	3195.5	3199.0	3258.9
Frequencies	3259.6	3264.4	3264.9
Rot.Consts	*3.697*	*1.906*	*1.297*

Hydroxyketene (12)			
Frequencies	261.3	350.4	598.7
Frequencies	663.5	759.2	1138.0
Frequencies	1304.5	1395.7	1574.9
Frequencies	2387.6	3392.7	4080.0
Rot.Consts	*50.951*	*4.772*	*4.417*

Methylisopropylketene (7)			
Frequencies	44.7	161.5	173.9
Frequencies	221.5	259.6	273.0
Frequencies	298.2	385.4	443.7
Frequencies	503.1	612.1	725.9
Frequencies	764.6	941.7	1004.3
Frequencies	1036.4	1088.9	1131.3
Frequencies	1197.5	1211.6	1256.6
Frequencies	1319.9	1471.2	1473.2
Frequencies	1533.0	1549.2	1556.5
Frequencies	1562.6	1616.0	1624.9
Frequencies	1630.4	1641.5	1647.1
Frequencies	1650.7	2353.4	3166.4
Frequencies	3181.3	3184.0	3189.6
Frequencies	3239.5	3249.2	3256.2
Frequencies	3262.7	3264.7	3267.7
Rot.Consts	*3.274*	*2.146*	*1.483*

Methyltertbutylketene (8)			
Frequencies	30.8	166.1	169.0
Frequencies	210.5	270.9	276.5
Frequencies	303.1	327.2	358.0
Frequencies	379.5	420.7	469.9
Frequencies	500.2	622.3	662.5
Frequencies	767.6	889.5	1002.0
Frequencies	1012.0	1041.7	1081.8
Frequencies	1124.5	1137.5	1157.7
Frequencies	1238.1	1340.8	1343.2
Frequencies	1394.2	1523.0	1539.6
Frequencies	1547.0	1557.8	1572.7
Frequencies	1614.3	1621.1	1627.9
Frequencies	1631.2	1639.9	1648.9
Frequencies	1651.9	1658.7	2349.9
Frequencies	3183.8	3184.4	3189.1
Frequencies	3195.6	3246.1	3251.8
Frequencies	3253.2	3255.7	3262.0
Frequencies	3264.2	3264.5	3269.4
Rot.Consts	*2.643*	*1.617*	*1.297*

Ethylisopropylketene (10)			
Frequencies	36.0	59.7	156.0
Frequencies	184.0	201.8	254.4
Frequencies	282.8	301.9	346.2
Frequencies	423.4	452.0	506.6
Frequencies	612.0	724.9	762.9
Frequencies	856.0	936.0	1004.3
Frequencies	1036.2	1040.3	1149.4
Frequencies	1176.0	1203.6	1210.8
Frequencies	1246.3	1313.1	1403.5
Frequencies	1466.4	1470.9	1486.7
Frequencies	1535.0	1545.0	1559.1
Frequencies	1569.0	1624.5	1629.2
Frequencies	1635.9	1637.0	1641.5
Frequencies	1644.4	1648.3	2348.1
Frequencies	3167.7	3178.2	3183.7
Frequencies	3189.2	3190.6	3207.5
Frequencies	3248.6	3256.1	3259.5
Frequencies	3264.0	3264.9	3266.4
Rot.Consts	*2.563*	*1.531*	*1.071*

Ethyltertbutylketene (11)			
Frequencies	11.7	57.8	164.0
Frequencies	183.8	199.8	258.9
Frequencies	290.4	300.7	328.8
Frequencies	332.9	357.5	384.1
Frequencies	455.3	488.5	499.3
Frequencies	620.2	664.7	764.2
Frequencies	859.5	883.7	1001.9
Frequencies	1012.1	1035.8	1041.6
Frequencies	1134.9	1135.8	1151.9
Frequencies	1201.5	1214.1	1340.1
Frequencies	1342.9	1386.6	1409.0
Frequencies	1479.2	1526.9	1540.1
Frequencies	1544.5	1562.3	1571.9
Frequencies	1619.6	1626.8	1628.3
Frequencies	1635.8	1637.5	1642.8
Frequencies	1645.6	1648.8	1658.6
Frequencies	2344.3	3184.0	3184.4
Frequencies	3189.1	3191.5	3196.9
Frequencies	3219.3	3249.8	3252.9
Frequencies	3255.5	3261.1	3263.9
Frequencies	3264.3	3265.3	3268.7
Rot.Consts	*2.041*	*1.258*	*0.950*

Methoxyketene (13)			
Frequencies	93.6	184.7	288.9
Frequencies	401.5	586.6	689.8
Frequencies	748.1	1064.4	1203.1
Frequencies	1288.2	1305.7	1361.8
Frequencies	1554.9	1624.0	1629.6
Frequencies	1643.0	2385.4	3183.0
Frequencies	3250.1	3306.5	3380.3
Rot.Consts	*21.642*	*2.676*	*2.577*

Dihydroxyketene (14)			
Frequencies	225.0	364.0	390.0
Frequencies	400.7	548.7	561.6
Frequencies	773.8	888.8	1346.6
Frequencies	1417.8	1431.4	1602.2
Frequencies	2422.9	4043.8	4046.5
Rot.Consts	*10.440*	*4.099*	*2.989*

Dimethoxyketene (15)			
Frequencies	93.3	103.3	151.8
Frequencies	154.6	199.2	253.3
Frequencies	343.0	514.3	545.5
Frequencies	659.5	766.4	830.1
Frequencies	1122.2	1173.1	1287.1
Frequencies	1288.9	1310.6	1333.8
Frequencies	1423.7	1551.4	1618.1
Frequencies	1620.1	1628.8	1629.3
Frequencies	1642.8	1646.2	2408.7
Frequencies	3202.5	3202.8	3280.6
Frequencies	3281.9	3317.6	3317.7
Rot.Consts	*3.088*	*2.438*	*1.501*

Methoxyhydroxyketene (16)			
Frequencies	104.2	156.8	237.2
Frequencies	242.8	388.6	493.0
Frequencies	551.4	586.4	765.3
Frequencies	863.2	1146.0	1287.9
Frequencies	1317.8	1389.1	1422.9
Frequencies	1575.0	1622.2	1628.5
Frequencies	1644.3	2415.2	3203.8
Frequencies	3283.6	3319.5	4046.1
Rot.Consts	*6.375*	*2.660*	*2.040*

Methylhydroxyketene (17)			
Frequencies	209.8	210.8	327.8
Frequencies	341.0	392.5	583.5
Frequencies	758.6	826.0	1097.9
Frequencies	1138.1	1358.1	1386.4
Frequencies	1544.5	1561.3	1605.1
Frequencies	1647.6	2383.3	3177.7
Frequencies	3239.3	3270.5	4063.4
Rot.Consts	*9.155*	*4.008*	*2.858*

Methylmethoxyketene (18)			
Frequencies	74.5	163.5	196.3
Frequencies	223.5	239.3	397.8
Frequencies	498.3	589.4	755.7
Frequencies	800.8	1068.7	1149.3
Frequencies	1177.3	1287.9	1315.5
Frequencies	1384.5	1526.6	1557.8
Frequencies	1604.3	1618.2	1633.5
Frequencies	1641.9	1649.6	2376.9
Frequencies	3182.9	3190.0	3244.6
Frequencies	3256.2	3269.7	3305.7
Rot.Consts	*5.474*	*2.716*	*1.982*

Ethylhydroxyketene (19)			
Frequencies	91.0	188.1	221.2
Frequencies	251.6	335.6	384.8
Frequencies	510.5	592.3	738.9
Frequencies	807.7	853.3	1039.2
Frequencies	1164.9	1174.1	1348.7
Frequencies	1374.8	1384.8	1492.8
Frequencies	1546.9	1576.8	1613.3
Frequencies	1629.1	1641.9	2378.5
Frequencies	3167.9	3194.6	3223.7
Frequencies	3262.3	3281.0	4064.3
Rot.Consts	*6.125*	*2.362*	*1.879*

Ethylmethoxyketene (22)			
Frequencies	68.4	79.5	152.1
Frequencies	170.6	209.1	285.1
Frequencies	319.7	436.3	508.8
Frequencies	589.4	757.3	779.6
Frequencies	863.4	1044.3	1127.5
Frequencies	1177.5	1204.9	1287.4
Frequencies	1309.0	1368.1	1390.7
Frequencies	1488.4	1528.4	1560.6
Frequencies	1619.1	1631.2	1635.9
Frequencies	1636.7	1643.5	1647.2
Frequencies	2371.2	3181.2	3190.0
Frequencies	3192.5	3214.0	3255.9
Frequencies	3260.7	3271.2	3304.7
Rot.Consts	*3.179*	*2.184*	*1.402*

isopropylhydroxyketene (20)			
Frequencies	66.1	158.0	226.0
Frequencies	253.1	273.2	311.1
Frequencies	339.8	373.3	483.7
Frequencies	523.4	591.8	730.3
Frequencies	797.3	953.0	1007.9
Frequencies	1040.3	1179.0	1213.8
Frequencies	1270.1	1343.0	1374.4
Frequencies	1468.4	1488.2	1537.2
Frequencies	1552.6	1565.1	1625.8
Frequencies	1627.0	1639.8	1649.1
Frequencies	2374.2	3148.4	3185.7
Frequencies	3191.0	3250.9	3256.6
Frequencies	3268.0	3283.4	4066.5
Rot.Consts	*3.476*	*2.161*	*1.502*

isopropylmethoxyketene (**23**)			
Frequencies	51.6	79.3	152.2
Frequencies	165.9	184.6	251.8
Frequencies	277.9	303.0	354.8
Frequencies	417.6	480.2	544.9
Frequencies	642.7	727.5	777.8
Frequencies	947.5	1007.3	1040.3
Frequencies	1133.3	1184.1	1219.7
Frequencies	1272.3	1289.5	1316.8
Frequencies	1369.1	1468.2	1487.3
Frequencies	1524.2	1544.1	1560.8
Frequencies	1618.4	1625.9	1627.2
Frequencies	1632.0	1639.8	1643.7
Frequencies	1649.1	2367.1	3166.9
Frequencies	3185.3	3189.2	3190.7
Frequencies	3250.6	3255.3	3257.2
Frequencies	3267.4	3281.3	3303.7
Rot.Consts	*2.128*	*1.863*	*1.170*

HC(CO)C(Me)CO (**40**)			
Frequencies	63.7	132.8	186.2
Frequencies	206.6	324.4	350.2
Frequencies	606.1	632.0	655.5
Frequencies	664.8	763.3	876.7
Frequencies	1089.7	1149.0	1221.9
Frequencies	1295.1	1497.4	1536.9
Frequencies	1554.2	1611.9	1643.4
Frequencies	2355.8	2376.2	3183.9
Frequencies	3246.8	3265.2	3351.9
Rot.Consts	*4.065*	*1.779*	*1.355*

(MeCCO)2 (**41**)			
Frequencies	52.6	121.3	148.5
Frequencies	172.0	178.3	217.7
Frequencies	255.2	425.6	428.2
Frequencies	619.7	627.3	641.1
Frequencies	758.4	760.9	999.1
Frequencies	1098.9	1142.8	1153.0
Frequencies	1177.9	1351.9	1498.3
Frequencies	1523.6	1551.0	1556.3
Frequencies	1609.7	1616.5	1642.6
Frequencies	1644.8	2348.5	2367.2
Frequencies	3183.7	3187.1	3246.4
Frequencies	3249.6	3265.7	3265.9
Rot.Consts	*2.509*	*1.469*	*1.247*

tertbutylhydroxyketene (**21**)			
Frequencies	62.3	162.0	205.6
Frequencies	247.3	275.1	302.3
Frequencies	307.7	351.1	364.7
Frequencies	381.8	415.7	500.8
Frequencies	531.4	609.1	666.9
Frequencies	796.3	899.5	1003.2
Frequencies	1017.4	1043.9	1133.6
Frequencies	1136.1	1253.0	1339.4
Frequencies	1347.1	1382.7	1429.2
Frequencies	1524.8	1537.3	1547.6
Frequencies	1570.0	1617.7	1627.4
Frequencies	1629.7	1640.0	1645.8
Frequencies	1660.5	2371.1	3182.8
Frequencies	3185.4	3193.8	3250.7
Frequencies	3254.3	3255.4	3257.4
Frequencies	3266.0	3281.0	4076.6
Rot.Consts	*2.764*	*1.619*	*1.321*

tertbutylmethoxyketene (**24**)			
Frequencies	55.5	88.0	154.8
Frequencies	168.9	173.9	249.7
Frequencies	269.6	306.5	320.7
Frequencies	328.7	359.9	398.4
Frequencies	439.7	495.5	536.3
Frequencies	642.0	678.6	793.0
Frequencies	891.9	1003.8	1017.4
Frequencies	1044.6	1114.3	1137.6
Frequencies	1148.2	1274.6	1291.7
Frequencies	1329.6	1343.1	1356.1
Frequencies	1425.1	1509.1	1536.8
Frequencies	1543.5	1569.9	1616.6
Frequencies	1618.6	1627.8	1629.3
Frequencies	1634.6	1639.8	1643.6
Frequencies	1647.3	1661.4	2359.0
Frequencies	3184.6	3185.1	3189.0
Frequencies	3194.6	3249.3	3253.9
Frequencies	3255.3	3260.4	3265.4
Frequencies	3270.4	3281.4	3303.7
Rot.Consts	*1.853*	*1.461*	*1.031*

(HCCO)2 (**39**)			
Frequencies	68.1	210.2	250.5
Frequencies	565.3	632.1	642.7
Frequencies	656.7	685.5	825.9
Frequencies	1053.7	1221.9	1273.7
Frequencies	1482.6	1550.1	2363.3
Frequencies	2383.6	3360.0	3362.4
Rot.Consts	*10.857*	*1.880*	*1.681*

HOC(CO)C(H)CO (42)			
Frequencies	75.7	139.0	219.6
Frequencies	337.3	368.8	411.2
Frequencies	593.5	632.6	655.9
Frequencies	691.8	790.2	904.7
Frequencies	1219.4	1318.0	1380.1
Frequencies	1514.0	1548.5	2361.0
Frequencies	2391.9	3357.5	4068.1
Rot.Consts	*4.250*	*1.812*	*1.378*

HOC(CO)C(Me)CO (43)			
Frequencies	65.8	119.4	155.8
Frequencies	164.8	220.4	268.5
Frequencies	360.7	461.5	488.0
Frequencies	598.7	624.7	642.5
Frequencies	757.8	791.9	1037.8
Frequencies	1149.7	1168.5	1362.0
Frequencies	1401.4	1506.4	1537.9
Frequencies	1551.0	1611.3	1643.8
Frequencies	2350.9	2383.9	3192.4
Frequencies	3262.5	3272.4	4066.7
Rot.Consts	*2.584*	*1.521*	*1.233*

CHMe(HCCO)2 (28)			
Frequencies	49.7	77.7	157.7
Frequencies	167.0	293.8	360.8
Frequencies	391.7	460.5	586.3
Frequencies	607.0	642.1	666.5
Frequencies	721.7	788.1	872.6
Frequencies	1019.9	1093.0	1184.8
Frequencies	1195.8	1238.3	1260.4
Frequencies	1444.1	1467.1	1539.7
Frequencies	1552.3	1566.4	1632.7
Frequencies	1635.8	2363.3	2376.6
Frequencies	3189.1	3191.9	3262.1
Frequencies	3268.0	3362.7	3366.3
Rot.Consts	*2.899*	*1.423*	*1.074*

HC(CO)CH2OH (33)			
Frequencies	101.0	220.7	370.6
Frequencies	428.2	615.4	672.5
Frequencies	706.2	970.3	1155.7
Frequencies	1185.2	1232.6	1308.9
Frequencies	1470.7	1542.4	1579.6
Frequencies	1649.0	2370.8	3188.2
Frequencies	3280.9	3378.4	4109.1
Rot.Consts	*21.165*	*2.427*	*2.382*

(HOCCO)2 (44)			
Frequencies	67.6	121.9	155.7
Frequencies	225.2	282.9	355.1
Frequencies	371.0	512.8	520.8
Frequencies	608.9	624.3	645.6
Frequencies	781.4	802.8	1136.8
Frequencies	1364.8	1373.0	1439.5
Frequencies	1513.0	1536.0	2357.7
Frequencies	2393.0	4067.2	4071.6
Rot.Consts	*2.706*	*1.498*	*1.258*

CH2(HCCO)2 (25)			
Frequencies	59.0	61.3	174.4
Frequencies	264.5	341.3	595.5
Frequencies	604.1	641.0	644.5
Frequencies	700.9	719.1	949.9
Frequencies	1064.1	1149.0	1237.7
Frequencies	1240.8	1330.7	1437.0
Frequencies	1566.4	1571.2	1623.0
Frequencies	2355.0	2384.5	3203.0
Frequencies	3242.0	3377.8	3378.0
Rot.Consts	*18.600*	*0.917*	*0.910*

CMe2(HCCO)2 (31)			
Frequencies	49.7	70.4	154.0
Frequencies	167.8	289.2	323.3
Frequencies	325.8	336.2	406.0
Frequencies	429.9	442.8	591.4
Frequencies	609.3	628.5	670.9
Frequencies	690.1	748.6	867.1
Frequencies	988.7	1018.9	1055.1
Frequencies	1125.0	1228.0	1230.7
Frequencies	1278.3	1313.8	1350.8
Frequencies	1536.9	1541.0	1548.6
Frequencies	1563.7	1622.1	1625.5
Frequencies	1638.8	1646.4	2361.5
Frequencies	2374.3	3185.3	3191.8
Frequencies	3255.3	3261.4	3268.0
Frequencies	3270.7	3358.8	3361.6
Rot.Consts	*1.839*	*1.342*	*0.939*

CH2(HCCO)(MeCCO) (26)			
Frequencies	57.0	59.5	164.7
Frequencies	177.2	213.3	244.8
Frequencies	332.7	433.0	599.0
Frequencies	607.4	643.1	698.4
Frequencies	754.0	820.2	969.3
Frequencies	1080.2	1110.1	1156.6
Frequencies	1237.5	1301.2	1336.1
Frequencies	1441.8	1548.0	1565.6
Frequencies	1567.4	1612.9	1620.0
Frequencies	1651.2	2351.0	2377.9
Frequencies	3183.0	3193.6	3236.6
Frequencies	3244.8	3271.8	3374.1
Rot.Consts	*5.553*	*0.911*	*0.819*

CH2(MeCCO)2 (27)			
Frequencies	43.5	61.5	134.1
Frequencies	156.5	178.4	182.3
Frequencies	222.8	297.9	312.5
Frequencies	364.2	478.8	606.8
Frequencies	610.2	741.2	754.7
Frequencies	799.3	825.1	997.1
Frequencies	1091.6	1103.7	1145.9
Frequencies	1147.5	1277.2	1320.7
Frequencies	1335.6	1445.0	1543.8
Frequencies	1552.2	1564.8	1565.7
Frequencies	1610.3	1614.6	1619.2
Frequencies	1647.1	1654.1	2347.6
Frequencies	2371.0	3182.5	3183.2
Frequencies	3185.9	3226.3	3243.6
Frequencies	3243.7	3270.9	3271.1
Rot.Consts	*3.158*	*0.859*	*0.758*

MeC(CO)CH2OH (34)			
Frequencies	103.5	164.6	198.2
Frequencies	215.1	316.8	396.2
Frequencies	523.6	617.3	750.1
Frequencies	804.1	1031.3	1105.7
Frequencies	1147.0	1176.9	1295.5
Frequencies	1329.1	1477.2	1541.6
Frequencies	1550.6	1575.5	1614.1
Frequencies	1644.1	1651.8	2361.2
Frequencies	3188.5	3189.1	3254.1
Frequencies	3264.9	3276.4	4104.7
Rot.Consts	*5.697*	*2.426*	*1.863*

CHMe(HCCO)(MeCCO) (29)			
Frequencies	49.2	56.2	154.1
Frequencies	164.7	172.9	205.2
Frequencies	263.6	285.2	379.8
Frequencies	455.3	500.7	594.1
Frequencies	617.1	639.0	729.6
Frequencies	778.1	790.9	941.1
Frequencies	1057.1	1108.4	1142.3
Frequencies	1173.1	1193.4	1253.4
Frequencies	1323.6	1412.4	1447.8
Frequencies	1536.9	1548.7	1557.9
Frequencies	1575.3	1616.4	1634.4
Frequencies	1640.8	1653.1	2347.3
Frequencies	2372.9	3188.7	3193.9
Frequencies	3195.7	3250.8	3262.4
Frequencies	3270.6	3277.8	3368.6
Rot.Consts	*3.357*	*0.814*	*0.804*

CMe2(HCCO)(MeCCO) (32)			
Frequencies	42.5	54.5	156.1
Frequencies	167.4	173.2	213.3
Frequencies	266.5	295.0	335.6
Frequencies	341.2	372.3	413.2
Frequencies	466.2	481.6	593.6
Frequencies	609.7	620.9	701.5
Frequencies	765.3	781.0	897.2
Frequencies	1022.1	1039.3	1088.7
Frequencies	1120.4	1149.6	1224.5
Frequencies	1230.2	1268.5	1334.8
Frequencies	1359.4	1521.4	1531.7
Frequencies	1548.3	1556.1	1564.6
Frequencies	1616.6	1627.2	1630.8
Frequencies	1641.9	1648.6	1655.5
Frequencies	2343.8	2369.2	3188.3
Frequencies	3190.6	3196.6	3252.8
Frequencies	3257.3	3263.4	3269.5
Frequencies	3275.8	3278.4	3363.9
Rot.Consts	*2.369*	*0.805*	*0.726*

CHMe(MeCCO)2 (30)			
Frequencies	42.4	51.0	132.0
Frequencies	159.2	165.5	173.7
Frequencies	183.9	238.2	275.1
Frequencies	288.5	315.1	399.6
Frequencies	479.5	522.3	607.3
Frequencies	620.3	714.3	762.4
Frequencies	783.6	821.3	1023.2
Frequencies	1078.1	1108.4	1140.0
Frequencies	1147.0	1176.5	1181.4
Frequencies	1291.8	1321.2	1411.9
Frequencies	1449.0	1533.3	1547.7
Frequencies	1554.4	1557.5	1573.1
Frequencies	1615.0	1616.3	1634.2
Frequencies	1640.2	1648.6	1653.4
Frequencies	2343.7	2365.6	3179.2
Frequencies	3183.9	3188.6	3195.8
Frequencies	3244.9	3250.1	3263.7
Frequencies	3269.8	3270.0	3277.2
Rot.Consts	*2.208*	*0.797*	*0.723*

HC(CO)C(CH3)2OH (37)			
Frequencies	68.0	158.7	261.7
Frequencies	303.0	343.3	354.6
Frequencies	385.0	436.5	463.4
Frequencies	493.9	609.9	673.2
Frequencies	709.5	842.1	1006.7
Frequencies	1018.4	1081.8	1110.6
Frequencies	1210.9	1231.9	1326.3
Frequencies	1366.9	1463.4	1533.4
Frequencies	1558.0	1562.4	1615.6
Frequencies	1624.7	1636.5	1645.8
Frequencies	2365.9	3187.1	3202.7
Frequencies	3254.1	3277.1	3281.2
Frequencies	3286.2	3368.7	4103.7
Rot.Consts	*4.717*	*1.648*	*1.611*

HC(CO)CH(CH3)OH (35)			
Frequencies	81.9	180.2	271.2
Frequencies	359.3	378.9	415.1
Frequencies	518.9	614.6	670.3
Frequencies	707.5	950.6	1037.6
Frequencies	1139.1	1196.8	1239.3
Frequencies	1254.7	1397.5	1438.2
Frequencies	1517.8	1559.1	1592.6
Frequencies	1621.7	1632.9	2368.3
Frequencies	3171.6	3201.3	3277.7
Frequencies	3282.9	3372.2	4113.6
Rot.Consts	*8.126*	*1.938*	*1.703*

MeC(CO)C(CH3)2OH (38)			
Frequencies	58.7	165.2	172.5
Frequencies	206.2	255.2	277.5
Frequencies	308.9	371.3	380.8
Frequencies	402.4	444.1	519.0
Frequencies	529.4	627.1	683.7
Frequencies	764.4	925.0	1016.1
Frequencies	1054.1	1091.4	1106.0
Frequencies	1151.2	1216.4	1233.9
Frequencies	1328.1	1382.9	1465.6
Frequencies	1525.2	1550.7	1556.9
Frequencies	1562.2	1614.0	1619.1
Frequencies	1628.5	1637.0	1646.7
Frequencies	1655.3	2353.9	3187.5
Frequencies	3194.0	3206.2	3255.3
Frequencies	3258.3	3276.2	3277.1
Frequencies	3286.1	3291.4	4097.0
Rot.Consts	*2.741*	*1.647*	*1.304*

MeC(CO)CH(CH3)OH (**36**)			
Frequencies	67.3	159.8	164.5
Frequencies	219.1	263.7	285.0
Frequencies	368.1	398.8	496.9
Frequencies	544.8	618.4	759.7
Frequencies	763.8	972.1	1075.5
Frequencies	1114.6	1152.8	1175.3
Frequencies	1232.0	1301.4	1382.6
Frequencies	1478.4	1537.4	1548.6
Frequencies	1554.1	1569.0	1614.3
Frequencies	1628.1	1635.5	1649.7
Frequencies	2358.1	3185.1	3188.5
Frequencies	3232.8	3254.1	3258.9
Frequencies	3276.7	3285.4	4089.7
Rot.Consts	*3.392*	*2.202*	*1.490*

Table C - Thermodynamic functions of 1,3-bisketenes- Treatment of MeCCO and HCCO hindered rotations as vibrations. Entropy and C_p are given in cal/(mol K).

1,3-Bisketenes	S^{298}	$C_p(300)$	$C_p(400)$	$C_p(500)$	$C_p(600)$	$C_p(800)$	$C_p(1000)$	$C_p(1500)$
CH2(HCCO)2 (**25**)	83.85	25.91	31.12	35.46	39.04	44.48	48.37	54.11
CH2(HCCO)(MeCCO) (**26**)	92.89	31.49	37.75	43.20	47.82	55.04	60.30	68.17
CH2(MeCCO)2 (**27**)	99.28	37.09	44.40	50.95	56.61	65.61	72.24	82.23
CHMe(HCCO)2 (**28**)	91.57	31.62	38.48	44.23	48.94	56.06	61.12	68.62
CHMe(HCCO)(MeCCO) (**29**)	99.66	37.08	44.88	51.71	57.46	66.40	72.86	82.56
CHMe(MeCCO)2 (**30**)	107.81	42.93	51.76	59.63	66.37	77.02	84.82	96.61
CMe2(HCCO)2 (**31**)	95.57	37.75	46.21	53.34	59.19	67.99	74.20	83.35
CMe2(HCCO)(MeCCO) (**32**)	104.69	43.33	52.77	60.97	67.85	78.44	86.03	97.34

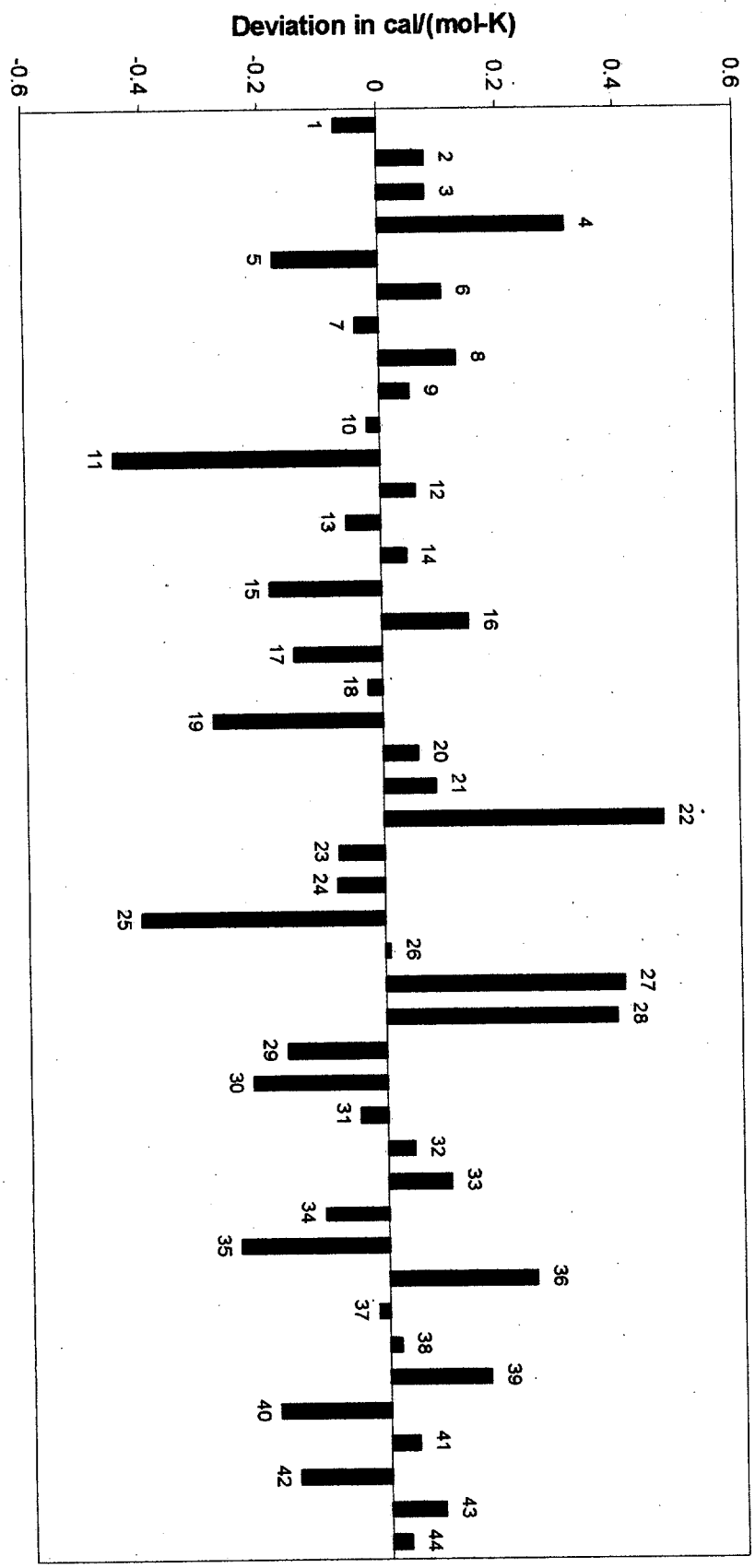

Figure A: Deviation between Calculated and Fitted S^{298}

Figure A

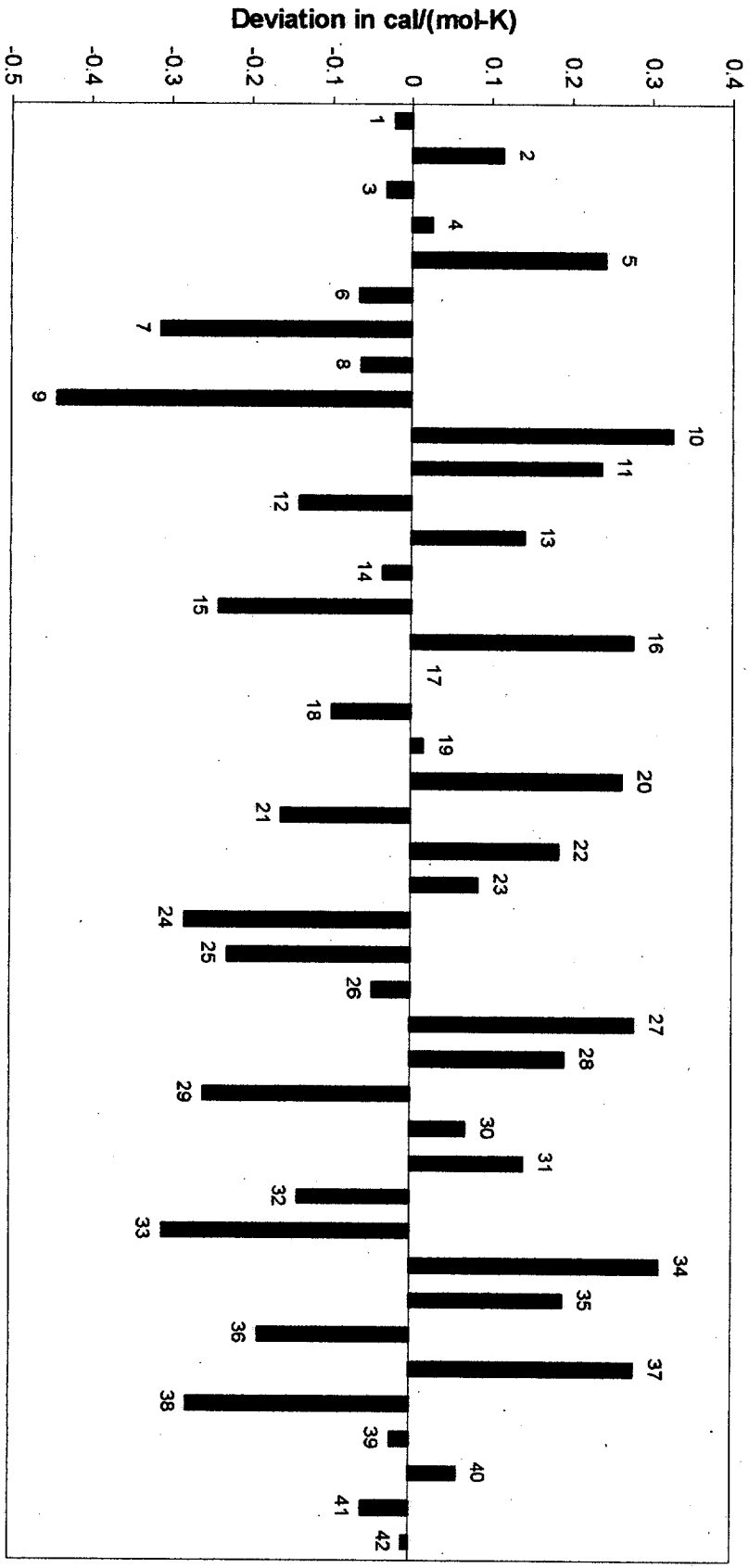

Figure B: Deviation between Calculated and Fitted Cp(300)

Figure B