Supporting Information

Dioxygen Promoted Regioselective Oxidative Heck Arylations of Electron-Rich Olefins with Arylboronic Acids

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EXPERIMENTAL SECTION	S2
Procedures	S2
Materials	S2
Analytical Data for New Compounds	S3
COMPUTATIONAL DETAILS	S4
APPENDIX	S13
NMR Spectra and GC-MS Chromatograms for New Enamides 8a, 8d, 9c and 10e	S13
NMR Spectra and GC-MS Chromatograms for Known Compounds 4b,c,d,f,g,h,i	S22
REFERENCES	S29

EXPERIMENTAL SECTION

Procedures

Analytical TLC was performed using Merck glass-backed 0.2 mm silica gel 60 F-254 plates. Visualization was done with UV light and staining with anisaldehyde solution [anisaldehyde (5.0 mL), AcOH (3.5 mL) and H₂SO₄ (6 mL) in EtOH (200 mL)] followed by heating. Centrifugal chromatography was used to purify the crude products using Merck silica gel 60 PF-254 containing gypsum (art. no. 1.07749.2500). Infrared spectra were recorded on a FTIR instrument. NMR spectra were recorded for ¹H at 270 MHz and 400 MHz, for ¹³C NMR at 67.8 MHz and 100 MHz at 25 °C. Chemical shifts for ¹H and ¹³C were referenced to TMS via the solvent signals (¹H, CHCl₃ at 7.26 ppm; ¹³C, CDCl₃ at 77.0 ppm). Low-resolution mass spectra were recorded on a GC-MS instrument equipped with a CP-Sil 8 CB capillary column (30 m × 0.25 mm, 0.25 μm) operating at an ionization energy of 70 eV. The oven temperature was 40-300 °C. To determine the regioselectivity in arylations of olefins **2** and **5-7**, small samples of the reaction mixture were removed after cooling. The samples were partitioned between diethyl ether and 0.1 M NaOH (aq) and subjected to GC-MS analyses. The regioisomers were considered to have identical response factors in GC-MS. High resolution MS was obtained using FAB⁺ ionization and the indicated values are calculated from the produced [M+H]⁺ ion.

Materials

Balloons (1L in. when 80% inflated) were procured from Aldrich. 2,9-Dimethyl-1,10-phenanthroline (Neocuproine) was obtained from Acros. All other reagents were purchased from commercial sources and used as received. All reagents were weighed in air and the reactions were conducted under an atmosphere of oxygen, unless otherwise indicated. All arylacetophenone products **4** are commercially available. All known products gave satisfactory analytical data corresponding to the reported literature values. The analytical data are provided

herewith for new arylated enamides, which are all sensitive to temperature and should be stored in the refrigerator. The instability of the α -arylated enamides **8-10** prevented elemental analysis.

Analytical Data for New Compounds

N-(1-[4-Phenoxyphenyl]ethenyl)-2-pyrrolidinone **9c**

Following the general procedure, the residue was purified by centrifugal chromatography (silica gel 60, 20% ethyl acetate in hexane) to afford the title product as a colorless solid (0.160 g, 60%). ^1H NMR (400 MHz, CDCl_3): δ 2.04 (s, 3H), 3.08 (s, 3H), 5.16 (s, 1H), 5.61 (s, 1H), 6.98 (m, 2H), 7.04 (m, 2H), 7.14 (t, 1H, $J = 7.3$ Hz), 7.32-7.40 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3): δ 21.7, 35.4, 111.3, 118.6, 119.4, 123.9, 127.1, 129.9, 130.1, 148.3, 156.3, 158.4, 170.9; (IR, CDCl_3): 1663, 1489, 1376, 1244 cm^{-1} ; MS (m/z , relative intensity) 267 (M^+ , 92), 266 (26), 224 (100); HRMS (FAB+) Calcd for $\{\text{C}_{17}\text{H}_{17}\text{NO}_2\}$: 267.1259; Found: 267.1246

N-(1-[4-Methylphenyl]ethenyl)-2-pyrrolidinone **8d**

Following the general procedure, the residue was purified by centrifugal chromatography (silica gel 60, 20% ethyl acetate in hexane as eluent) to afford the title product as a colorless liquid (0.193 g, 96%). ^1H NMR (270 MHz, CDCl_3): δ 2.05-2.12 (m, 2H), 2.33 (s, 3H), 2.54

(dd, 2H, $J = 8.2$, $J = 7.9$ Hz), 3.52 (dd, 2H, $J = 7.0$, $J = 7.1$ Hz), 5.22 (s, 1H), 5.36 (s, 1H), 7.14 (m, 2H), 7.22 (m, 2H); ^{13}C NMR (67.5 MHz, CDCl_3): δ 18.4, 21.7, 31.8, 49.5, 108.5, 126.4, 129.3, 133.1, 138.3, 143.3, 174.6; (IR, CDCl_3): 1701 cm^{-1} ; MS (m/z , relative intensity 70 eV) 201 (M^+ , 100), 158 (32), 117 (22); HRMS (FAB+) Calcd for $\{\text{C}_{13}\text{H}_{15}\text{NO}\}$: 201.1154; Found: 201.1153

***N*-(1-[4-*n*-Butylphenyl]ethenyl)-2-pyrrolidinone 10e**

Following the general procedure, the residue was purified by centrifugal chromatography (silica gel 60, 25% ethyl acetate in hexane) to afford the title product as a colorless liquid (0.240 g, 89%). ^1H NMR (400 MHz, CDCl_3): δ 0.91 (m, 3H), 1.29-1.39 (m, 2H), 1.52-1.62 (m, 2H), 1.7-1.89 (m, 6H), 2.58 (dd, $J = 7.8$, $J = 7.7$ Hz, 2H), 2.68 (m, 2H), 3.50 (m, 2H), 5.10 (s, 1H), 5.58 (s, 1H), 7.13 (m, 2H), 7.32 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 13.9, 22.3, 23.5, 28.7, 30.0, 33.4, 35.3, 37.6, 51.8, 110.3, 125.7, 128.5, 133.5, 143.4, 149.0, 175.8; (IR, CDCl_3): 2928, 2857, 1664 cm^{-1} ; MS (m/z , relative intensity) 271 (M^+ , 100), 242 (49), 228 (23); HRMS (FAB+) Calcd for $\{\text{C}_{18}\text{H}_{25}\text{NO}\}$: 271.1936; Found: 271.1932

COMPUTATIONAL DETAILS

Geometries and energies of all intermediates and transition states were fully optimized using the gradient-corrected hybrid density functional method B3LYP.¹ We used a basis set of double- ζ valence quality labeled LANL2DZ in the Gaussian98 program.² For Pd the core electrons were replaced by a relativistic electron core potential (ECP) developed by Hay and

Wadt.³ For non-metal atoms the double- ζ basis sets of Huzinaga and Dunning were assigned.⁴

All relative energies were recalculated using a valence triple- ζ quality basis set at the B3LYP level. For all non metal atoms the 6-311G(d,p) basis set⁵ was employed and for Pd the primitive LANL2DZ basis set was recontracted to 4s4p3d and an f-function(1.472) was added. The atomic charges were calculated using the Merz-Singh-Kollman scheme as implemented in Gaussian98.⁶

Cartesian coordinates [$\text{\AA}$] and energies [Hartree] of calculated structures.

A, R=OMe
-739.574007836

C	-3.264133	1.425823	-.196548
C	-3.938702	.115045	-.096617
N	-1.969687	1.482819	-.158529
N	-3.166594	-.928751	-.001898
H	-3.862006	2.331867	-.300896
H	-5.027353	.049724	-.101527
C	-1.238605	2.759784	-.250898
C	-3.712242	-2.299115	.084804
Pd	-1.039262	-.372361	.037491
C	.820854	.114152	.071938
C	1.424538	.365997	1.314449
C	2.818631	.294466	1.396185
C	3.581734	-.009906	.240993
C	1.555949	-.080955	-1.092324
C	2.945470	-.174552	-1.008187
H	.845895	.579443	2.215341
H	3.334224	.445555	2.340244
O	4.935251	-.140166	.453235
H	1.072460	-.229154	-2.056515
H	3.516132	-.376907	-1.905336
H	-1.933624	3.606048	-.328979
H	-.606943	2.878972	.632889
H	-.584690	2.741969	-1.125622
H	-4.810078	-2.321133	.060109
H	-3.306651	-2.885313	-.748996
H	-3.352104	-2.751928	1.020614
C	5.814541	-.499201	-.660248
H	6.812725	-.560328	-.226908
H	5.533108	-1.474118	-1.079642
H	5.798703	.267512	-1.443530

B, R=OMe
-1103.74522414

C	-.484010	3.540658	1.202483
C	-1.735319	3.517197	.424812
N	.345535	2.545134	1.088758
N	-1.991293	2.478348	-.314485
H	-.279484	4.395735	1.848734
H	-2.403073	4.379610	.482091
C	1.610792	2.531719	1.846177
C	-3.208811	2.444302	-1.142518
Pd	-.311139	1.012865	-.241657

C	1.460288	.043109	-.139731
C	-1.014337	-.423551	-1.775448
C	-1.153878	-1.421232	-.801336
H	-.103143	-.440974	-2.369217
H	-1.892831	-.004425	-2.261548
H	-.273763	-1.945985	-.437544
N	-2.321420	-1.885748	-.264959
C	1.775466	-.849731	.909576
C	3.058545	-1.415739	.992135
C	4.037525	-1.106420	.021243
C	2.434558	.345334	-1.109620
C	3.726546	-.226634	-1.036806
H	1.037571	-1.121046	1.660900
H	3.316430	-2.106286	1.788970
O	5.265369	-1.727259	.201088
H	2.215280	1.022668	-1.933577
H	4.459110	.018470	-1.799673
C	-2.321151	-2.831506	.820202
C	-3.699343	-1.536636	-.689487
C	-3.765737	-3.208335	1.103299
O	-1.286559	-3.200251	1.390369
C	-4.555572	-2.704456	-.129404
H	-3.848366	-4.284864	1.274843
H	-4.079328	-2.708471	2.029792
H	-3.992370	-.575125	-.246113
H	-3.756515	-1.456283	-1.779518
H	-5.567673	-2.377751	.121724
H	-4.633323	-3.498949	-.878979
H	1.731107	3.434709	2.457394
H	1.631064	1.642860	2.484535
H	2.443154	2.438368	1.142048
H	-3.831988	3.339039	-1.016287
H	-2.917795	2.357931	-2.196142
H	-3.797270	1.557942	-.882045
C	6.330004	-1.501717	-.773218
H	7.177557	-2.088474	-.414466
H	6.034644	-1.852909	-1.771841
H	6.609755	-.439802	-.818867

TS α , R=OMe
-1103.72967876

Pd	1.656442	-0.212040	0.119691
C	0.861364	-2.096308	0.433912
C	-0.500440	-1.686505	0.759165

C	-0.378825	0.311476	0.152146
C	3.843191	1.711779	-0.300996
C	4.495601	0.391589	-0.212979
N	2.550418	1.763403	-0.175904
N	3.748507	-0.656262	-0.019864
H	4.459057	2.598038	-0.466126
H	5.580795	0.326667	-0.311192
C	1.828332	3.043020	-0.247474
C	4.343306	-2.000570	0.078012
H	1.431556	-2.449525	1.298693
H	0.999430	-2.713023	-0.456361
N	-1.634980	-2.207755	0.149697
H	-0.702793	-1.432149	1.797410
C	-0.865375	0.550667	-1.171254
C	-1.794932	1.559438	-1.425810
C	-2.292175	2.351217	-0.355763
C	-0.896661	1.110925	1.204264
C	-1.837023	2.126038	0.964902
H	-0.496789	-0.043835	-2.003885
H	-2.163628	1.759921	-2.427513
O	-3.223593	3.301713	-0.716487
H	-0.582151	0.930484	2.229522
H	-2.228786	2.700840	1.797580
C	-2.920785	-1.974349	0.707453
C	-1.704318	-2.911082	-1.151395
C	-3.953687	-2.602316	-0.215229
O	-3.095803	-1.348729	1.768121
C	-3.131502	-3.526345	-1.148012
H	-1.574689	-2.196138	-1.975151
H	-0.923076	-3.673546	-1.225216
H	-4.718049	-3.124101	0.366549
H	-4.457044	-1.798384	-0.769216
H	-3.545304	-3.584525	-2.157851
H	-3.096694	-4.540982	-0.737726
H	2.493224	3.892188	-0.451805
H	1.064683	2.973231	-1.029458
H	1.306436	3.204558	0.702190
H	5.433717	-1.986593	-0.044044
H	4.095342	-2.428613	1.055667
H	3.899878	-2.641722	-0.691740
C	-3.849772	4.141037	0.309602
H	-4.542910	4.781711	-0.236576
H	-4.399078	3.525700	1.033008
H	-3.099711	4.755801	0.823618

TS β , R=OMe
-1103.72368672

Pd	0.457296	-0.805011	0.248232
C	1.548243	0.888569	1.146725
C	0.247917	1.126038	1.687410
C	-1.319902	0.259989	0.588299
C	-2.246360	-0.332842	1.489590
C	-1.819004	1.072264	-0.456722
C	-3.623561	-0.147963	1.324370
C	-3.203359	1.261347	-0.633138
C	-4.111779	0.651411	0.261815
C	0.356137	-3.358034	-1.225244
C	1.714399	-3.310697	-0.655280
N	-0.471372	-2.404060	-0.923357
N	2.070512	-2.270661	0.039193
H	0.077504	-4.199896	-1.862488
H	2.376134	-4.166084	-0.802491
C	-1.849882	-2.398108	-1.439151

C	3.383826	-2.254613	0.714697
N	2.158048	1.769586	0.228235
H	2.271837	0.313491	1.721042
H	0.033361	0.670910	2.649718
H	-0.240353	2.081074	1.530066
H	-1.892350	-0.936469	2.322753
H	-4.339147	-0.593958	2.008497
O	-5.486456	0.777366	0.198762
H	-1.137409	1.565427	-1.145574
H	-3.554693	1.886607	-1.447760
C	3.500975	1.621049	-0.157045
C	1.509227	2.928250	-0.438926
O	4.234629	0.688655	0.234356
C	3.858497	2.752010	-1.109783
C	2.709397	3.775049	-0.941947
H	0.884280	2.581758	-1.272959
H	0.877449	3.483530	0.261666
H	4.847444	3.150838	-0.869536
H	3.910447	2.347147	-2.129746
H	2.469538	4.302101	-1.868946
H	2.977774	4.522430	-0.187943
H	3.974833	-3.149410	0.481405
H	3.928151	-1.348156	0.436417
H	3.212230	-2.214319	1.798519
H	-2.069464	-3.280075	-2.054202
H	-2.543181	-2.354082	-0.592671
H	-2.003115	-1.488619	-2.030230
C	-6.089400	1.628353	-0.827638
H	-7.162849	1.575751	-0.643737
H	-5.745539	2.665994	-0.728262
H	-5.866413	1.249871	-1.833854

A, R=Me

-664.349426586

C	2.796836	1.608457	.113694
C	3.601188	.374150	.016001
N	1.497118	1.521374	.117639
N	2.968200	-.758249	-.065226
H	3.302272	2.572201	.185936
H	4.689712	.450219	.021467
C	.641503	2.721618	.220684
C	3.687186	-2.039676	-.156575
Pd	.786431	-.425255	-.033932
C	-1.151485	-.063835	.006979
C	-1.845642	.242540	-1.181136
C	-3.250150	.151242	-1.185738
C	-3.971719	-.188874	-.013986
C	-1.836989	-.356123	1.201740
C	-3.245488	-.440230	1.172428
H	-1.321192	.513707	-2.095593
H	-3.790500	.353691	-2.108563
C	-5.483931	-.260404	-.038971
H	-1.308788	-.528362	2.138392
H	-3.777993	-.693110	2.086373
H	1.240651	3.638077	.281113
H	-.017198	2.764069	-.651976
H	.008731	2.629916	1.108735
H	4.777245	-1.917246	-.141006
H	3.379912	-2.677140	.681153
H	3.390125	-2.544003	-1.083960
H	-5.895484	-.530431	.939056
H	-5.925000	.701787	-.332515
H	-5.833376	-1.006691	-.765341

B, R=Me
-1028.52126649

C	0.224229	3.424727	1.280153
C	-1.043361	3.584648	0.544984
N	0.927015	2.345600	1.094161
N	-1.442117	2.617623	-0.227779
H	0.546851	4.218430	1.955794
H	-1.602125	4.515933	0.661089
C	2.204727	2.149787	1.804962
C	-2.675387	2.767154	-1.018635
Pd	0.055855	0.957410	-0.270997
C	1.690167	-0.230491	-0.255459
C	-0.869050	-0.343721	-1.815900
C	-1.114967	-1.313069	-0.833325
H	0.018508	-0.481752	-2.429470
H	-1.691523	0.195378	-2.281712
H	-0.300343	-1.950521	-0.497552
N	-2.313377	-1.625343	-0.254861
C	1.925906	-1.172226	0.766434
C	3.133838	-1.900822	0.781784
C	4.117838	-1.716346	-0.213831
C	2.660576	-0.031722	-1.260342
C	3.862372	-0.769912	-1.231340
H	1.189367	-1.357841	1.545469
H	3.302648	-2.627072	1.574430
C	5.398476	-2.532216	-0.211669
H	2.501797	0.689193	-2.061205
H	4.603927	-0.608059	-2.011798
C	-2.386409	-2.551739	0.842587
C	-3.654336	-1.121810	-0.640215
C	-3.854327	-2.756179	1.178184
O	-1.382877	-3.039177	1.378794
C	-4.621890	-2.175012	-0.034204
H	-4.054644	-3.814224	1.365971
H	-4.076839	-2.215589	2.108378
H	-3.821543	-0.127993	-0.203794
H	-3.738057	-1.048456	-1.728943
H	-5.579029	-1.728310	0.246193
H	-4.819135	-2.962150	-0.769218
H	2.450172	3.003650	2.448504
H	2.139640	1.236176	2.404268
H	2.998195	1.992430	1.067750
H	-3.177527	3.727605	-0.844732
H	-2.423972	2.682367	-2.082599
H	-3.363245	1.952635	-0.770227
H	6.254919	-1.937889	-0.551922
H	5.629982	-2.915025	0.788521
H	5.314610	-3.397810	-0.883345

TS α , R=OMe
-1028.50157213

Pd	1.414812	-0.381126	0.148009
C	0.275614	-2.026041	0.645290
C	-0.990193	-1.324753	0.842583
C	-0.469340	0.584299	0.267364
C	3.937751	1.000102	-0.487435
C	4.294313	-0.422515	-0.328013
N	2.693402	1.339393	-0.329013
N	3.350657	-1.269445	-0.035625
H	4.723330	1.718967	-0.728978
H	5.334292	-0.728045	-0.457184
C	2.265373	2.740333	-0.460598

C	3.650611	-2.701843	0.136857
H	0.740220	-2.378829	1.570875
H	0.322037	-2.754501	-0.166733
N	-2.150621	-1.651003	0.142109
H	-1.227219	-1.003968	1.854842
C	-0.937091	0.972082	-1.019694
C	-1.547044	2.220795	-1.213624
C	-1.737643	3.118187	-0.131151
C	-0.670259	1.479650	1.350483
C	-1.282570	2.727040	1.150981
H	-0.814650	0.305408	-1.870515
H	-1.888530	2.505559	-2.206939
C	-2.459425	4.434620	-0.330218
H	-0.369109	1.194250	2.356431
H	-1.438671	3.390318	1.998821
C	-3.406310	-1.130775	0.553325
C	-2.243449	-2.417032	-1.122182
C	-4.453277	-1.589541	-0.450603
O	-3.548852	-0.422541	1.565472
C	-3.760760	-2.731955	-1.233551
H	-1.892839	-1.806547	-1.966382
H	-1.635117	-3.325484	-1.076560
H	-5.371262	-1.890564	0.060363
H	-4.703091	-0.738971	-1.099672
H	-4.085448	-2.792804	-2.275365
H	-3.972176	-3.694736	-0.756228
H	3.089476	3.409353	-0.740082
H	1.469644	2.796934	-1.210420
H	1.834087	3.065645	0.492406
H	4.714312	-2.926928	-0.011041
H	3.353837	-3.009240	1.145653
H	3.055709	-3.278842	-0.579586
H	-2.016931	5.234605	0.274514
H	-2.452989	4.748630	-1.379693
H	-3.511305	4.343405	-0.021929

TS β , R=Me
-1028.49766012

Pd	-0.107831	0.775894	0.262832
C	-1.406227	-0.777303	1.129429
C	-0.136449	-1.198441	1.637937
C	1.489239	-0.576324	0.505725
C	2.536820	-0.191880	1.373506
C	1.792090	-1.381447	-0.618954
C	3.862724	-0.576490	1.099379
C	3.120026	-1.753401	-0.887603
C	4.180688	-1.364649	-0.032230
C	0.348633	3.337609	-1.132938
C	-0.995476	3.466050	-0.541782
N	1.036414	2.267706	-0.872152
N	-1.488652	2.465404	0.126201
H	0.734341	4.150525	-1.751750
H	-1.530623	4.411056	-0.652455
C	2.393519	2.083975	-1.409801
C	-2.785121	2.613037	0.817492
N	-2.145759	-1.560153	0.217115
H	-2.034707	-0.118001	1.725458
H	0.151950	-0.794065	2.603445
H	0.199527	-2.215362	1.470302
H	2.329742	0.399880	2.262361
H	4.656481	-0.273130	1.778836
C	5.604636	-1.806966	-0.309200
H	1.004988	-1.715301	-1.289869

H	3.337047	-2.364414	-1.761930
C	-3.444269	-1.201394	-0.182316
C	-1.704264	-2.839013	-0.400725
O	-4.014097	-0.149972	0.178931
C	-3.982003	-2.283431	-1.106900
C	-3.031010	-3.483780	-0.885052
H	-1.025105	-2.641577	-1.239337
H	-1.183195	-3.467338	0.328272
H	-5.028912	-2.495036	-0.874400
H	-3.946638	-1.910336	-2.139605
H	-2.882158	-4.082144	-1.787324
H	-3.430411	-4.141336	-0.105556
H	-3.237638	3.595607	0.632680
H	-3.457485	1.810504	0.502033
H	-2.615873	2.496027	1.896081
H	2.707088	2.919920	-2.048058
H	3.092099	1.974580	-0.573696
H	2.425708	1.150274	-1.980213
H	6.318690	-1.302736	0.350547
H	5.717658	-2.888880	-0.154648
H	5.895080	-1.597697	-1.346819

A, R=H

-625.019343864

C	2.403310	1.657295	.121469
C	3.243075	.444392	.049331
N	1.106223	1.533864	.100585
N	2.644297	-.705675	-.042325
H	2.881078	2.635133	.193784
H	4.328816	.552011	.077105
C	.215204	2.710432	.172500
C	3.400128	-1.966314	-.114289
Pd	.457105	-.431607	-.047594
C	-1.492873	-.120250	-.006434
C	-2.195584	.113826	-1.205213
C	-3.602036	-.004109	-1.198222
C	-4.282377	-.308292	-.001946
C	-2.159533	-.379618	1.208557
C	-3.566464	-.497098	1.196587
H	-1.679218	.356685	-2.132024
H	-4.157221	.145497	-2.120671
H	-5.366359	-.384901	-.001315
H	-1.616704	-.501611	2.144397
H	-4.093240	-.721778	2.120331
H	.786931	3.643911	.236675
H	-.424515	2.725888	-.715360
H	-.435073	2.609441	1.047033
H	4.485591	-1.813515	-.071868
H	3.091137	-2.611287	.716932
H	3.141246	-2.480468	-1.047581

B, R=H

-989.192929863

C	1.610385	2.924905	1.301007
C	.466764	3.531292	.595654
N	1.886380	1.672020	1.085382
N	-.255010	2.781207	-.182783
H	2.204990	3.543533	1.974964
H	.274086	4.597291	.736268
C	3.031174	1.029645	1.761204
C	-1.365773	3.370912	-.949637
Pd	.556832	.704519	-.269151
C	1.678231	-.977490	-.290762

C	-.775155	-.174777	-1.816005
C	-1.330386	-1.023443	-.848841
H	.006368	-.591824	-2.446724
H	-1.368272	.623696	-2.256562
H	-.783164	-1.908335	-.532625
N	-2.558388	-.910877	-.259232
C	1.557633	-1.969290	.706757
C	2.433421	-3.077449	.697852
C	3.419438	-3.199196	-.299858
C	2.658940	-1.099834	-1.298855
C	3.529197	-2.212652	-1.297947
H	.793595	-1.905038	1.478699
H	2.333814	-3.841860	1.464779
H	4.087642	-4.055916	-.304313
H	2.761078	-.346187	-2.078194
H	4.283403	-2.303068	-2.076045
C	-2.944882	-1.775383	.824157
C	-3.638734	.040828	-.616863
C	-4.387779	-1.454525	1.177640
O	-2.172346	-2.595529	1.337371
C	-4.910657	-.615720	-.014117
H	-4.947637	-2.377290	1.351965
H	-4.397390	-.888459	2.119236
H	-3.438625	1.019406	-.159692
H	-3.699151	.162736	-1.702635
H	-5.646386	.133820	.287713
H	-5.379001	-1.267963	-.758636
H	3.572306	1.735197	2.403146
H	2.663357	.188163	2.357268
H	3.704044	.617568	1.002353
H	-1.493776	4.442363	-.750148
H	-1.173562	3.227706	-2.019066
H	-2.294982	2.847427	-.701662

TS α , R=H

-989.170830422

Pd	-1.207748	-0.348861	-0.217388
C	0.105355	-1.694881	-1.055289
C	1.281155	-0.833376	-0.990689
C	0.486364	0.936917	-0.346507
C	-3.829951	0.505962	0.825488
C	-3.994193	-0.910998	0.444835
N	-2.662090	1.048698	0.648971
N	-2.968083	-1.538215	-0.052855
H	-4.684467	1.048595	1.234241
H	-4.963640	-1.391990	0.584705
C	-2.429825	2.463251	0.997429
C	-3.086713	-2.954771	-0.457136
H	-0.280251	-1.863350	-2.063985
H	0.110678	-2.593928	-0.436794
N	2.362700	-1.132414	-0.161947
H	1.617843	-0.363598	-1.911635
C	0.973066	1.369632	0.915584
C	1.328631	2.714813	1.119668
C	1.217650	3.643864	0.061218
C	0.398489	1.876994	-1.405939
C	0.752459	3.223037	-1.201472
H	1.081142	0.661080	1.733982
H	1.701906	3.037739	2.088541
H	1.514081	4.678438	0.214679
H	0.079084	1.556454	-2.395798
H	0.693756	3.930558	-2.023996
C	3.597108	-0.456716	-0.325672

C 2.354484 -2.052320 0.995737
 C 4.553472 -0.941434 0.751924
 O 3.793879 0.389168 -1.215394
 C 3.856572 -2.168446 1.393844
 H 1.739527 -1.643520 1.810163
 H 1.937559 -3.025235 0.715896
 H 5.525966 -1.175055 0.309297
 H 4.716915 -0.124464 1.466686
 H 3.975130 -2.193088 2.480345
 H 4.276766 -3.096287 0.994341
 H -3.334882 2.949515 1.381809
 H -1.635453 2.516933 1.748936
 H -2.076347 2.992717 0.106623
 H -4.098952 -3.343731 -0.293695
 H -2.830599 -3.046388 -1.517822
 H -2.372791 -3.552782 0.119140

TS β , R=H

-989.168608299

Pd 0.308759 0.631808 0.234918
 C -1.329173 -0.522524 1.126869
 C -0.207716 -1.274428 1.610606
 C 1.482284 -1.114354 0.453062
 C 2.611232 -1.035750 1.305043
 C 1.534553 -1.937100 -0.699520
 C 3.783620 -1.749568 0.991203
 C 2.713956 -2.638707 -1.013622
 C 3.838898 -2.550778 -0.168367
 C 1.462007 3.025328 -1.059184
 C 0.208870 3.497552 -0.447457
 N 1.813527 1.789946 -0.869155
 N -0.550516 2.645244 0.174756
 H 2.067893 3.726990 -1.635184
 H -0.038654 4.558367 -0.507782
 C 3.058393 1.256859 -1.448853
 C -1.755743 3.120248 0.884579
 N -2.269466 -1.082210 0.235343
 H -1.743037 0.281451 1.732201
 H 0.198266 -0.972605 2.571352
 H -0.176950 -2.345051 1.439462
 H 2.576977 -0.431706 2.209215
 H 4.643671 -1.690198 1.653514
 H 4.740742 -3.110414 -0.401458
 H 0.669948 -2.030528 -1.351732
 H 2.749295 -3.262000 -1.903722
 C -3.410383 -0.374462 -0.181920
 C -2.221170 -2.454881 -0.337202
 O -3.650734 0.806376 0.143402
 C -4.237901 -1.276609 -1.085595
 C -3.668979 -2.694468 -0.845139
 H -1.493463 -2.503626 -1.156667
 H -1.932402 -3.183731 0.426589
 H -5.300670 -1.176126 -0.850619
 H -4.102578 -0.944496 -2.124328
 H -3.679704 -3.312680 -1.746487
 H -4.251851 -3.211110 -0.075975
 H -1.932728 4.189753 0.716262
 H -2.618208 2.528147 0.568813
 H -1.609788 2.949352 1.959994
 H 3.655136 2.035543 -1.940246
 H 3.644900 0.784813 -0.654877
 H 2.804838 0.476682 -2.175396

A, R=CF₃

-962.144235284

C 3.683405 1.579700 .090236
 C 4.469054 .332411 .001075
 N 2.383290 1.512697 .099322
 N 3.818622 -.789969 -.065008
 H 4.202315 2.536883 .149402
 H 5.558155 .392540 -.003828
 C 1.543517 2.725633 .192665
 C 4.513917 -2.084940 -.151070
 Pd 1.650709 -.424637 -.025197
 C -.283957 -.023481 .016761
 C -.977744 .249481 -1.180161
 C -2.383789 .201448 -1.178187
 C -3.073588 -.081921 .019067
 C -.966473 -.266723 1.225011
 C -2.375721 -.315601 1.217129
 H -.452782 .470388 -2.106860
 H -2.932613 .384432 -2.098115
 C -4.574893 -.115111 -.010415
 H -.434321 -.426186 2.160835
 H -2.917842 -.522313 2.134479
 H 2.156312 3.633333 .241583
 H .883365 2.770503 -.678856
 H .913876 2.653635 1.084992
 H 5.605415 -1.980362 -.146068
 H 4.204145 -2.708959 .695651
 H 4.201108 -2.593149 -1.070995
 F -5.129598 -.406458 1.235832
 F -5.118726 1.112118 -.424641
 F -5.060066 -1.076984 -.910746

B, R=CF₃

-1326.32076270

C 1.510122 -3.457824 1.273767
 C 2.751368 -3.233372 0.512128
 N 0.514318 -2.638467 1.105597
 N 2.825498 -2.193709 -0.264659
 H 1.451000 -4.311106 1.950643
 H 3.563675 -3.956307 0.608997
 C -0.750837 -2.833669 1.839973
 C 4.025800 -1.970426 -1.089706
 Pd 0.914031 -1.054516 -0.265524
 C -0.991919 -0.390466 -0.215603
 C 1.412225 0.458117 -1.813796
 C 1.336919 1.470062 -0.844791
 H 0.536237 0.317615 -2.443456
 H 2.366785 0.193287 -2.263013
 H 0.363046 1.833054 -0.524964
 N 2.373542 2.136735 -0.259398
 C -1.462396 0.483382 0.790002
 C -2.823195 0.842035 0.830854
 C -3.711317 0.326583 -0.131165
 C -1.889640 -0.897791 -1.181053
 C -3.250267 -0.539091 -1.139556
 H -0.790442 0.902076 1.534730
 H -3.183167 1.511815 1.606785
 C -5.153584 0.743448 -0.110878
 H -1.549423 -1.571126 -1.964473
 H -3.940527 -0.937101 -1.877946
 C 2.145384 3.048668 0.832240
 C 3.809587 2.071017 -0.629165
 C 3.471950 3.705460 1.170573

O	1.035037	3.194436	1.359966
C	4.393440	3.380109	-0.030817
H	3.330008	4.775135	1.345471
H	3.844807	3.272370	2.109043
H	4.271295	1.182998	-0.176364
H	3.923312	2.015468	-1.716160
H	5.439326	3.257118	0.260792
H	4.342466	4.181898	-0.774529
H	-0.717175	-3.719510	2.485219
H	-0.952572	-1.942515	2.443246
H	-1.568315	-2.927812	1.118554
H	4.795241	-2.736844	-0.933008
H	3.732837	-1.969365	-2.146315
H	4.446732	-0.986599	-0.856370
F	-5.999620	-0.244954	-0.634659
F	-5.605917	1.028864	1.185219
F	-5.390708	1.904792	-0.872931

TS α , R=CF₃
-989.170830422

Pd	-1.207748	-0.348861	-0.217388
C	0.105355	-1.694881	-1.055289
C	1.281155	-0.833376	-0.990689
C	0.486364	0.936917	-0.346507
C	-3.829951	0.505962	0.825488
C	-3.994193	-0.910998	0.444835
N	-2.662090	1.048698	0.648971
N	-2.968083	-1.538215	-0.052855
H	-4.684467	1.048595	1.234241
H	-4.963640	-1.391990	0.584705
C	-2.429825	2.463251	0.997429
C	-3.086713	-2.954771	-0.457136
H	-0.280251	-1.863350	-2.063985
H	0.110678	-2.593928	-0.436794
N	2.362700	-1.132414	-0.161947
H	1.617843	-0.363598	-1.911635
C	0.973066	1.369632	0.915584
C	1.328631	2.714813	1.119668
C	1.217650	3.643864	0.061218
C	0.398489	1.876994	-1.405939
C	0.752459	3.223037	-1.201472
H	1.081142	0.661080	1.733982
H	1.701906	3.037739	2.088541
H	1.514081	4.678438	0.214679
H	0.079084	1.556454	-2.395798
H	0.693756	3.930558	-2.023996
C	3.597108	-0.456716	-0.325672
C	2.354484	-2.052320	0.995737
C	4.553472	-0.941434	0.751924
O	3.793879	0.389168	-1.215394
C	3.856572	-2.168446	1.393844
H	1.739527	-1.643520	1.810163
H	1.937559	-3.025235	0.715896
H	5.525966	-1.175055	0.309297
H	4.716915	-0.124464	1.466686
H	3.975130	-2.193088	2.480345
H	4.276766	-3.096287	0.994341
H	-3.334882	2.949515	1.381809
H	-1.635453	2.516933	1.748936
H	-2.076347	2.992717	0.106623
H	-4.098952	-3.343731	-0.293695
H	-2.830599	-3.046388	-1.517822
H	-2.372791	-3.552782	0.119140

TS β , R=CF₃
-989.168608299

Pd	0.308759	0.631808	0.234918
C	-1.329173	-0.522524	1.126869
C	-0.207716	-1.274428	1.610606
C	1.482284	-1.114354	0.453062
C	2.611232	-1.035750	1.305043
C	1.534553	-1.937100	-0.699520
C	3.783620	-1.749568	0.991203
C	2.713956	-2.638707	-1.013622
C	3.838898	-2.550778	-0.168367
C	1.462007	3.025328	-1.059184
C	0.208870	3.497552	-0.447457
N	1.813527	1.789946	-0.869155
N	-0.550516	2.645244	0.174756
H	2.067893	3.726990	-1.635184
H	-0.038654	4.558367	-0.507782
C	3.058393	1.256859	-1.448853
C	-1.755743	3.120248	0.884579
N	-2.269466	-1.082210	0.235343
H	-1.743037	0.281451	1.732201
H	0.198266	-0.972605	2.571352
H	-0.176950	-2.345051	1.439462
H	2.576977	-0.431706	2.209215
H	4.643671	-1.690198	1.653514
H	4.740742	-3.110414	-0.401458
H	0.669948	-2.030528	-1.351732
H	2.749295	-3.262000	-1.903722
C	-3.410383	-0.374462	-0.181920
C	-2.221170	-2.454881	-0.337202
O	-3.650734	0.806376	0.143402
C	-4.237901	-1.276609	-1.085595
C	-3.668979	-2.694468	-0.845139
H	-1.493463	-2.503626	-1.156667
H	-1.932402	-3.183731	0.426589
H	-5.300670	-1.176126	-0.850619
H	-4.102578	-0.944496	-2.124328
H	-3.679704	-3.312680	-1.746487
H	-4.251851	-3.211110	-0.075975
H	-1.932728	4.189753	0.716262
H	-2.618208	2.528147	0.568813
H	-1.609788	2.949352	1.959994
H	3.655136	2.035543	-1.940246
H	3.644900	0.784813	-0.654877
H	2.804838	0.476682	-2.175396

A, R=CHO
-777.699556094

C	3.336324	1.618815	-.071250
C	4.155505	.392383	.005779
N	2.037651	1.515800	-.096313
N	3.536081	-.749443	.043045
H	3.829050	2.590846	-.108653
H	5.242617	.482614	.027463
C	1.167002	2.707156	-.181693
C	4.266975	-2.025189	.118278
Pd	1.359557	-.440330	-.004611
C	-.583359	-.074849	-.002313
C	-1.298430	-.204663	-1.208801
C	-2.707957	-.240567	-1.164006
C	-3.389941	-.111289	.066277
C	-1.243811	.093477	1.232828

C	-2.648287	.052140	1.260809
H	-.789896	-.280814	-2.168083
H	-3.259224	-.360596	-2.092001
C	-4.900143	-.116858	.164593
H	-.691567	.234899	2.159849
H	-3.192005	.153724	2.196145
H	1.755780	3.631208	-.217045
H	.545086	2.627335	-1.078551
H	.499868	2.722805	.685214
H	5.355152	-1.889411	.144711
H	3.945751	-2.563643	1.018148
H	3.997406	-2.638269	-.750376
O	-5.441463	.004758	1.286615
C	-5.728031	-.255032	-1.099607
H	-6.787518	-.220950	-.836372
H	-5.510949	.555989	-1.807159
H	-5.518690	-1.206273	-1.606606

B, R=CHO

-1141.87670413

C	3.336324	1.618815	-.071250
C	4.155505	.392383	.005779
N	2.037651	1.515800	-.096313
N	3.536081	-.749443	.043045
H	3.829050	2.590846	-.108653
H	5.242617	.482614	.027463
C	1.167002	2.707156	-1.81693
C	4.266975	-2.025189	.118278
Pd	1.359557	-.440330	-.004611
C	-.583359	-.074849	-.002313
C	-1.298430	-.204663	-1.208801
C	-2.707957	-.240567	-1.164006
C	-3.389941	-.111289	.066277
C	-1.243811	.093477	1.232828
C	-2.648287	.052140	1.260809
H	-.789896	-.280814	-2.168083
H	-3.259224	-.360596	-2.092001
C	-4.900143	-.116858	.164593
H	-.691567	.234899	2.159849
H	-3.192005	.153724	2.196145
H	1.755780	3.631208	-.217045
H	.545086	2.627335	-1.078551
H	.499868	2.722805	.685214
H	5.355152	-1.889411	.144711
H	3.945751	-2.563643	1.018148
H	3.997406	-2.638269	-.750376
O	-5.441463	.004758	1.286615
C	-5.728031	-.255032	-1.099607
H	-6.787518	-.220950	-.836372
H	-5.510949	.555989	-1.807159
H	-5.518690	-1.206273	-1.606606

TS α , R=CHO

-1141.85139248

Pd	-1.751154	0.003636	0.106694
C	-1.418913	2.005451	0.460052
C	0.003685	1.884875	0.778894
C	0.373035	-0.054160	0.304579
C	-3.451696	-2.356649	-0.359596
C	-4.367674	-1.200495	-0.342850
N	-2.181800	-2.133207	-0.200503
N	-3.869425	-0.014494	-0.147214
H	-3.864480	-3.357016	-0.502756

H	-5.435424	-1.365856	-0.495538
C	-1.210135	-3.238521	-0.196538
C	-4.739404	1.175050	-0.113685
H	-2.053697	2.202549	1.328855
H	-1.690598	2.593225	-0.418903
N	0.990946	2.633259	0.135962
H	0.255603	1.742832	1.828636
C	0.956206	-0.285441	-0.973786
C	2.018075	-1.190533	-1.122413
C	2.531815	-1.881021	0.002536
C	0.915690	-0.728094	1.431097
C	1.972641	-1.636547	1.279002
H	0.574466	0.235614	-1.848954
H	2.441204	-1.357476	-2.108977
C	3.666545	-2.875063	-0.101601
H	0.529320	-0.525658	2.427291
H	2.394725	-2.155396	2.134774
C	2.307456	2.675993	0.665180
C	0.878483	3.341238	-1.159330
C	3.164810	3.509097	-0.274329
O	2.631422	2.097208	1.717798
C	2.144841	4.242806	-1.180273
H	0.878487	2.622893	-1.991602
H	-0.045119	3.926159	-1.207451
H	3.815564	4.178188	0.294655
H	3.814172	2.830831	-0.844453
H	2.513295	4.395658	-2.197670
H	1.905270	5.223812	-0.756930
H	-1.678684	-4.213432	-0.381356
H	-0.451055	-3.041343	-0.960800
H	-0.699630	-3.254397	0.772572
H	-5.785304	0.932600	-0.338752
H	-4.681502	1.629280	0.882066
H	-4.371592	1.907046	-0.840494
O	3.971531	-3.562869	0.898927
C	4.416064	-3.022060	-1.413959
H	5.226243	-3.742323	-1.281072
H	3.752600	-3.382062	-2.212164
H	4.838397	-2.062162	-1.738294

TS β , R=CHO

-1141.85050030

Pd	0.624446	0.773856	-0.254657
C	1.725457	-0.894084	-1.168721
C	0.399308	-1.180855	-1.633671
C	-1.137726	-0.349242	-0.549989
C	-2.086732	0.233394	-1.425272
C	-1.594866	-1.134936	0.539708
C	-3.463390	0.068399	-1.190964
C	-2.969048	-1.290298	0.768980
C	-3.919618	-0.692255	-0.091459
C	0.519665	3.302259	1.276936
C	1.847447	3.304614	0.636163
N	-0.302774	2.339968	0.989524
N	2.199744	2.287305	-0.092796
H	0.259578	4.117052	1.956375
H	2.491288	4.176886	0.765536
C	-1.649405	2.287952	1.581929
C	3.474313	2.327461	-0.840726
N	2.395553	-1.712782	-0.241829
H	2.404118	-0.326877	-1.803085
H	0.140797	-0.786492	-2.611771

H	-0.033987	-2.152657	-1.420882	Cl	-2,826392	-1,446473	-1,178811
H	-1.756466	0.811650	-2.285310	B', R=Me			
H	-4.171136	0.528610	-1.874266	-1488.97955940			
C	-5.383733	-0.898381	0.208934	Pd	0,092940	0,709040	-0,440410
H	-0.886004	-1.620678	1.205393	C	1,816640	-0,356880	-0,275340
H	-3.332760	-1.876387	1.608330	C	-1,009340	-1,383560	-0,749200
C	3.760552	-1.525067	0.054432	C	-0,703900	-0,719800	-1,933790
C	1.813234	-2.854833	0.512541	C	1,993410	-1,340000	0,714720
O	4.449669	-0.605124	-0.432696	C	3,214140	-2,024800	0,825400
C	4.189767	-2.592868	1.047442	C	4,282450	-1,757520	-0,045400
C	3.060099	-3.648955	0.987835	C	4,096160	-0,771520	-1,030390
H	1.224300	-2.484756	1.362376	C	2,883330	-0,077870	-1,146380
H	1.160640	-3.457411	-0.127586	N	0,877300	2,080740	1,012950
H	5.178048	-2.980250	0.786880	C	0,870100	1,650490	2,417170
H	4.273097	-2.131194	2.041064	C	1,282970	3,260470	0,694120
H	2.883545	-4.136219	1.949999	C	1,275700	3,759750	-0,684910
H	3.306600	-4.425420	0.256097	N	1,126900	2,964900	-1,679750
H	4.079552	3.202025	-0.569177	C	0,997670	3,495910	-3,034580
H	4.034192	1.405321	-0.665394	H	1,613460	3,955210	1,471110
H	3.239584	2.377362	-1.912861	H	1,366380	4,846420	-0,804140
H	-1.846726	3.138478	2.246833	H	0,196900	-1,002410	-2,467230
H	-2.389549	2.271471	0.775268	H	-1,464340	-0,187520	-2,493630
H	-1.756833	1.352628	2.141478	H	-0,279020	-2,028340	-0,275190
O	-5.717763	-1.486171	1.263171	N	-2,263510	-1,476380	-0,171350
C	-6.427019	-0.383306	-0.766749	H	1,185840	-1,587950	1,398920
H	-7.410852	-0.741860	-0.457187	H	3,330700	-2,779850	1,599570
H	-6.443469	0.716107	-0.775345	C	5,584410	-2,524950	0,052390
H	-6.224776	-0.719831	-1.790721	H	2,774810	0,689410	-1,906150
A', R=Me				H	4,910260	-0,540290	-1,714200
-1124.80841567				C	-2,422990	-1,936400	1,139150
Pd	-0,687938	-0,634706	-0,299121	C	-3,531160	-1,004680	-0,778350
C	1,248394	-0,189965	-0,142968	C	-3,900990	-1,863760	1,483470
C	2,174060	-1,253325	-0,082590	O	-1,484930	-2,295810	1,872460
C	3,557935	-0,986780	-0,157815	C	-4,609230	-1,653260	0,126190
C	4,042152	0,335075	-0,272481	H	-4,215410	-2,763280	2,018950
C	3,101231	1,389321	-0,304549	H	-4,051880	-1,011410	2,159030
C	1,716281	1,137380	-0,232900	H	-3,555470	0,089490	-0,757080
N	-0,947869	-0,096611	1,689125	H	-3,590230	-1,343190	-1,817300
C	-0,312152	-0,907581	2,746830	H	-5,496120	-1,020520	0,205950
C	-1,672040	0,939084	1,992816	H	-4,920670	-2,618130	-0,289370
C	-2,356789	1,761422	0,975875	H	1,274080	2,422460	3,084470
N	-1,944545	1,774830	-0,249035	H	-0,159840	1,418040	2,700880
C	-2,719998	2,450369	-1,294490	H	1,462160	0,736210	2,503680
H	-1,840496	1,197224	3,042419	H	1,150940	4,583530	-3,097880
H	-3,247192	2,303248	1,323286	H	1,708660	2,985470	-3,691160
H	1,832091	-2,284289	0,004549	H	-0,012300	3,255250	-3,383210
H	4,262857	-1,816287	-0,124531	H	6,444940	-1,888770	-0,185030
C	5,531537	0,616533	-0,376463	H	5,733800	-2,931910	1,058330
H	1,009835	1,963710	-0,261108	H	5,605050	-3,371720	-0,647940
H	3,451848	2,417483	-0,386018	Cl	-2,000070	2,139780	-0,591570
H	-0,519526	-0,508264	3,749683	TS'α, R=Me			
H	-0,688823	-1,933143	2,674874	-1488.93926745			
H	0,767925	-0,924554	2,571566	Pd	1,414810	-0,381130	0,148010
H	-3,587275	3,016369	-0,916373	C	-0,469340	0,584300	0,267360
H	-2,059739	3,117216	-1,860898	C	0,275610	-2,026040	0,645290
H	-3,072656	1,667467	-1,978571	C	-0,990190	-1,324750	0,842580
H	5,801483	1,546772	0,138607	N	-2,138739	-1,635645	0,099728
H	6,124673	-0,195919	0,059750	C	-2,153450	-2,364275	-1,182797
H	5,842017	0,722761	-1,426091				

C	-3,660601	-2,645940	-1,414956	C	-1,406230	-0,777300	1,129430
C	-4,390949	-1,551187	-0,606882	C	-0,136450	-1,198440	1,637940
C	-3,393955	-1,142338	0,466682	N	-2,192024	-1,527431	0,235951
O	-3,608865	-0,474391	1,490904	C	-3,585277	-1,416354	0,265639
C	-0,665748	1,464411	1,355746	C	-1,696906	-2,249819	-0,947582
C	-1,193419	2,744410	1,165195	C	-2,961154	-2,965804	-1,488010
C	-1,577851	3,182233	-0,115728	C	-4,133991	-2,102478	-0,976774
C	-1,411844	2,298542	-1,199510	O	-4,225338	-0,846429	1,162829
C	-0,885795	1,017181	-1,013077	C	2,553766	-0,203362	1,351355
C	-2,188703	4,551198	-0,312361	C	3,868524	-0,579959	1,058989
N	2,563187	1,402051	-0,365013	C	4,169976	-1,358395	-0,072997
C	2,867631	2,303481	0,755581	C	3,104445	-1,745733	-0,905941
C	3,126195	1,605051	-1,505894	C	1,785254	-1,376861	-0,618374
C	2,957858	0,752157	-2,687586	C	5,588472	-1,787765	-0,377216
N	1,999171	-0,088067	-2,828118	N	1,161491	2,357425	-0,495673
C	1,974005	-0,944554	-4,014552	C	1,509069	2,244154	-1,918529
H	3,825320	2,439596	-1,625572	C	1,461088	3,427437	0,154758
H	3,736450	0,874988	-3,453769	C	1,115288	3,678519	1,559543
H	0,756696	-2,385922	1,554643	N	0,690267	2,769734	2,360147
H	0,348726	-2,728387	-0,183046	C	0,316235	3,137979	3,727395
H	-1,253808	-1,022358	1,850590	H	1,976331	4,246877	-0,357345
H	-0,742545	0,370202	-1,871607	H	1,236386	4,722188	1,881672
H	-1,693550	2,624294	-2,197993	H	-2,032727	-0,138278	1,746604
H	-0,409588	1,140241	2,361013	H	0,169377	-0,787039	2,592607
H	-1,332375	3,402176	2,019433	H	0,192629	-2,215771	1,458794
H	-1,722203	-1,742143	-1,977370	H	2,349505	0,408962	2,223904
H	-1,563478	-3,281009	-1,110470	H	4,673642	-0,264514	1,718141
H	-5,329329	-1,880964	-0,155144	H	0,991910	-1,702961	-1,281350
H	-4,615675	-0,667905	-1,219769	H	3,307617	-2,349200	-1,787604
H	-3,913885	-2,634056	-2,477804	H	-1,291814	-1,530070	-1,671796
H	-3,915649	-3,636143	-1,022701	H	-0,903715	-2,954744	-0,677605
H	3,520344	3,134149	0,455863	H	-5,035698	-2,670726	-0,738303
H	1,928686	2,695340	1,154675	H	-4,413368	-1,322153	-1,696889
H	3,356521	1,718058	1,539299	H	-2,936687	-3,055583	-2,576803
H	2,783260	-0,734112	-4,731147	H	-3,025050	-3,976503	-1,069633
H	2,057286	-1,983755	-3,681039	H	0,479255	4,201947	3,958924
H	1,008156	-0,833727	-4,517600	H	-0,743395	2,899921	3,866512
H	-1,678725	5,309164	0,293046	H	0,886278	2,523045	4,431710
H	-2,142913	4,864638	-1,360120	H	2,103287	3,098184	-2,269340
H	-3,245320	4,558451	-0,012091	H	2,066176	1,315517	-2,068209
Cl	3,498406	-1,687629	0,222817	H	0,574649	2,185823	-2,483980
				H	6,311340	-1,235437	0,231661
				H	5,736705	-2,857211	-0,175046
				H	5,841064	-1,622525	-1,431601
				Cl	-2,021484	2,100848	-0,536998
TS'β, R=Me							
-1488.93846385							
Pd	-0,107830	0,775890	0,262830				
C	1,489240	-0,576320	0,505720				

APPENDIX

NMR Spectra and GC-MS Chromatograms for New Enamides 8a, 8d, 9c and 10e

N-(1-[4-Methoxyphenyl]ethenyl)-2-pyrrolidinone **8a**

Print Date: 26 Sep 2003 11:23:28

Chromatogram Plot

8a

File: c:\saturnws\data\v2_2003_v36\mu_ox147_ch6.sms
Sample: mu_ox147_ch6
Scan Range: 1 - 1809 Time Range: 0.00 - 16.99 min.
Sample Notes: ROUTINE

Operator: Andrei
Date: 2003-09-04 19:48

8a

N-(1-[4-Methylphenyl]ethenyl)-2-pyrrolidinone **8d**

Print Date: 26 Sep 2003 11:28:32

8d

Chromatogram Plot

File: c:\saturnws\data\v2_2003_v34\mu_ox105_ch4.sms
Sample: mu_ox105_ch4
Scan Range: 1 - 1811 Time Range: 0.00 - 16.98 min.
Sample Notes: today

Operator: Andrei
Date: 2003-08-18 14:21

N-(1-[4-Phenoxyphenyl]ethenyl)-2-pyrrolidinone **9c**

9c

Print Date: 26 Sep 2003 11:19:33

9C

Chromatogram Plot

File: c:\saturnws\data\lv2_2003_v37\mu1_ox153_ch3.sms

Sample: mu1_ox153_ch3

Operator: Andrei

Scan Range: 1 - 1815 Time Range: 0.00 - 16.98 min.

Date: 2003-09-12 15:23

Sample Notes: today

N-(1-[4-*n*-Butylphenyl]ethenyl)-2-pyrrolidinone **10e**

10e

Print Date: 26 Sep 2003 10:57:54

Chromatogram Plot

10e

File: c:\saturnws\data\v2_2003_v36\mu_ox142_ch2001.sms

Sample: mu_ox142_ch2

Scan Range: 1 - 1808 Time Range: 0.00 - 16.99 min.

Sample Notes: today

Operator: Andrei

Date: 2003-09-04 16:48

NMR Spectra and GC-MS Chromatograms for Known Compounds 4b,c,d,f,g,h,i

1-(2-Methoxy-phenyl)-ethanone 4b

Print Date: 05 Mar 2004 12:42:25

4b

Chromatogram Plot

File: k:\2omeacetophenone.sms

Sample: prnskak

Scan Range: 1 - 1228 Time Range: 0.00 - 11.99 min.

Sample Notes: ROUTINE

Operator: Operator

Date: 2004-02-26 14:24

1-(4-Phenoxy-phenyl)-ethanone 4c

Print Date: 05 Mar 2004 13:49:42

4c

Chromatogram Plot

File: k:\mu_ox149_ch5.sms

Sample: mu_ox149_ch5

Scan Range: 1 - 1811 Time Range: 0.00 - 16.98 min.

Sample Notes: today

Operator: Andrei

Date: 2003-09-22 13:10

1-(4-Methyl-phenyl)-ethanone **4d**

Print Date: 05 Mar 2004 13:26:58

4d

Chromatogram Plot

File: k:\4meacetophenonedist.sms

Sample: mu_mic93H_ch8

Scan Range: 1 - 1809 Time Range: 0.00 - 16.98 min.

Sample Notes: today

Operator: Andrei

Date: 2003-10-23 15:19

1-Phenyl-ethanone **4f**

rint Date: 05 Mar 2004 17:50:03

Chromatogram Plot

File: k:\acetophenoneprod.sms

Sample: acetophenoneprod

Scan Range: 1 - 1344 Time Range: 0.00 - 12.99 min.

Sample Notes: today

Operator: Operator

Date: 2004-03-05 17:34

49

1-(4-Chloro-phenyl)-ethanone **4h**

int Date: 05 Mar 2004 13:34:55

4h

Chromatogram Plot

File: k:\mu_ox158_hyd.sms

Sample: mu_ox158_hyd

Scan Range: 1 - 1810 Time Range: 0.00 - 16.99 min.

Sample Notes: today

Operator: Andrei

Date: 2003-10-10 12:55

1-(4-Acetyl-phenyl)-ethanone **4i**

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