Supporting Information

Carboxyketenes, Methyleneketenes, Vinylketenes, Oxetanediones, Ynols, and Ylidic Ketenes from Meldrum's Acid Derivatives

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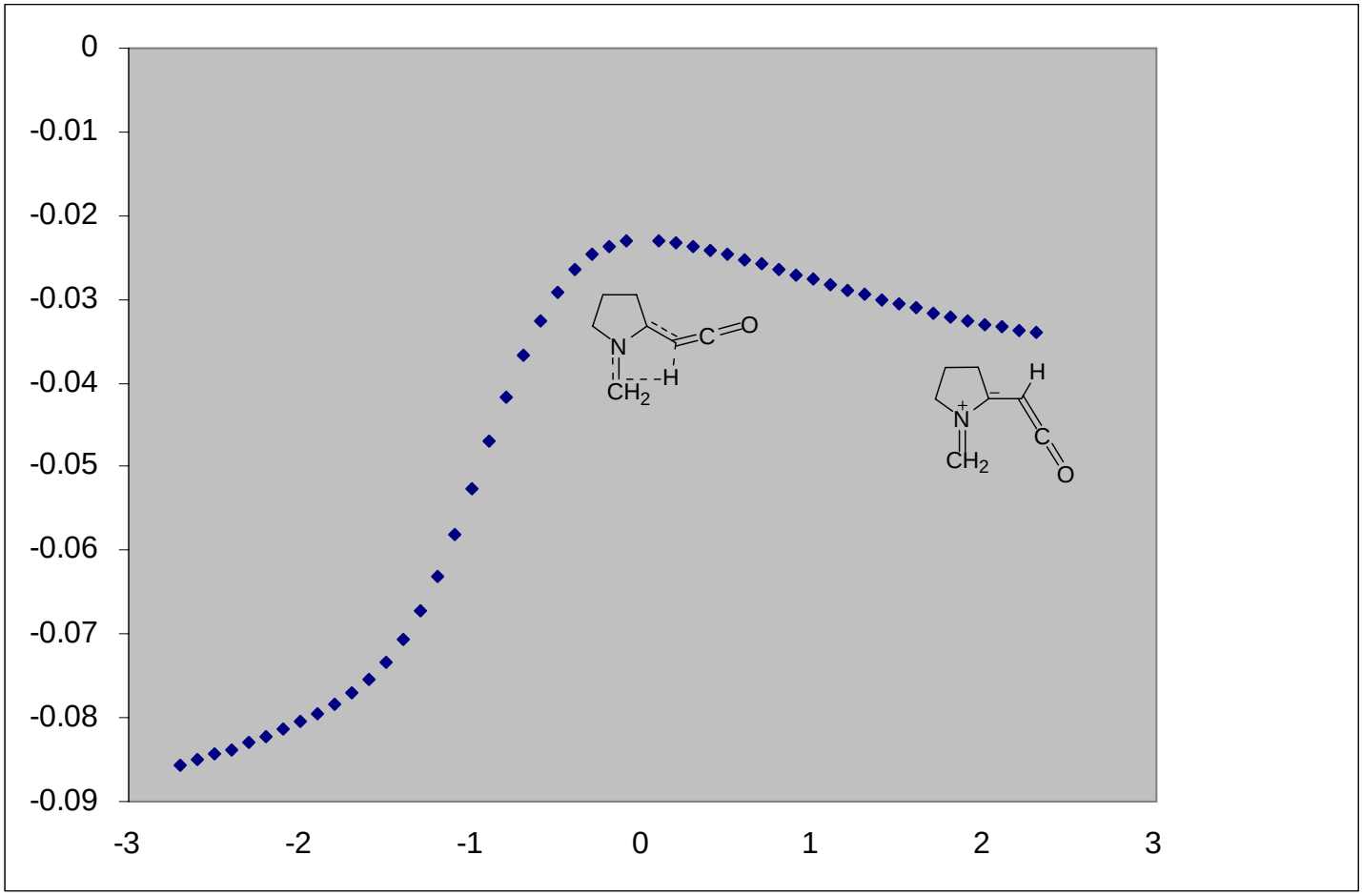
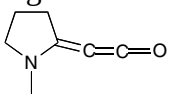
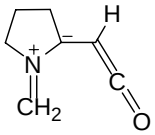


Figure S1. IRC curve for TS**24**, transition state connecting methyleneketene **21** (-3)



and ylidic ketene **25**



(*cf.* Scheme 2)

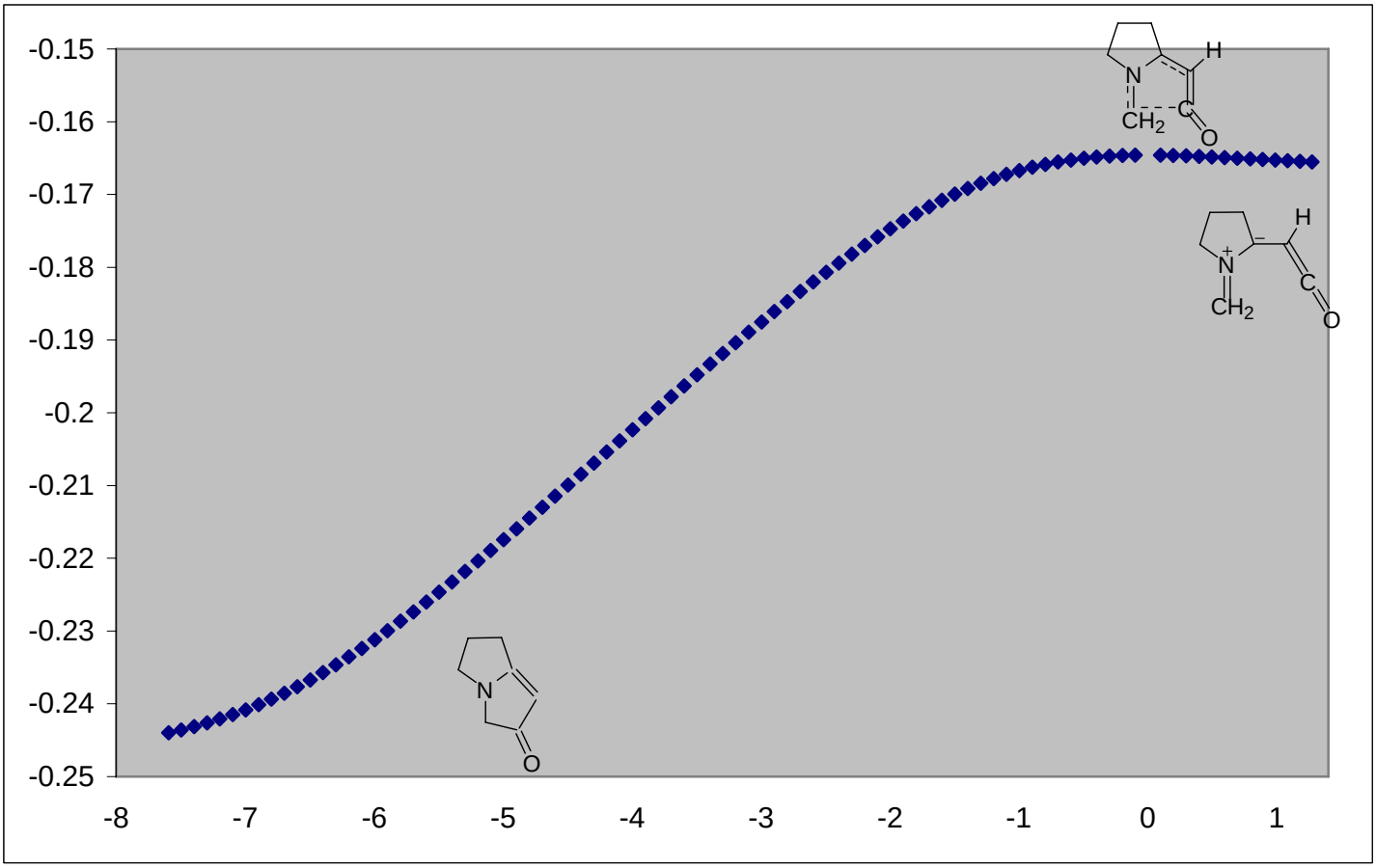


Figure S2. IRC curve of TS**26**, transition state connecting structures **25** and **27** (Scheme 2).

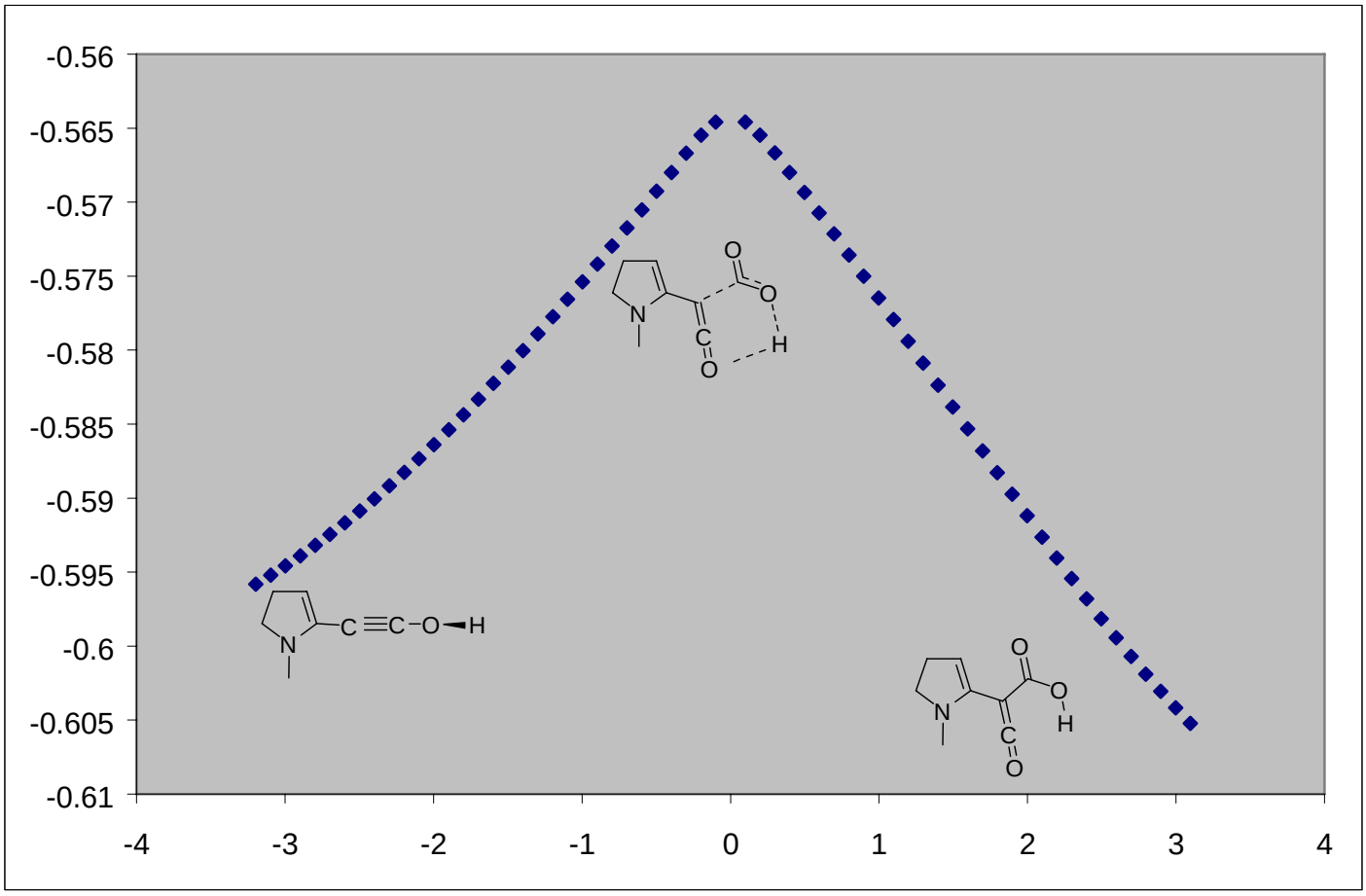


Figure S3. IRC curve of TS**33**, transition state connecting structures **32** and **34** (eq. 2).

Ser.No.	Structures	ΔE (kcal/mol)B3LYP/6-311+G(2d,p)	ΔE (kcal/mol)B3LYP/6-31G(d)
1	**12**	0	0
2	**13**	23.22	27.28
3	**19**	8.81	14.02
4	TS**14**	37.03	42.73
4a	TS**15**	41.17	48.89
5	**19**	0	0
6	**16**	20.86	27.82
7	**18**	9.42	17.52
8	TS**17**	65.43	71.75
9	1**21**	1.61	8.90
10	TS**23**	33.12	38.59
11	TS**22**	64.49	73.23
12	TS**20**	18.88	22.98
13	**25**	30.16	39.68
14	**27**	-17.34	-11.58
15	TS**24**	39.66	48.20
16	TS**26**	31.15	40.51
17	**32**	26.62	33.92
18	**34**	40.44	52.60
19	TS**33**	65.53	73.48

Relative energies of various species obtained by B3LYP/6-311+G(2d,p) and B3LYP/6-31G(d). Relative energy of 13, TS 14 and TS 15 are relative to 12. Relative energies of all others are relative to 19. The energy of 19 + acetone is 21.36 kcal/mol above that of 12.

Tables of Cartesian coordinates and energies for all the calculated species at B3LYP/6-311+G(2d,p) level

A: CO_2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.000000	0.000000
2	8	0.000000	0.000000	1.160367
3	8	0.000000	0.000000	-1.160367

Energy = -188.6506395

E+ZPVE = -188.638985

B: Acetone

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000079	0.183884	0.000000
2	8	-0.000012	1.394477	0.000000
3	6	-0.000012	-0.611430	1.289585
4	1	0.000006	0.062746	2.143691
5	1	-0.878517	-1.261796	1.332731
6	1	0.878393	-1.261925	1.332784
7	6	-0.000012	-0.611430	-1.289585
8	1	0.878393	-1.261925	-1.332784
9	1	-0.878517	-1.261796	-1.332731
10	1	0.000006	0.062746	-2.143691

Energy = -193.2228467
E+ZPVE = -193.139795

C: 5-(*N*-Methylpyrrolidin-2-ylidene)dioxanedione 12

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	0.304132	-2.315569	-0.887396
2	6	0.737678	-1.236576	-0.544843
3	6	0.596424	1.193345	0.137987

4	8	0.057647	2.208827	0.526177
5	8	2.092723	-1.053614	-0.620488
6	8	1.959851	1.224990	-0.030177
7	6	2.702727	0.013120	0.110174
8	6	4.050407	0.259275	-0.538196
9	1	4.661965	-0.640989	-0.476472
10	1	3.908918	0.521818	-1.586262
11	1	4.561917	1.077602	-0.031201
12	6	2.812133	-0.363402	1.585123
13	1	1.825088	-0.529226	2.019439
14	1	3.395224	-1.278905	1.689398
15	1	3.302173	0.440071	2.135713
16	6	-0.054139	-0.073842	-0.149477
17	6	-2.100961	-1.489393	0.557316
18	6	-3.708491	0.280824	0.309553
19	6	-3.606164	-1.243979	0.384045
20	1	-1.819380	-1.588563	1.611279
21	1	-1.726238	-2.368311	0.041717
22	1	-3.887754	0.738954	1.287940
23	1	-4.478623	0.637399	-0.374961
24	1	-4.202056	-1.661173	1.194503
25	1	-3.954657	-1.684960	-0.551578
26	6	-1.444277	-0.233131	0.021237
27	7	-2.382503	0.685597	-0.186234
28	6	-2.248045	1.939646	-0.912861
29	1	-1.387507	1.883839	-1.574329
30	1	-3.153860	2.077371	-1.506535
31	1	-2.106276	2.783503	-0.240269

Energy = -784.1150593
E+ZPVE = -783.861423

D: Enol 13

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.695921	1.234570	0.164196
2	6	-0.622433	-0.967796	-0.824411
3	8	-0.098504	-1.906398	-1.367813
4	8	-2.022075	1.246754	0.166859
5	8	-2.008292	-0.890814	-0.839545
6	6	-2.668428	-0.059492	0.100177
7	6	-4.058959	0.201135	-0.437568
8	1	-4.597493	0.875602	0.228268
9	1	-3.992113	0.650438	-1.427800
10	1	-4.602936	-0.740195	-0.511616
11	6	-2.667108	-0.682397	1.490574

12	1	-1.652207	-0.812279	1.865779
13	1	-3.218299	-0.045984	2.183349
14	1	-3.148211	-1.659617	1.444121
15	6	0.057217	0.160574	-0.216290
16	6	2.286509	1.162579	-0.821465
17	6	3.702447	-0.389662	0.258944
18	6	3.733430	0.995540	-0.416832
19	1	1.916864	1.888738	-1.530206
20	1	4.371926	-0.473891	1.116319
21	1	3.965385	-1.177707	-0.463294
22	1	4.047432	1.773057	0.291144
23	1	4.429385	1.026592	-1.256839
24	6	1.530603	0.248249	-0.177424
25	7	2.300381	-0.553701	0.676538
26	6	1.897514	-1.889731	1.072757
27	1	0.864690	-1.883711	1.418053
28	1	1.982336	-2.616794	0.255141
29	1	2.526259	-2.213122	1.904928
30	8	-0.211444	2.404702	0.560856
31	1	0.757603	2.369407	0.428102

Energy = -784.0768303
E+ZPVE = -783.824412

E: Z-carboxyketene 16

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.905550	-0.882093	0.285440
2	6	1.428465	1.252696	-0.635374
3	8	1.856254	2.260059	-0.988459
4	8	3.089146	-0.658178	0.325657
5	6	0.910369	0.099940	-0.221247
6	6	-2.642240	-1.035751	-0.778117
7	6	-2.779165	0.127712	0.222371
8	1	-3.036712	-0.761185	-1.763847
9	1	-3.185245	-1.924782	-0.452279
10	1	-3.576988	0.828874	-0.024083
11	1	-2.965531	-0.261098	1.234279
12	6	-0.546926	-0.135399	-0.293695
13	7	-1.463797	0.803427	0.205585
14	6	-1.166293	1.570365	1.407077
15	1	-1.167501	0.943441	2.311613
16	1	-0.198512	2.061484	1.327692
17	1	-1.924188	2.345770	1.525675
18	6	-1.144786	-1.207628	-0.849470
19	1	-0.642877	-1.943485	-1.460859

20	8	1.395290	-2.051254	0.719617
21	1	0.428770	-2.057092	0.586292

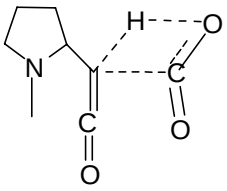
Energy = -590.8367668
E+ZPVE = -590.674343

F: Pyrrolinylketene 18

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.187266	-1.061101	0.280955
2	6	2.293533	-0.436396	-0.060796
3	8	3.297116	0.080982	-0.336952
4	6	-1.973523	0.831375	-0.119085
5	6	-2.494983	-0.611746	-0.220755
6	1	-2.206356	1.244250	0.874225
7	1	-2.383331	1.504465	-0.873390
8	1	-3.361661	-0.778720	0.422984
9	1	-2.805516	-0.849889	-1.246496
10	7	-0.505144	0.720651	-0.266216
11	6	0.214025	1.831748	0.339858
12	1	0.071232	1.881306	1.430976
13	1	1.281096	1.783251	0.129402
14	1	-0.153600	2.762241	-0.095649
15	1	1.344669	-2.060885	0.670178
16	6	-1.271120	-1.398583	0.168564
17	1	-1.245023	-2.469076	0.307423
18	6	-0.185601	-0.606855	0.101172

Energy = -402.2004313
E+ZPVE = -402.053582

G: TS17, connecting 16 and 18



Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.857991	-0.795381	0.689391
2	6	1.408898	1.018975	-1.063628
3	8	1.985295	1.896417	-1.527705

4	8	1.917238	-0.437489	1.818562
5	6	0.853732	-0.073546	-0.531078
6	6	-2.818844	-0.899096	-0.682410
7	6	-2.729205	0.179018	0.415684
8	1	-3.307955	-0.509916	-1.583848
9	1	-3.389859	-1.770874	-0.357472
10	1	-3.497775	0.948931	0.340267
11	1	-2.803128	-0.285916	1.409776
12	6	-0.619326	-0.212969	-0.406485
13	7	-1.382517	0.770135	0.258302
14	6	-0.864496	1.412988	1.458554
15	1	-0.827631	0.729619	2.318225
16	1	0.140989	1.796870	1.290196
17	1	-1.506295	2.258870	1.709781
18	6	-1.362318	-1.183141	-0.952016
19	1	-0.990381	-1.962843	-1.598890
20	8	2.340288	-1.726961	-0.036218
21	1	1.558489	-1.132503	-0.941332

Energy = -590.7590005
E+ZPVE = -590.603312
Imaginary frequency = -1739.4 cm^{-1}

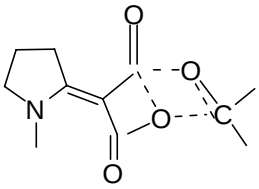
H: Oxetanedione 19

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.854389	-1.064358	0.015122
2	6	1.829664	0.939773	-0.034732
3	8	1.979077	2.122243	-0.071882
4	8	2.860615	-0.038909	-0.028203
5	8	2.041331	-2.238450	0.036739
6	6	0.780118	-0.079752	0.012270
7	6	-2.715903	-1.268153	-0.261812
8	6	-2.883998	0.212284	0.094431
9	1	-2.852340	-1.408888	-1.335474
10	1	-3.432731	-1.904917	0.254500
11	1	-3.540710	0.752627	-0.590277
12	1	-3.267182	0.357562	1.111976
13	6	-0.582543	-0.214420	0.033158
14	7	-1.518351	0.741477	-0.003386
15	6	-1.295836	2.176923	0.049108
16	1	-1.629407	2.574618	1.012865
17	1	-0.241534	2.408298	-0.080240
18	1	-1.870184	2.664118	-0.742206
19	6	-1.258682	-1.563932	0.130114
20	1	-0.767747	-2.310620	-0.491389

21	1	-1.181143	-1.912397	1.164757

Energy = -590.8718072
E+ZPVE = -590.707581

I: TS14 connecting 12 and 19

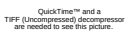


Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	0.469222	2.587737	0.206723
2	6	0.449787	1.433050	0.088935
3	6	0.538103	-1.135952	0.638374
4	8	-0.154981	-1.701240	1.490438
5	8	2.201840	1.008140	-0.815946
6	8	1.641562	-1.472571	0.161982
7	6	3.038953	0.235298	-0.328289
8	6	3.460585	0.324249	1.114774
9	1	4.351273	0.962460	1.158885
10	1	2.685552	0.778017	1.730176
11	1	3.715789	-0.655729	1.511928
12	6	3.911549	-0.574713	-1.246084
13	1	3.465014	-0.627348	-2.236536
14	1	4.894271	-0.096032	-1.317285
15	1	4.047086	-1.577499	-0.842422
16	6	-0.148897	0.202320	0.138356
17	6	-2.368229	1.542971	-0.021009
18	6	-3.763628	-0.382145	-0.403464
19	6	-3.806687	1.036845	0.165299
20	1	-2.241045	2.065354	-0.974891
21	1	-2.046826	2.225991	0.762199
22	1	-4.080994	-0.429306	-1.451332
23	1	-4.366707	-1.094181	0.162836
24	1	-4.545277	1.662051	-0.334254
25	1	-4.054596	1.005154	1.227212
26	6	-1.541917	0.272007	-0.043241
27	7	-2.343585	-0.752343	-0.313505
28	6	-1.954528	-2.114933	-0.654006
29	1	-0.988895	-2.114966	-1.156054
30	1	-1.872340	-2.729824	0.241511
31	1	-2.708915	-2.518248	-1.330881

Energy = -784.0506531

E+ZPVE = -783.802404
Imaginary frequency = - 219.5cm^{-1}

Ia: TS 15 connecting **13** and **16**



Atom type Coordinates (angstroms):
X Y Z
C -0.59172700 1.35429600 0.38307800
C -0.49209000 -0.88730700 -0.79625900
O -0.26178000 -1.94447100 -1.25547700
O -1.78075000 1.45282400 0.67137500
O -2.21330700 -0.47462700 -1.08716900
C -3.00261900 -0.32439900 -0.13669700
C -4.28544100 0.40161600 -0.39741000
H -4.39580300 1.19789600 0.34000300
H -4.28908000 0.82256000 -1.40005700
H -5.12700700 -0.28710600 -0.27775800
C -2.87168900 -1.05967500 1.16250200
H -1.84676800 -1.36032300 1.36164700
H -3.24840000 -0.45537200 1.98532800
H -3.49155500 -1.96097000 1.08726200
C 0.09120100 0.21156100 -0.21198500
C 2.36617600 0.88272800 -1.09776000
C 3.72676500 -0.49303500 0.25748700
C 3.81431900 0.70817300 -0.70497800
H 2.00717800 1.50873700 -1.90075300
H 4.42912300 -0.43947900 1.09054600
H 3.90822700 -1.43298900 -0.28691700
H 4.19954900 1.59888700 -0.19228500
H 4.47830500 0.51264000 -1.54891400
C 1.58173600 0.19598500 -0.24638500
N 2.33614100 -0.46827800 0.74194400
C 1.85998700 -1.68677800 1.36678300
H 0.83176200 -1.55499400 1.70058200
H 1.90240700 -2.55392200 0.69135300

H 2.47238500 -1.90002500 2.24507800
O 0.19834400 2.40807200 0.68248700
H 1.09692800 2.22902400 0.35130400

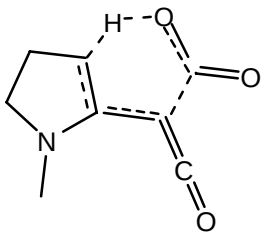
Imaginary Frequency: -156.2626 cm^{-1}
HF = -784.0438062 Hartree
Zero-point correction = 0.247990 (Hartree/Particle)
Sum of electronic and zero-point Energies = -783.795816 Hartree

J: Methyleneketene 21

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.342163	0.428172	-0.022454
2	6	2.555888	0.027961	-0.014865
3	8	3.712463	-0.190976	-0.013773
4	6	-2.277238	-0.066792	0.114074
5	6	-1.845676	-1.506220	-0.199862
6	1	-2.667294	0.036276	1.135275
7	1	-3.039095	0.313418	-0.570535
8	1	-2.419570	-2.241448	0.363229
9	1	-1.989973	-1.710652	-1.262342
10	7	-1.040007	0.695157	-0.031281
11	6	-1.048661	2.141704	-0.022101
12	1	-1.413399	2.522958	0.937650
13	1	-0.030761	2.492986	-0.180721
14	1	-1.696630	2.520528	-0.816515
15	6	0.078674	-0.059772	0.012727
16	6	-0.346474	-1.512788	0.141445
17	1	0.250407	-2.155505	-0.503654
18	1	-0.165403	-1.830442	1.172973

Energy = -402.214556
E+ZPVE = -402.066031

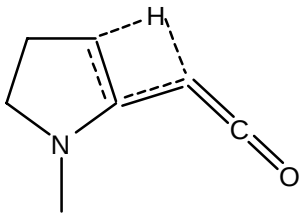
K: TS23, connecting 16 and 21



Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.909522	0.142069	-0.176214
2	6	1.526650	1.291392	-0.407239
3	8	2.075726	2.275936	-0.642599
4	6	1.838083	-1.036616	0.253320
5	8	3.022959	-0.790733	0.381362
6	8	1.219875	-2.142693	0.455032
7	1	0.015192	-1.971559	0.132108
8	6	-2.808583	0.153971	0.012305
9	6	-2.506449	-1.335848	-0.272237
10	1	-3.374558	0.307168	0.932833
11	1	-3.349645	0.649075	-0.801096
12	1	-2.755068	-1.951769	0.594931
13	1	-3.098578	-1.705162	-1.109143
14	7	-1.471532	0.766793	0.163596
15	6	-1.308866	2.065283	0.786373
16	1	-1.538339	2.874642	0.086790
17	1	-1.982296	2.147098	1.641648
18	1	-0.287667	2.184450	1.144123
19	6	-0.514380	-0.065842	-0.256974
20	6	-1.003163	-1.358463	-0.572094
21	1	-0.673683	-1.777243	-1.521161

Energy = -590.8121828
E+ZPVE = -590.654797
Imaginary frequency = -1439.8 cm^{-1}

L: TS22, connecting 18 and 21



Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.248112	-0.781413	-0.098818
2	6	2.447838	-0.322528	0.002226
3	8	3.580742	-0.045601	0.137726
4	6	-2.194605	0.559182	-0.030893
5	6	-2.337570	-0.956716	0.279731
6	1	-2.610957	1.198005	0.751033
7	1	-2.666062	0.835889	-0.980066

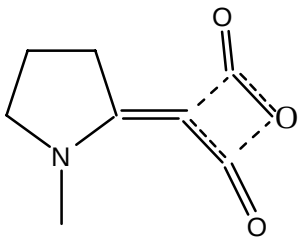
8	1	-2.563964	-1.103245	1.339720
9	1	-3.154113	-1.401575	-0.289975
10	7	-0.734545	0.783382	-0.113957
11	6	-0.135182	2.092117	0.012866
12	1	-0.579848	2.634174	0.851643
13	1	0.933863	1.978802	0.189725
14	1	-0.276012	2.683615	-0.896568
15	1	0.460192	-1.867842	0.417676
16	6	-0.961705	-1.514515	-0.093558
17	1	-0.890010	-2.246637	-0.892863
18	6	-0.093089	-0.381135	-0.203961

Energy = - 402.1070418

E+ZPVE = - 401.965826

Imaginary frequency = -1891.2 cm^{-1}

M: TS20, connecting 19 and 21



Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.002886	-1.028979	-0.059602
2	6	1.478306	1.248080	0.068970
3	8	1.957609	2.288102	0.156615
4	8	3.096477	-0.428237	-0.085323
5	8	1.682085	-2.209697	-0.084989
6	6	0.842117	0.058799	0.013867
7	6	-2.604982	-1.364203	-0.133458
8	6	-2.858893	0.125049	0.110806
9	1	-2.772057	-1.601872	-1.185434
10	1	-3.260331	-1.997827	0.461672
11	1	-3.552711	0.575463	-0.600162
12	1	-3.225386	0.331099	1.122544
13	6	-0.535816	-0.166492	0.041548
14	7	-1.520879	0.722799	-0.058070
15	6	-1.357277	2.161532	-0.181508
16	1	-1.045905	2.613402	0.763918
17	1	-0.616077	2.392411	-0.946983
18	1	-2.307994	2.598672	-0.480479

19	6	-1.119275	-1.543499	0.220202
20	1	-0.574334	-2.277568	-0.368647
21	1	-0.970806	-1.836426	1.264687

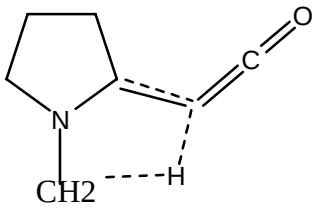
Energy = -590.8390145
E+ZPVE = -590.677492
Imaginary frequency = -288.1cm^{-1}

N: Ylidic ketene 25

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.370784	-1.407317	0.154892
2	6	0.298136	1.858471	-0.001479
3	6	2.343283	-0.390689	-0.024120
4	1	-1.503084	-1.777831	1.182534
5	1	-1.329238	-2.288541	-0.492237
6	1	1.368535	1.770070	0.034225
7	1	-0.179294	2.818831	-0.082119
8	7	-0.479054	0.764773	0.011980
9	8	3.410236	0.079383	-0.026068
10	6	1.183589	-1.033917	-0.018589
11	1	1.316162	-2.111318	-0.058127
12	6	-0.159196	-0.534352	0.016231
13	6	-2.510307	-0.450044	-0.238769
14	1	-2.699884	-0.517331	-1.311486
15	1	-3.445121	-0.655596	0.283394
16	6	-1.951943	0.928135	0.111534
17	1	-2.266585	1.722280	-0.564994
18	1	-2.186682	1.229239	1.135294

Energy = -402.1662874
E+ZPVE = -402.020527

O: TS24, connecting 21 and 25



Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.278923	0.407199	-0.183762
2	6	2.481012	-0.079733	-0.059599
3	8	3.599801	-0.396685	0.058363
4	6	-2.299917	0.154042	0.083369
5	6	-2.029617	-1.337572	-0.190581
6	1	-2.758022	0.331632	1.060771
7	1	-2.929795	0.627378	-0.671630
8	1	-2.682495	-1.986574	0.391249
9	1	-2.193301	-1.559785	-1.245979
10	7	-0.962317	0.763477	0.059324
11	6	-0.626523	2.141015	-0.016503
12	1	-0.317647	2.555872	0.942412
13	1	0.947294	1.569086	-0.422206
14	1	-1.398157	2.727394	-0.508194
15	6	0.007590	-0.140573	0.027801
16	6	-0.531171	-1.529688	0.156091
17	1	-0.016926	-2.225681	-0.507660
18	1	-0.394920	-1.898317	1.178165

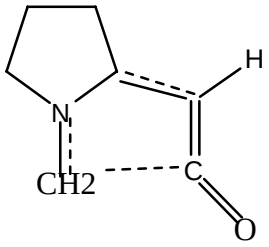
Energy = -402.1484942
E+ZPVE = -402.005393
Imaginary frequency = - 898.9 cm^{-1}

P: Bicyclic pyrrolinone 27

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.667015	1.251395	0.063921
2	6	-1.017221	-1.186667	-0.042827
3	6	-1.910382	0.086847	0.008850
4	1	1.785458	1.705805	1.051309
5	1	1.887367	2.025125	-0.672737
6	1	-1.318900	-1.845723	-0.858150
7	1	-1.104323	-1.731966	0.903081
8	7	0.318367	-0.642127	-0.220491
9	8	-3.126596	0.059907	0.035840
10	6	-0.993826	1.211838	0.021991
11	1	-1.284943	2.247608	0.086430
12	6	0.271991	0.714659	-0.067661
13	6	2.552119	-0.011801	-0.102382
14	1	2.913629	-0.081966	-1.129270
15	1	3.419065	-0.007514	0.557133
16	6	1.602673	-1.191717	0.191046
17	1	1.852211	-2.088688	-0.377734
18	1	1.600419	-1.454373	1.259020

Energy = -402.2464502
E+ZPVE = -402.096226

Q: TS26, connecting 25 and 27



Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.435883	-1.391389	0.023543
2	6	0.458546	1.748787	-0.110712
3	6	2.271782	-0.348141	0.097653
4	1	-1.477480	-1.903034	0.995373
5	1	-1.513033	-2.168320	-0.742075
6	1	1.331243	1.613439	-0.729100
7	1	0.079975	2.747472	0.036218
8	7	-0.446849	0.739689	-0.062932
9	8	3.373480	0.031844	0.062009
10	6	1.142970	-1.059022	-0.045328
11	1	1.304512	-2.130056	0.034295
12	6	-0.188695	-0.566559	-0.091582
13	6	-2.554972	-0.337814	-0.115190
14	1	-2.911771	-0.304029	-1.145934
15	1	-3.410820	-0.544184	0.527506
16	6	-1.873096	0.985865	0.242016
17	1	-2.228420	1.836432	-0.338791
18	1	-1.958017	1.229349	1.304566

Energy = -402.1645706
E+ZPVE = -402.018958
Imaginary frequency = - 262.8cm^{-1}

R: E-carboxyketene 32

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.976468	-0.878945	0.141823
2	6	1.181744	1.334419	-0.446836
3	8	1.519342	2.405437	-0.722253
4	8	1.806520	-2.064001	0.205074

5	6	0.873894	0.087375	-0.100584
6	6	-2.606410	-1.368696	-0.214685
7	6	-2.786388	0.150542	-0.435159
8	1	-3.066809	-1.940077	-1.023543
9	1	-3.052601	-1.728846	0.720243
10	1	-2.975643	0.357183	-1.491090
11	1	-3.601096	0.584429	0.144155
12	6	-0.546233	-0.289381	-0.097360
13	7	-1.492571	0.787645	-0.060349
14	6	-1.551451	1.503011	1.223250
15	1	-1.893779	0.864376	2.050464
16	1	-0.568735	1.894933	1.486080
17	1	-2.229686	2.351447	1.127394
18	6	-1.102386	-1.499092	-0.203186
19	1	-0.557376	-2.424979	-0.285715
20	8	3.237734	-0.377716	0.280884
21	1	3.249531	0.582853	0.381234

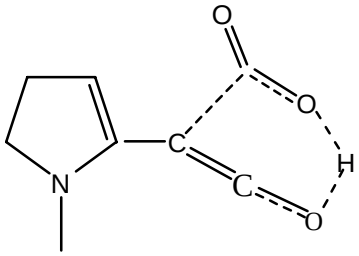
Energy = -590.8269446
E+ZPVE = -590.665154

S:Ynol 34

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.270282	-0.302837	-0.003755
2	6	2.468942	-0.225456	-0.009095
3	6	-2.319759	0.371346	0.035691
4	6	-2.344379	-1.165397	-0.055666
5	1	-2.520613	0.690511	1.071401
6	1	-3.039845	0.863538	-0.619691
7	1	-3.024055	-1.612437	0.672704
8	1	-2.672552	-1.495957	-1.050266
9	7	-0.941490	0.737487	-0.332537
10	6	-0.508884	2.051032	0.107282
11	1	-0.586499	2.176100	1.199787
12	1	0.525847	2.218929	-0.188798
13	1	-1.128784	2.812634	-0.369496
14	6	-0.148441	-0.393945	-0.016055
15	6	-0.892096	-1.500577	0.168511
16	1	-0.493858	-2.492079	0.317027
17	8	3.770652	-0.086301	0.066059
18	1	4.211572	-0.638237	-0.594850

Energy = -402.150622
E+ZPVE = -402.004157

T: TS 33, connecting 32 and 34



Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.839090	0.748461	-0.793225
2	6	-1.665809	-1.118201	0.736571
3	8	-2.878442	-1.240068	0.955263
4	8	-1.081650	1.396356	-1.410595
5	6	-0.616998	-0.663394	0.252113
6	6	2.954300	-0.864189	-0.762486
7	6	2.887857	0.393457	0.125544
8	1	3.487771	-1.679438	-0.256682
9	1	3.468783	-0.679435	-1.707259
10	1	3.717184	0.477804	0.828975
11	1	2.871512	1.298784	-0.501512
12	6	0.788669	-0.545266	0.019926
13	7	1.605548	0.268930	0.840949
14	6	1.079953	1.499808	1.401973
15	1	0.930744	2.282204	0.642175
16	1	0.129253	1.305007	1.897860
17	1	1.777379	1.876373	2.152343
18	6	1.494810	-1.204091	-0.914524
19	1	1.089877	-1.949836	-1.580518
20	8	-3.040886	0.595372	-0.541762
21	1	-3.205647	-0.306762	0.219379

Energy = -590.7592025
E+ZPVE = -590.603148
Imaginary frequency = -1231.2 cm^{-1}

Tables of Cartesian coordinates and energies for species **35**–**39** at

B3LYP/6-31G(2df,p) level

35a

Energy = -628.20344

C	-0.38981	0.00606	-0.39309
C	0.95200	0.00908	-0.29022
C	-1.36141	0.01620	-1.22600
O	-2.34941	0.02278	-1.86293
N	1.61749	-0.00695	0.87904
H	1.62096	0.02620	-1.15476
C	0.94952	-0.03528	2.16711
H	1.70136	-0.01255	2.95774
H	0.34183	-0.94038	2.26945
H	0.28396	0.82718	2.27267
H	2.62299	-0.01038	0.85824

36a

Energy = -628.14291

H	1.45787	0.94094	1.72077
H	1.25631	-0.39655	2.93724
O	0.17733	0.13876	-2.86185
C	0.05453	-0.19647	-0.41624
C	0.05905	-0.02647	-1.71060
C	-0.92915	-0.01611	0.56209
H	1.00531	-0.46401	0.30674
N	-0.43151	0.04436	1.79332
H	-2.00063	0.02388	0.41651
C	0.97368	-0.00612	1.96240
H	-1.06552	-0.05383	2.57433

37a

Energy = -628.15438

C	0.77826	-0.16650	0.48018
O	-0.04113	0.31023	-2.89900
C	-0.14792	0.00888	-1.77650
H	-1.17483	-0.87569	-0.24426
C	-0.24664	-0.37226	-0.51771
N	0.43650	0.03639	1.75832
C	-0.75041	0.16021	2.36239
H	-1.64316	0.23175	1.76472
H	-0.76826	0.20782	3.43728
H	1.22950	0.06031	2.38778
H	1.83052	-0.14282	0.24806

38a

Energy = -628.15248

C	-1.25793	0.04946	1.14197
C	-0.01517	-0.09923	-1.30885
C	1.07501	0.02484	-0.53914
C	1.13045	0.03752	0.88090
H	-2.03855	-0.10713	1.87086
H	2.00482	-0.05983	-1.09503
H	-1.46178	0.69351	0.29968
O	-0.80328	-0.07340	-2.17125
N	0.01586	0.01053	1.60652
H	2.07413	0.06486	1.40200
H	0.14249	-0.15343	2.59761

39a

Energy = -628.24957

C	1.11777	0.03140	-0.36601
C	-0.37614	0.01235	-0.79214
C	-1.12826	0.00600	0.45759
C	-0.24081	-0.01093	1.48424
H	1.57895	0.97633	-0.67491
H	-2.20383	-0.00669	0.53463
H	1.66429	-0.79084	-0.83694
O	-0.76064	-0.00104	-1.94214
N	1.06795	-0.10108	1.08669
H	-0.46042	0.00896	2.54538
H	1.79511	0.29520	1.66010

35b

Energy = -285.37379

C	-0.60954	0.00000	-0.69384
C	0.71863	0.00000	-0.65936
C	-1.72256	0.00000	-1.32601
O	-2.80804	0.00000	-1.77094
S	1.70927	0.00000	0.76576
H	1.34569	0.00000	-1.55335
C	0.46145	0.00000	2.08437
H	1.00608	0.00000	3.02955
H	-0.16182	-0.89143	2.00410
H	-0.16182	0.89143	2.00410

36b

Energy = -285.30664

H	0.25688	-0.90954	-2.22665
H	-0.34661	0.64246	-2.99065
O	2.25416	-0.34160	2.30137
C	0.62423	0.11194	0.49008
C	1.45641	-0.11474	1.48720

37b

Energy = -285.32590

C	1.50368	-0.00195	-0.99174
C	-0.09165	0.00679	1.73386
C	-1.14687	0.00219	0.93103
C	-1.22325	-0.00362	-0.50108
H	2.29456	-0.00389	-1.72656

C	-0.76618	0.07532	0.49822
H	0.94345	0.33462	-0.61190
S	-1.52603	0.10838	-1.02198
H	-1.38671	-0.01188	1.38162
C	-0.16176	0.08467	-2.07745
H	-2.08108	0.00316	1.48809
H	1.74068	0.00260	0.05952
O	0.78028	0.01103	2.50755
S	-0.01521	-0.00649	-1.62254
H	-2.20464	-0.00669	-0.95329

38b

Energy = -285.32408

C	1.56600	0.10564	-0.48759
C	-1.19591	-0.11093	-1.10910
C	-1.39848	-0.18009	0.21393
C	-0.47226	-0.02985	1.27796
H	2.53013	0.51436	-0.75239
H	-2.45721	-0.24157	0.45799
H	1.10320	-0.61819	-1.14124
O	-1.24471	-0.18882	-2.26956
S	1.16289	0.20539	1.12031
H	-0.82074	-0.13897	2.29603

39b

Energy = -285.40841

C	0.93983	0.00011	-0.69580
C	-0.57309	0.00004	-1.02142
C	-1.35460	-0.00010	0.21750
C	-0.60637	-0.00013	1.33478
H	1.41366	0.88704	-1.12113
H	-2.43627	-0.00017	0.19927
H	1.41377	-0.88670	-1.12126
O	-0.98961	0.00009	-2.15788
S	1.12953	-0.00001	1.12155
H	-0.98131	-0.00022	2.35091

35C

Energy = -305.22928

C	-0.37159	0.00000	-0.34090
C	0.96110	0.00000	-0.26027
C	-1.33204	0.00000	-1.19737
O	-2.30597	0.00000	-1.84542
O	1.67007	0.00000	0.86296
H	1.64134	0.00000	-1.11263
C	0.93525	0.00000	2.09387
H	1.68448	0.00000	2.88523
H	0.30250	-0.88933	2.15752
H	0.30250	0.88933	2.15752

36C

Energy = -305.15034

H	1.40828	0.87910	1.66086
H	1.12264	-0.26592	3.06327
O	0.05818	0.21706	-2.84537
C	0.10939	-0.20500	-0.40453
C	0.03845	0.00416	-1.70148
C	-0.86292	-0.03430	0.58280
H	1.05248	-0.53877	0.17445
O	-0.43957	-0.01949	1.80772
H	-1.93634	0.02316	0.45903
C	0.94909	-0.04453	2.01381

37C

Energy = -305.1565

C	-1.22423	0.40723	1.25903
C	0.01351	-0.38060	-1.32909
C	1.04791	-0.18781	-0.51580
C	1.09327	0.20160	0.85186
H	-1.53848	0.13498	0.26506
H	2.00126	-0.36510	-1.00660
H	-1.89966	0.66180	2.05735
O	-0.82053	-0.57533	-2.12110
O	0.04857	0.45178	1.58551
H	2.02977	0.31413	1.37289

38C

Energy = -305.15955

C	0.90444	-0.12690	0.38959
O	-1.32822	1.30597	-1.98438
C	-0.72122	0.62881	-1.25775
H	-0.58693	-1.33529	-0.66286
C	-0.18096	-0.33173	-0.52778
O	1.48527	1.03639	0.48837
C	1.28430	2.12807	-0.21507
H	0.71416	2.08299	-1.13042
H	1.86713	2.97496	0.10402
H	1.31223	-0.87644	1.04822

39C

Energy = -305.27

C	1.11707	0.00011	-0.31395
C	-0.34829	0.00006	-0.79333
C	-1.12207	-0.00017	0.44764
C	-0.23942	-0.00017	1.46494
H	1.65410	0.89233	-0.64666
H	-2.19751	-0.00028	0.52387
H	1.65415	-0.89203	-0.64679

O	-0.70564	0.00016	-1.94968
O	1.06328	0.00000	1.12519
H	-0.41565	-0.00028	2.53373