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Supplementary Material

Palladium-mediated CO_2 extrusion followed by insertion of ketenes: translating mechanistic studies to develop a one-pot method for the synthesis of ketones

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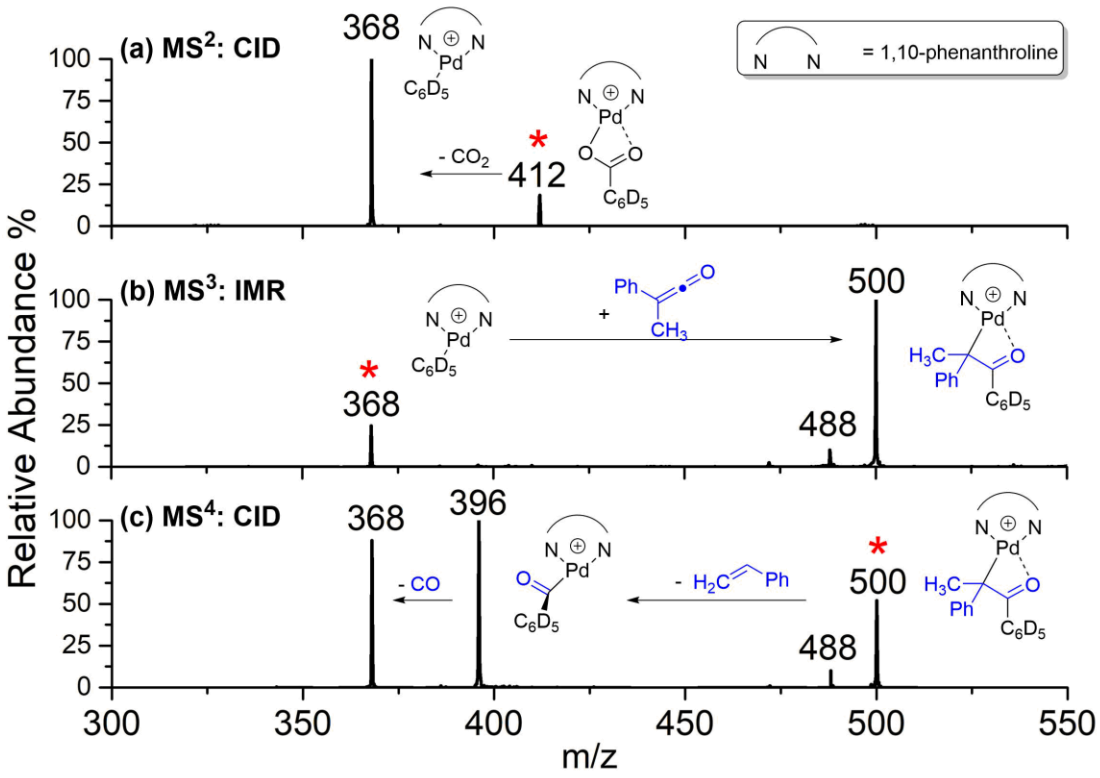

Figure S1: MS^n spectra of unimolecular and bimolecular reactions associated with key steps of the ExIn reaction: (a) MS^2 experiment involving extrusion of CO_2 from $[(phen)Pd(O_2CC_6D_5)]^+$ (*m/z* 407) under CID conditions at a normalised collision energy of 17; (b) MS^3 experiment involving an ion–molecule reaction (IMR) between the organometallic cation $[(phen)Pd(C_6D_5)]^+$ (*m/z* 368) and phenylmethylketene at 10-ms reaction time; (c) MS^4 CID of the enolate $[(phen)Pd(CPhMeC(O)C_6D_5)]^+$ (*m/z* 500). The concentration of phenylmethylketene in the ion–molecule reactions is 1.27×10^{10} molecules cm^{-3}.The mass-selected ions are denoted by asterisks.

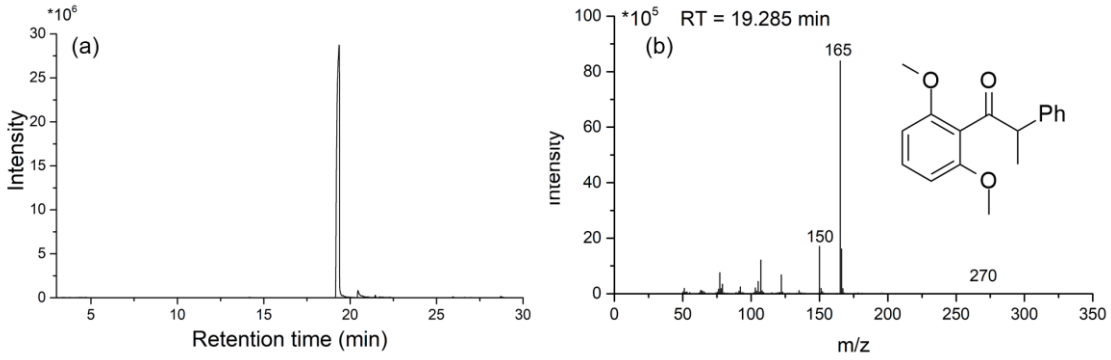

Figure S2: GC-MS analysis of ketone **25a** (Ar = 2,6-dimethoxyphenyl, X = O, Y = CMePh) synthesised by an alternative route developed by Joshi et al.[1] (a) TIC trace spectrum, (b) EI-MS spectrum at the retention time of 19.285 min**.**

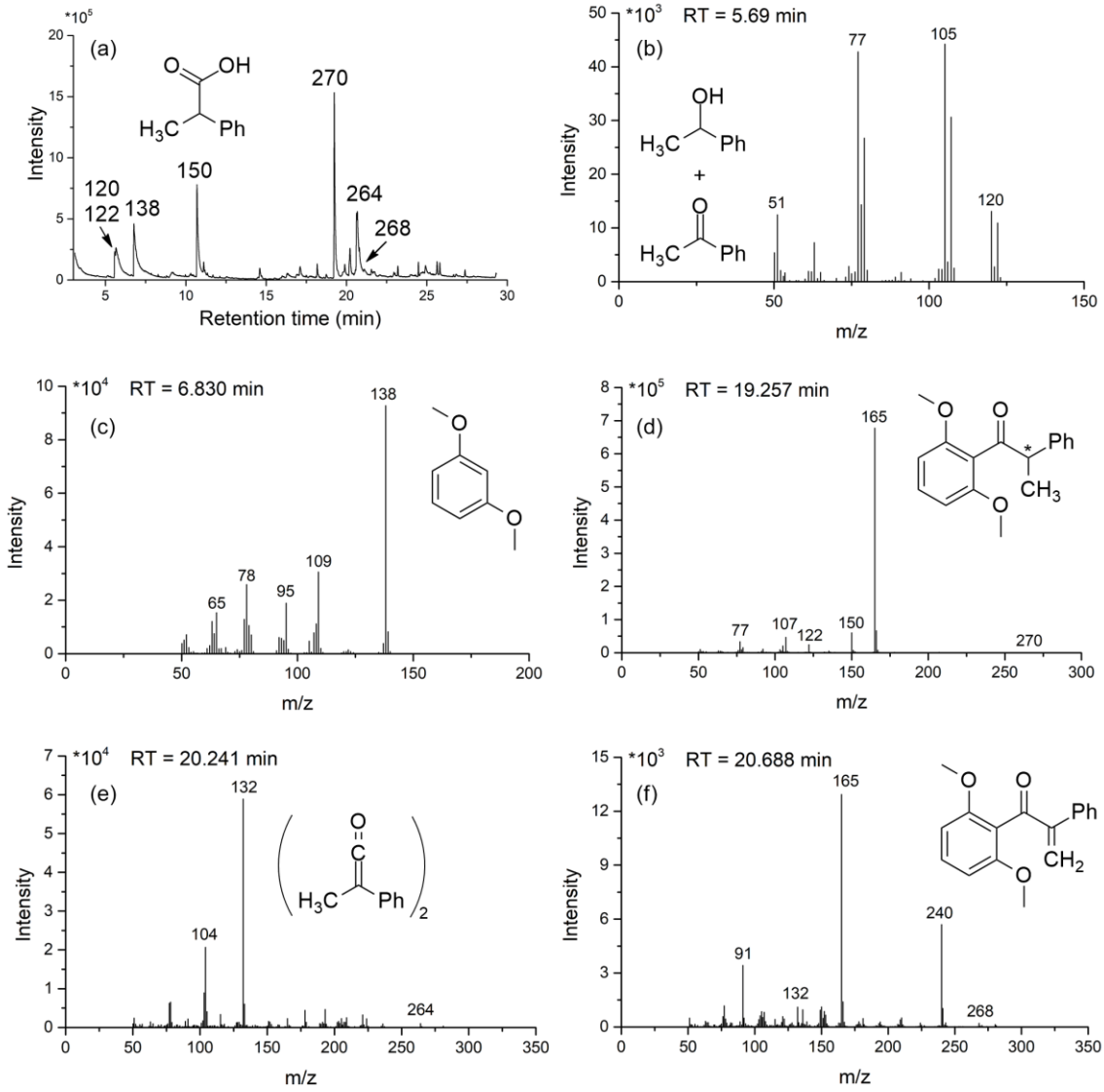

Figure S3: GC-MS analysis of the Ex-In one-pot reaction mixture using 2,6-dimethoxybenzoic acid **1a** and methylphenylketene **3a** quenched with $NaBH_4$ (entry 5, table 1): (a) TIC trace spectrum, (b) EI-MS spectrum at the retention time of 5.690 min, (c) EI-MS spectrum at the retention time of 6.830 min, (d) EI-MS spectrum at the retention time of 19.257 min, (e) EI-MS spectrum at the retention time of 20.241 min and (f) EI-MS spectrum at the retention time of 20.688 min. Note: there seems to be a significant peak at 122 in Figure S2b, which is likely due to the formation of 1-phenylethanol.

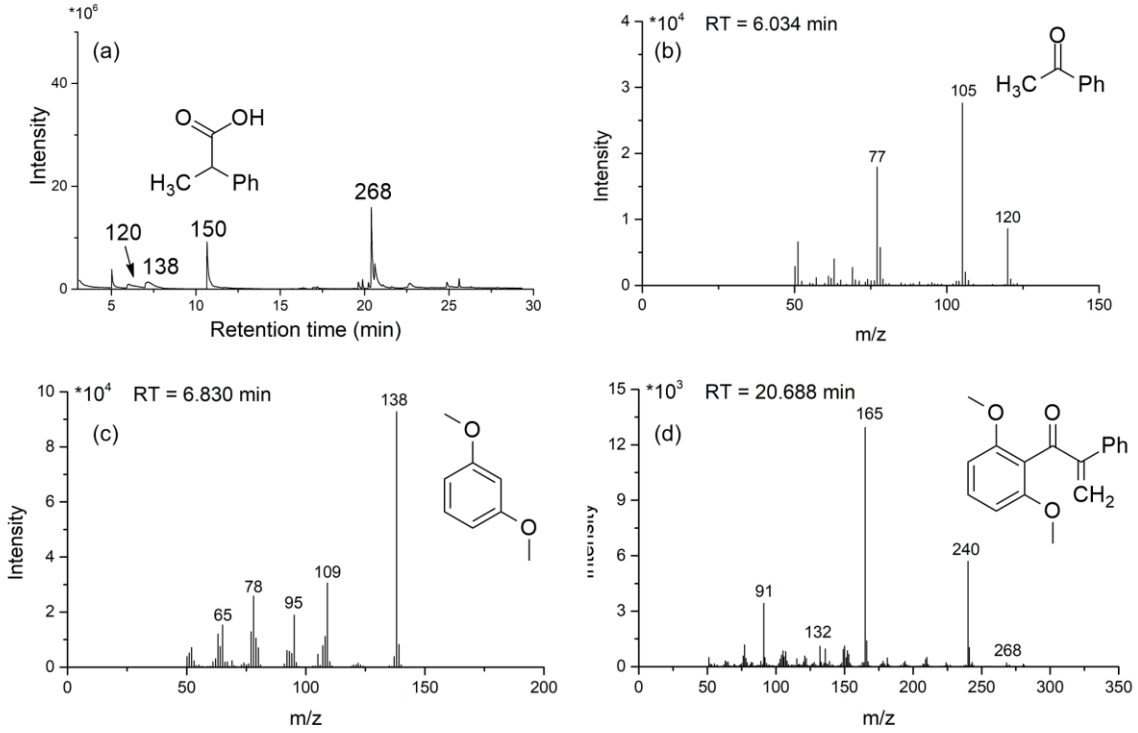

Figure S4: GC-MS analysis of the Ex-In one-pot reaction mixture using 2,6-dimethoxybenzoic acid **1a** and methylphenylketene **3a** quenched with HCl (entry 6, table 1): (a) TIC trace spectrum, (b) EI-MS spectrum at the retention time of 6.034 min, (c) EI-MS spectrum at the retention time of 6.830 min, (d) EI-MS spectrum at the retention time of 20.688 min.

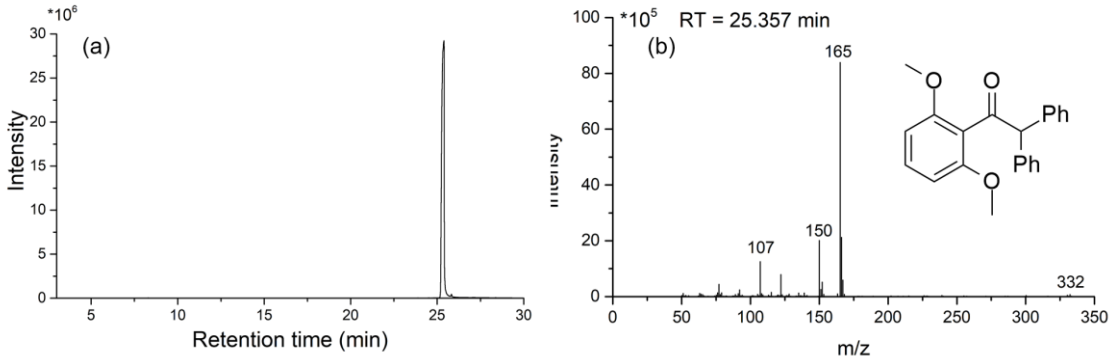

Figure S5: GC-MS analysis of ketone **25b** (Ar = 2,6-dimethoxyphenyl, X = O, Y = CPh_2) synthesised by an alternative route developed by Joshi et al.[1] (a) TIC trace spectrum, (b) EI-MS spectrum at the retention time of 25.357 min.

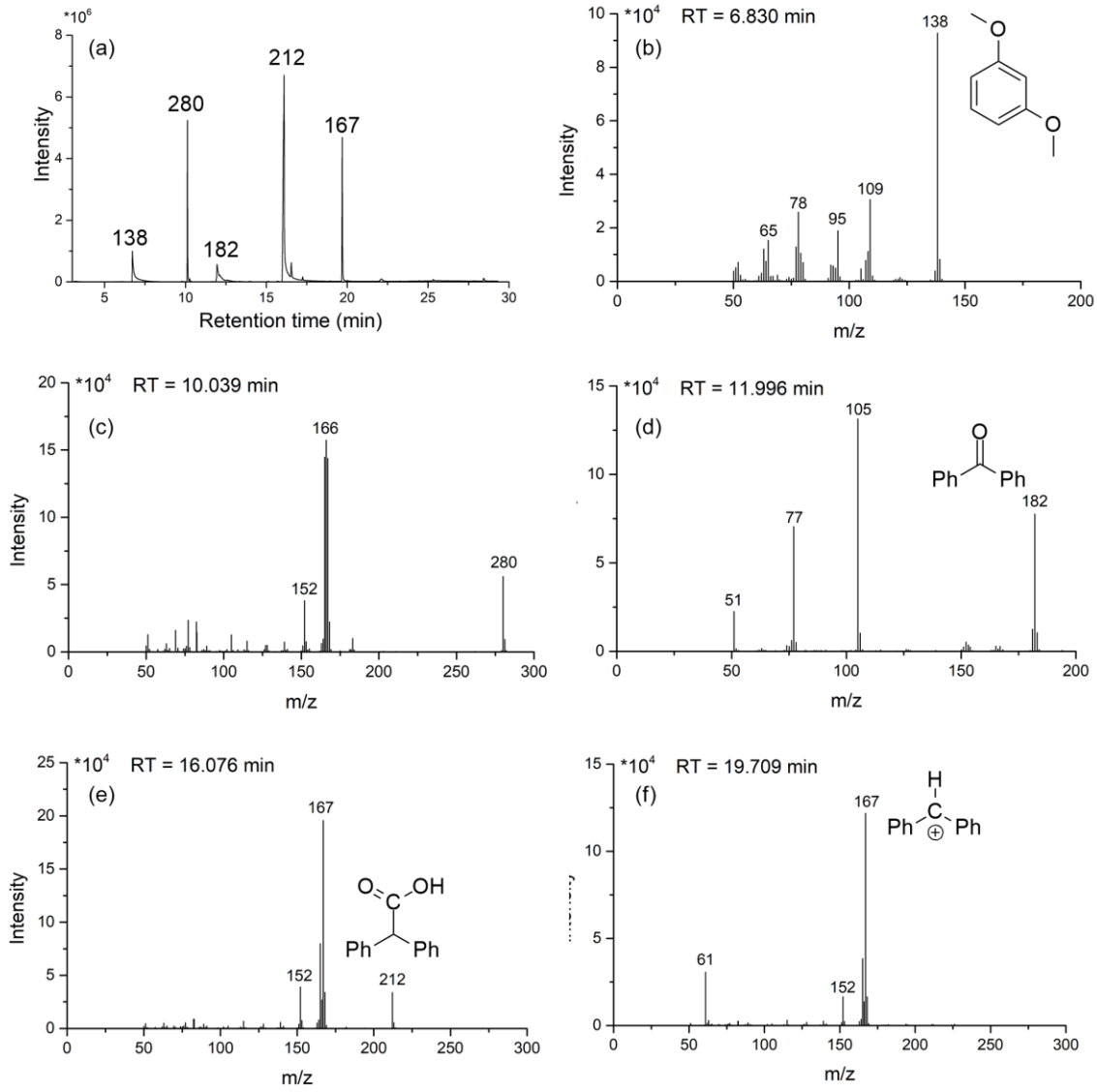

Figure S6: GC-MS analysis of the Ex-In one-pot reaction mixture using 2,6-dimethoxybenzoic acid **1a** and diphenylketene **3b** quenched with HCl (entry 7, table 1). (a) TIC trace spectrum, (b) EI-MS spectrum at the retention time of 6.830 min, (c) EI-MS spectrum of unknown product at the retention time of 10.039 min, (d) EI-MS spectrum at the retention time of 11.996 min, (e) EI-MS spectrum at the retention time of 16.076 min and (f) EI-MS spectrum at the retention time of 19.709 min.

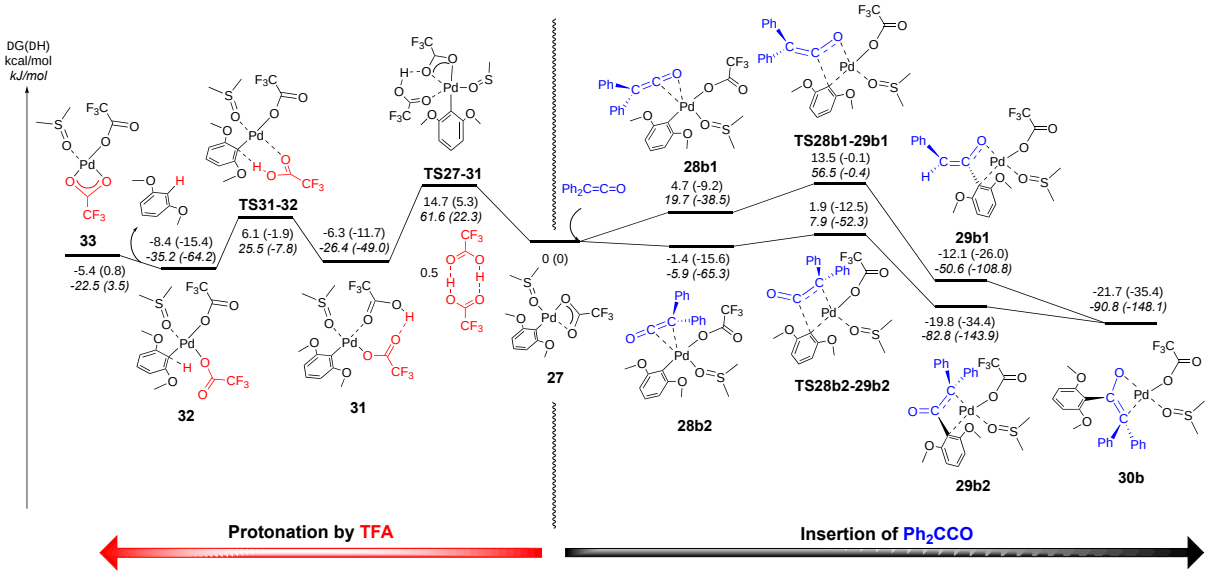

Figure S7: DFT calculated energy surface showing protonation (left) and insertion (right) of diphenylketene into [(DMSO)(CF_3CO_2)Pd(Ar)] with comparation of conformers. The relative Gibbs energies (and enthalpies in parentheses) are given in kilocalories per mole (kilojoules per mole, in italic) and were calculated at the B3LYP-D3BJ/BS2//M06/BS1 level of theory in DMSO using the CPCM approach.

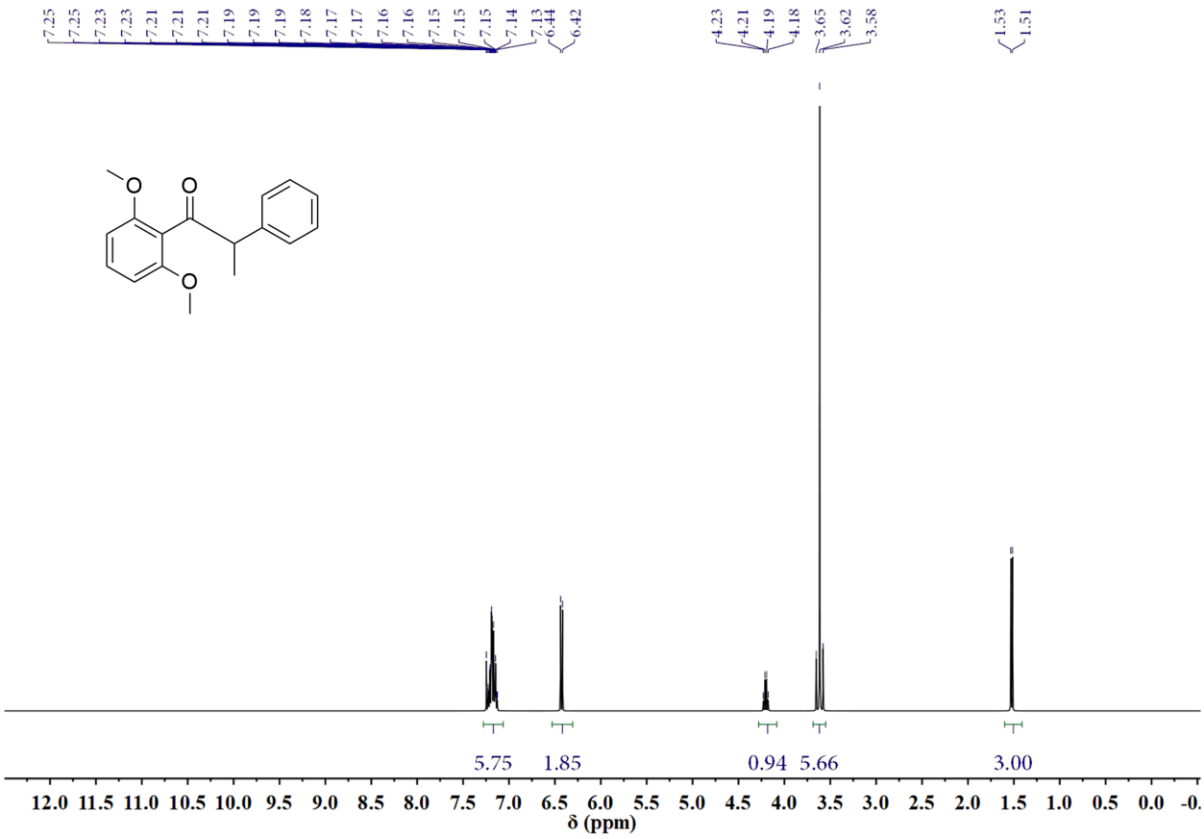

Figure S8. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of 1-(2,6-dimethoxyphenyl)-2-phenyl,1-propanone), **25a**, formed by reaction of ortholithiated 1,3-dimethoxybenzene with methylphenylacetyl chloride.

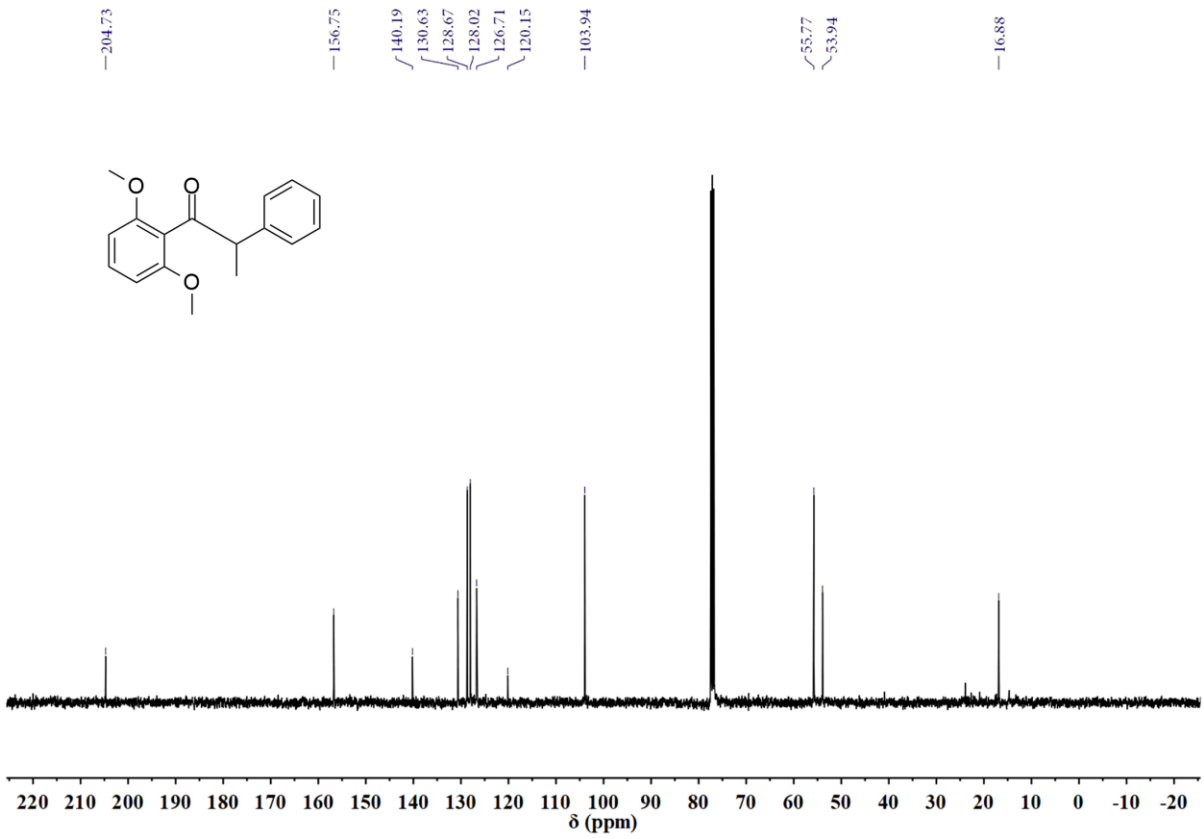

Figure S9. ^{13}C NMR spectra (400 MHz, $CDCl_3$) of 1-(2,6-dimethoxyphenyl)-2-phenyl,1-propanone, **25a**, formed by reaction of ortholithiated 1,3-dimethoxybenzene with methylphenylacetyl chloride.

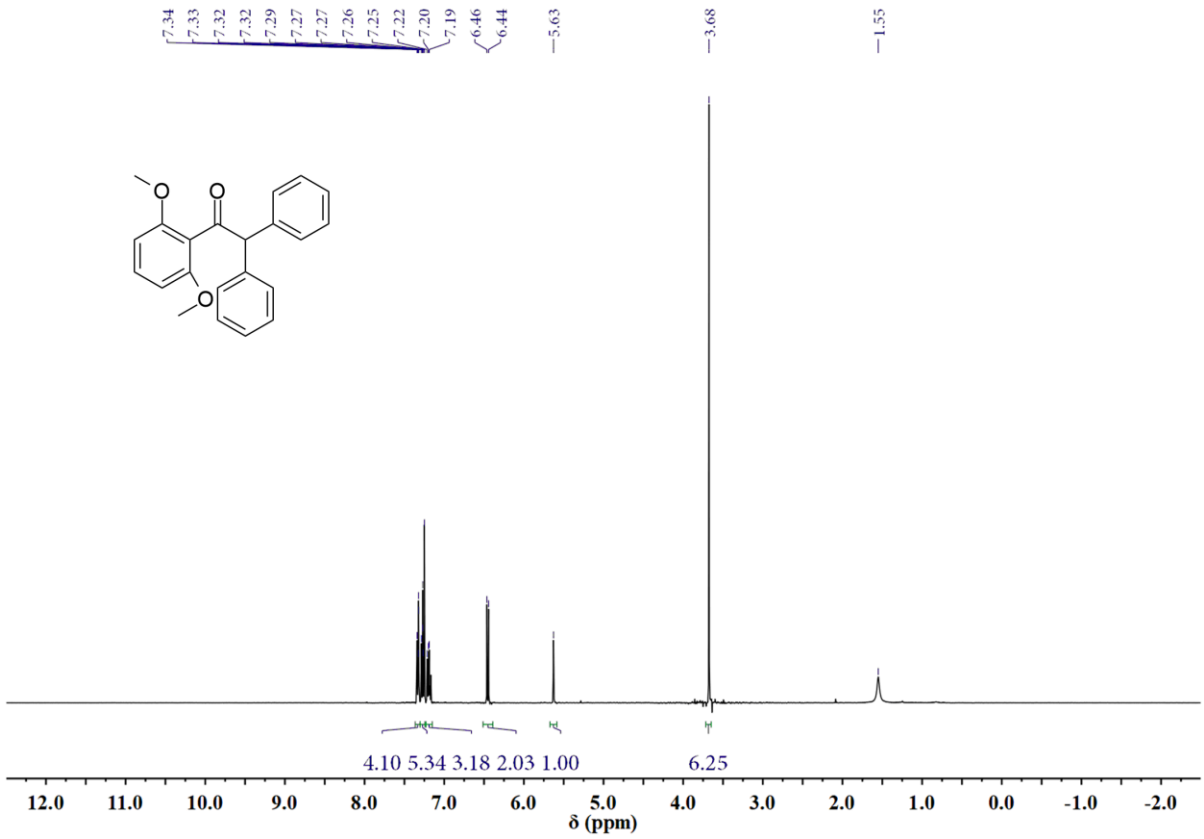

Figure S10. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of 1-(2,6-dimethoxyphenyl)-2-phenyl,1-propanone, **25b**, formed by reaction of ortholithiated 1,3-dimethoxybenzene with diphenylacetyl chloride.

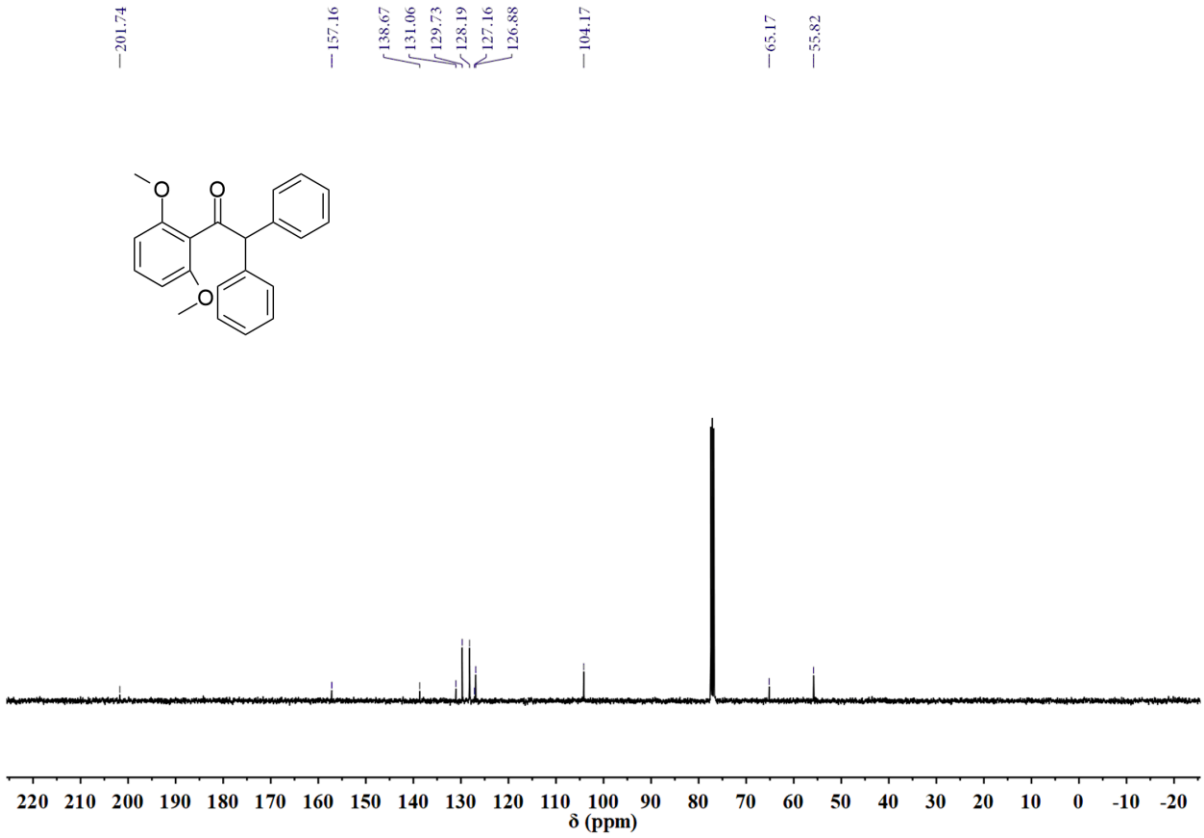

Figure S11. ^{13}C NMR spectra (400 MHz, $CDCl_3$) of 1-(2,6-dimethoxyphenyl)-2,2-diphenylethanone, **25b**, formed by reaction of ortholithiated 1,3-dimethoxybenzene with diphenylacetyl chloride.

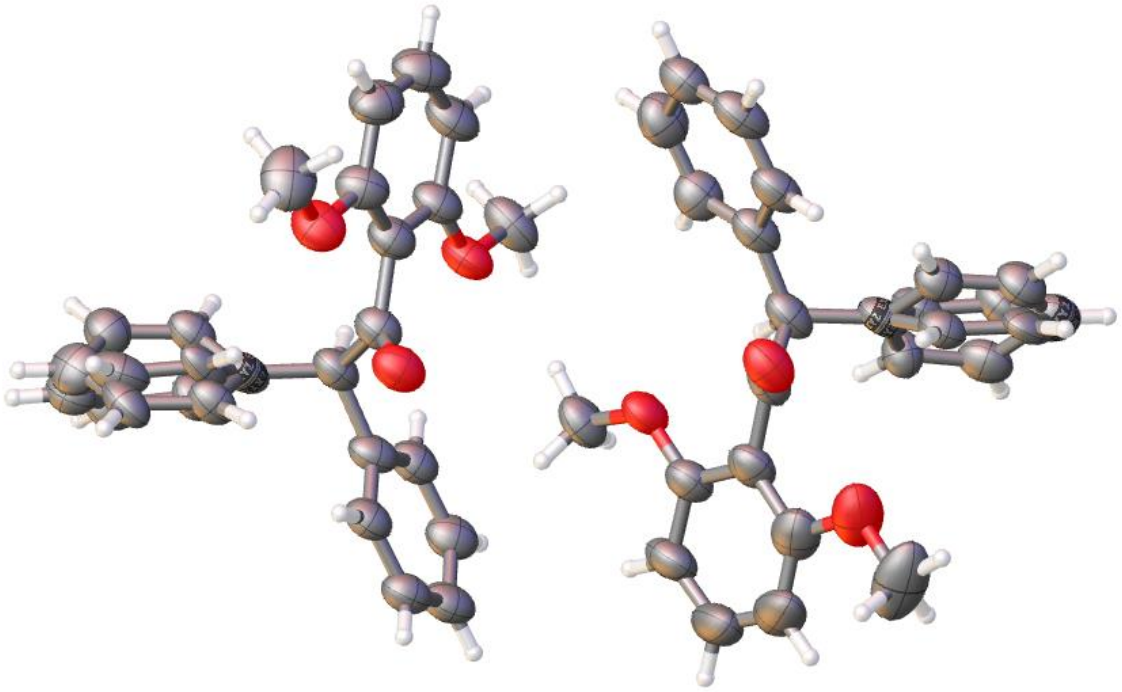

Figure S12: X-ray structure of the 1-(2,6-dimethoxyphenyl)-2,2-diphenylethanone, **25b**, formed by reaction of ortholithiated 1,3-dimethoxybenzene with diphenyl acetic acid chloride.

Table S1. Crystal data and structure refinement for 1-(2,6-dimethoxyphenyl)-2,2-diphenylethanone.

CCDC	2240016
Empirical formula	$C_{22}H_{20}O_3$
Formula weight	332.38
Temperature	100.0(2) K
Wavelength	0.71088 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	A =5.7780(12) Å □ = 85.39(3)°
	b = 11.878(2) Å □ = 89.47(3)°
	c = 25.251(5) Å □ = 87.70(3)°
Volume	1726.0(6) $Å^3$
Z	4
Density (calculated)	1.279 Mg m^{-3}
Absorption coefficient	0.084 mm^{-1}
F(000)	704
Crystal size	0.05 x 0.04 x 0.03 mm^3
Theta range for data collection	0.809 to 29.225°.
Index ranges	-6<=h<=6, -15<=k<=15, -32<=l<=31
Reflections collected	22310
Independent reflections	6243 [R(int) = 0.59]
Completeness to theta = 25.247°	88.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8622 and 0.59
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6243 / 0 / 534
Goodness-of-fit on F^2	1.003
Final R indices [I>2sigma(I)]	R1 = 0.1218, wR2 = 0.2920
R indices (all data)	R1 = 0.1945, wR2 = 0.3630
Extinction coefficient	n/a
Largest diff. peak and hole	0.701 and –0.420 e.$Å^{-3}$

Cartesian coordinates and energies for all DFT calculated structures

17a

Zero-point correction= 0.407444 (Hartree/Particle)
Thermal correction to Energy= 0.434206
Thermal correction to Enthalpy= 0.435151
Thermal correction to Gibbs Free Energy= 0.348112
Sum of electronic and zero-point Energies= -1351.474150
Sum of electronic and thermal Energies= -1351.447388
Sum of electronic and thermal Enthalpies= -1351.446443
Sum of electronic and thermal Free Energies= -1351.533482
HF = -1351.8815941

Single Point Energy Calculations with extended basis set:
HF = -1354.6235854

Optimised Geometry:
Charge = 1 Multiplicity = 1

C	-2.078564	-1.536331	0.711273
H	6.854276	-1.029801	-0.413791
C	5.879543	-0.548886	-0.349637
C	4.720723	-1.372394	-0.198189
C	5.766980	0.803315	-0.412883
C	3.447822	-0.773539	-0.111919
C	4.779748	-2.778942	-0.129757
C	4.489127	1.441063	-0.330340
H	6.649319	1.430597	-0.528735
N	2.314753	-1.503690	0.032764
C	3.328759	0.655385	-0.178910
C	3.620631	-3.506174	0.015022
H	5.747232	-3.275490	-0.193286
C	4.330733	2.839098	-0.394099
C	2.397431	-2.822374	0.093394
N	2.089222	1.219123	-0.094454
H	3.636662	-4.591196	0.069563
C	3.072387	3.387447	-0.308758
H	5.210276	3.470879	-0.511177
H	1.456017	-3.359126	0.208665
C	1.966580	2.540323	-0.158464
H	2.916419	4.461544	-0.355773
H	0.955970	2.936098	-0.085072
Pd	0.565688	-0.176358	0.131597
C	-0.904139	1.143479	0.207728
C	-1.754086	1.262807	-0.889246
C	-1.162489	1.819246	1.398214
C	-2.902146	2.048464	-0.777272

H -1.549970 0.730213 -1.819568
C -2.313381 2.604044 1.495955
H -0.483907 1.735676 2.248837
C -3.182384 2.712719 0.413274
H -3.586026 2.123803 -1.622006
H -2.527374 3.131627 2.424642
H -4.082191 3.319365 0.496865
C -3.313328 -1.292681 1.070892
O -0.947372 -1.741896 0.395105
C -4.337780 -1.013978 0.044426
C -5.527115 -0.377240 0.407596
C -4.125338 -1.340430 -1.301055
C -6.473127 -0.056015 -0.560258
H -5.715547 -0.116620 1.447552
C -5.068262 -1.012736 -2.263564
H -3.215611 -1.867412 -1.595973
C -6.246693 -0.365381 -1.896775
H -7.395574 0.439177 -0.263085
H -4.890473 -1.276635 -3.304357
H -6.990617 -0.115332 -2.650271
C -3.609303 -1.215737 2.549805
H -3.850566 -0.181975 2.830775
H -4.464993 -1.856370 2.796424
H -2.757792 -1.536761 3.158581

17b

Zero-point correction= 0.407602 (Hartree/Particle)
Thermal correction to Energy= 0.434165
Thermal correction to Enthalpy= 0.435109
Thermal correction to Gibbs Free Energy= 0.349554
Sum of electronic and zero-point Energies= -1351.490655
Sum of electronic and thermal Energies= -1351.464093
Sum of electronic and thermal Enthalpies= -1351.463148
Sum of electronic and thermal Free Energies= -1351.548704
HF = -1351.8982574

Single Point Energy Calculations with extended basis set:
HF = -1354.6378369

Optimised Geometry:
Charge = 1 Multiplicity = 1
C 0.015629 2.155998 1.531402
H -2.773743 -5.232643 0.132902
C -1.957186 -4.515470 0.066027
C -2.254947 -3.128787 0.240795
C -0.686765 -4.927549 -0.173823
C -1.223514 -2.167889 0.157830
C -3.560047 -2.668905 0.502004
C 0.383410 -3.984172 -0.255884
H -0.456540 -5.983597 -0.304914

N	-1.458662	-0.838093	0.312681
C	0.121584	-2.606570	-0.092843
C	-3.782532	-1.323613	0.667540
H	-4.375068	-3.388304	0.572108
C	1.714342	-4.377661	-0.492289
C	-2.697730	-0.441135	0.561886
N	1.114640	-1.678944	-0.159321
H	-4.774126	-0.930845	0.875006
C	2.704064	-3.426327	-0.553014
H	1.942200	-5.434999	-0.621730
H	-2.850851	0.630330	0.681864
C	2.361574	-2.079194	-0.378938
H	3.741744	-3.694440	-0.730625
H	3.122132	-1.301453	-0.419589
Pd	0.465978	0.353835	0.130124
C	2.347670	0.995760	-0.007754
C	2.895559	1.213354	-1.269989
C	3.130390	1.084783	1.139456
C	4.251991	1.519287	-1.381120
H	2.278049	1.144271	-2.167780
C	4.486736	1.395990	1.015444
H	2.705277	0.905508	2.128216
C	5.045748	1.610980	-0.240296
H	4.686977	1.687634	-2.365162
H	5.104607	1.468165	1.909158
H	6.102763	1.852638	-0.331346
C	-0.167688	2.486363	0.213733
O	0.127055	2.033266	2.681868
C	-1.585947	2.560982	-0.266557
C	-1.886699	2.186958	-1.579164
C	-2.596658	3.064977	0.556827
C	-3.188296	2.293165	-2.052689
H	-1.093999	1.801009	-2.221785
C	-3.901026	3.166508	0.079598
H	-2.364334	3.387780	1.572778
C	-4.198412	2.776053	-1.222296
H	-3.416645	1.998560	-3.074946
H	-4.682436	3.562066	0.725353
H	-5.216520	2.859870	-1.596805
C	0.776299	3.528734	-0.377203
H	0.930640	3.330456	-1.443840
H	0.305288	4.515364	-0.274064
H	1.756033	3.543649	0.108920

TS17a-18a

Zero-point correction= 0.407110 (Hartree/Particle)
Thermal correction to Energy= 0.432824
Thermal correction to Enthalpy= 0.433768
Thermal correction to Gibbs Free Energy= 0.349526
Sum of electronic and zero-point Energies= -1351.449362

Sum of electronic and thermal Energies= -1351.423648
Sum of electronic and thermal Enthalpies= -1351.422704
Sum of electronic and thermal Free Energies= -1351.506945
HF = -1351.8564719

Single Point Energy Calculations with extended basis set:
HF = -1354.599842

Optimised Geometry:
Charge = 1 Multiplicity = 1

C	-2.206599	0.066417	0.279634
H	6.166330	-2.612868	-0.318104
C	5.370474	-1.870872	-0.280086
C	4.027071	-2.320074	-0.080525
C	5.649869	-0.547492	-0.416597
C	2.987396	-1.372957	-0.029845
C	3.670184	-3.675148	0.074768
C	4.611010	0.435699	-0.367668
H	6.673921	-0.209120	-0.565600
N	1.693307	-1.727586	0.161892
C	3.279039	0.020167	-0.178675
C	2.350709	-4.018578	0.266945
H	4.445959	-4.439047	0.041557
C	4.847708	1.818073	-0.497330
C	1.380354	-3.004968	0.305282
N	2.244063	0.904897	-0.126359
H	2.049241	-5.055126	0.389440
C	3.792006	2.698806	-0.434238
H	5.866090	2.175424	-0.644232
H	0.324503	-3.228723	0.454870
C	2.494653	2.202355	-0.246282
H	3.943273	3.770538	-0.527537
H	1.636047	2.870379	-0.196094
Pd	0.398969	-0.021410	0.175283
C	-0.746831	1.664733	0.210056
C	-0.886684	2.391463	-0.983491
C	-0.851777	2.310008	1.449899
C	-1.075460	3.767235	-0.931387
H	-0.840047	1.875997	-1.943358
C	-1.052355	3.689223	1.493844
H	-0.767870	1.736085	2.373213
C	-1.146972	4.412495	0.306458
H	-1.173887	4.340338	-1.851581
H	-1.132018	4.198167	2.452501
H	-1.296425	5.490093	0.343214
C	-3.456138	0.463038	0.067620
O	-1.422705	-0.863427	0.515275
C	-4.437364	-0.648470	-0.104992
C	-4.284879	-1.890222	0.521705
C	-5.563057	-0.437593	-0.911084

C -5.229006 -2.892957 0.343477
H -3.429578 -2.068813 1.172211
C -6.506110 -1.443504 -1.085020
H -5.704549 0.518454 -1.412267
C -6.343344 -2.675556 -0.461206
H -5.098519 -3.848528 0.848366
H -7.374183 -1.259780 -1.715553
H -7.083931 -3.461118 -0.596742
C -3.929171 1.878000 -0.058208
H -4.012352 2.196829 -1.107279
H -4.924607 1.967161 0.392801
H -3.268267 2.578851 0.457890
Imaginary Vibrational Frequency = -386.7514 cm^{-1}

TS17b-18b
Zero-point correction= 0.407412 (Hartree/Particle)
Thermal correction to Energy= 0.433110
Thermal correction to Enthalpy= 0.434054
Thermal correction to Gibbs Free Energy= 0.351004
Sum of electronic and zero-point Energies= -1351.482246
Sum of electronic and thermal Energies= -1351.456548
Sum of electronic and thermal Enthalpies= -1351.455604
Sum of electronic and thermal Free Energies= -1351.538654
HF = -1351.8896581

Single Point Energy Calculations with extended basis set:
HF = -1354.6259689

Optimised Geometry:
Charge = 1 Multiplicity = 1
C 2.053200 -1.982021 0.161822
H -3.384218 4.905927 -0.044937
C -3.126201 3.848900 -0.003116
C -1.758428 3.476429 -0.189472
C -4.081002 2.908893 0.216636
C -1.389881 2.115636 -0.139114
C -0.741236 4.420397 -0.429450
C -3.741931 1.521314 0.270398
H -5.122817 3.193636 0.354734
N -0.104920 1.705166 -0.313571
C -2.399445 1.123577 0.098816
C 0.552585 3.991464 -0.605603
H -0.994254 5.479051 -0.473503
C -4.698376 0.510299 0.486962
C 0.828756 2.618131 -0.538477
N -2.022787 -0.179711 0.145499
H 1.362804 4.690472 -0.793574
C -4.301373 -0.805923 0.520979
H -5.743754 0.784833 0.622847
H 1.847065 2.252216 -0.668672

C -2.944257 -1.111162 0.344811
H -5.014649 -1.609399 0.682500
H -2.594233 -2.142422 0.373539
Pd 0.104191 -0.477308 -0.174824
C -0.002961 -2.536357 -0.080191
C -0.330654 -3.202517 -1.268567
C -0.320560 -3.135465 1.150870
C -0.960398 -4.447057 -1.225656
H -0.130742 -2.749809 -2.239095
C -0.950617 -4.369947 1.189980
H -0.040267 -2.640527 2.082039
C -1.269472 -5.027738 -0.001460
H -1.209014 -4.959144 -2.153316
H -1.186486 -4.830456 2.147674
H -1.755122 -6.001182 0.030549
C 2.146516 -0.817406 -0.629699
O 2.495045 -2.714743 0.952918
C 3.024269 0.213791 0.017714
C 2.934792 0.485147 1.390218
C 3.933760 0.946433 -0.753225
C 3.724641 1.466005 1.971263
H 2.225562 -0.066500 2.009237
C 4.722597 1.933254 -0.165835
H 4.036448 0.753047 -1.818859
C 4.618888 2.199871 1.193815
H 3.639585 1.661709 3.038226
H 5.426844 2.489992 -0.781069
H 5.236216 2.970639 1.650195
C 2.255836 -1.011779 -2.129464
H 1.591809 -1.802074 -2.487871
H 1.995521 -0.083395 -2.652702
H 3.280203 -1.293723 -2.412631
Imaginary Vibrational Frequency = -364.9818 cm^{-1}

18a
Zero-point correction= 0.410002 (Hartree/Particle)
Thermal correction to Energy= 0.435435
Thermal correction to Enthalpy= 0.436379
Thermal correction to Gibbs Free Energy= 0.352901
Sum of electronic and zero-point Energies= -1351.490230
Sum of electronic and thermal Energies= -1351.464797
Sum of electronic and thermal Enthalpies= -1351.463852
Sum of electronic and thermal Free Energies= -1351.547331
HF = -1351.9002317

Single Point Energy Calculations with extended basis set:
HF = -1354.6403984

Optimised Geometry:
Charge = 1 Multiplicity = 1

C	2.135369	0.894317	0.277321
H	-4.977667	-3.843871	-0.492352
C	-4.463579	-2.887352	-0.414447
C	-3.063968	-2.886655	-0.116267
C	-5.139389	-1.721308	-0.599825
C	-2.396709	-1.654153	-0.010744
C	-2.292467	-4.051074	0.077698
C	-4.475420	-0.456398	-0.503943
H	-6.203790	-1.729730	-0.828565
N	-1.072801	-1.576958	0.268162
C	-3.100868	-0.428383	-0.206333
C	-0.946036	-3.947439	0.352090
H	-2.770423	-5.027075	0.004403
C	-5.117546	0.783379	-0.694985
C	-0.356067	-2.676848	0.441329
N	-2.395611	0.731583	-0.100454
H	-0.331390	-4.831059	0.499119
C	-4.392402	1.948953	-0.588168
H	-6.181594	0.806797	-0.926468
H	0.704690	-2.531777	0.647027
C	-3.023560	1.882155	-0.286761
H	-4.860170	2.919037	-0.731219
H	-2.418046	2.784100	-0.191235
Pd	-0.356159	0.367505	0.361858
C	1.188171	2.063873	0.239962
C	0.566409	2.500567	1.440296
C	0.901308	2.759342	-0.958757
C	-0.245162	3.636850	1.442272
H	0.808480	1.990816	2.372272
C	0.109768	3.895577	-0.938453
H	1.345306	2.403141	-1.887423
C	-0.452553	4.343083	0.263511
H	-0.681041	3.984415	2.376558
H	-0.070318	4.445398	-1.860102
H	-1.055066	5.249987	0.273531
C	3.396513	0.862663	-0.224474
O	1.483256	-0.146874	0.817311
C	4.194306	-0.372226	-0.222774
C	5.195397	-0.553539	-1.191106
C	4.012248	-1.390086	0.729210
C	5.951940	-1.716545	-1.233217
H	5.373921	0.220474	-1.936075
C	4.774859	-2.550099	0.688754
H	3.291493	-1.248099	1.530707
C	5.743147	-2.723671	-0.295328
H	6.713134	-1.835371	-2.002262
H	4.627338	-3.316654	1.448170
H	6.344071	-3.630708	-0.321596
C	4.040917	2.115608	-0.745800
H	4.099626	2.131339	-1.844662

H 3.500234 3.020115 -0.441631
H 5.069581 2.202562 -0.372470

18b

Zero-point correction= 0.409781 (Hartree/Particle)
Thermal correction to Energy= 0.435477
Thermal correction to Enthalpy= 0.436421
Thermal correction to Gibbs Free Energy= 0.353128
Sum of electronic and zero-point Energies= -1351.515340
Sum of electronic and thermal Energies= -1351.489644
Sum of electronic and thermal Enthalpies= -1351.488700
Sum of electronic and thermal Free Energies= -1351.571993
HF = -1351.9251215

Single Point Energy Calculations with extended basis set:
HF = -1354.6524906

Optimised Geometry:
Charge = 1 Multiplicity = 1

C	2.849865	-1.101360	-0.020707
H	-5.102270	2.946075	-0.227841
C	-4.419861	2.106503	-0.105260
C	-3.037865	2.306129	-0.412862
C	-4.869154	0.904244	0.336438
C	-2.124748	1.238718	-0.270813
C	-2.535981	3.546096	-0.852024
C	-3.970741	-0.195411	0.498020
H	-5.920346	0.755676	0.578329
N	-0.798609	1.386789	-0.533428
C	-2.603911	-0.037323	0.182280
C	-1.193404	3.678680	-1.113124
H	-3.218963	4.385955	-0.973551
C	-4.388849	-1.453808	0.971862
C	-0.357178	2.567944	-0.934694
N	-1.714036	-1.051548	0.305693
H	-0.768126	4.620836	-1.447613
C	-3.469607	-2.466733	1.113756
H	-5.437044	-1.606946	1.225898
C	-2.134367	-2.219622	0.763412
H	-3.757528	-3.445906	1.486574
H	-1.380434	-3.001344	0.854505
Pd	0.365738	-0.472592	-0.292648
C	1.888476	-2.244153	-0.180994
C	1.141359	-2.507362	-1.358093
C	1.791981	-3.145915	0.907847
C	0.333965	-3.653525	-1.428653
H	1.288164	-1.930076	-2.267070
C	1.000194	-4.269378	0.816869
H	2.391841	-2.940411	1.792736
C	0.274158	-4.528188	-0.359467

H -0.207332 -3.868081 -2.347404
H 0.950843 -4.968809 1.649027
H -0.328588 -5.431927 -0.432346
C 2.349413 0.172717 -0.648560
O 3.805708 -1.179133 0.719503
C 2.528885 1.370211 0.201805
C 2.227145 1.309417 1.575799
C 2.943417 2.602066 -0.327973
C 2.296793 2.440999 2.372444
H 1.937425 0.358117 2.023514
C 3.031776 3.732369 0.477169
H 3.218383 2.681812 -1.378471
C 2.696078 3.659459 1.824902
H 2.053886 2.371675 3.430726
H 3.371740 4.673170 0.048588
H 2.762609 4.544880 2.453760
H 0.715478 2.654129 -1.105067
C 2.660987 0.333976 -2.119729
H 2.607593 -0.606321 -2.675433
H 1.994741 1.057013 -2.608825
H 3.693853 0.695595 -2.237999

19

Zero-point correction= 0.410756 (Hartree/Particle)
Thermal correction to Energy= 0.436014
Thermal correction to Enthalpy= 0.436958
Thermal correction to Gibbs Free Energy= 0.354445
Sum of electronic and zero-point Energies= -1351.529293
Sum of electronic and thermal Energies= -1351.504035
Sum of electronic and thermal Enthalpies= -1351.503091
Sum of electronic and thermal Free Energies= -1351.585604
HF = -1351.9400488

Single Point Energy Calculations with extended basis set:
HF = -1354.6718643

Optimised Geometry:
Charge = 1 Multiplicity = 1
C 2.165351 -1.001350 0.487356
H -6.560439 -0.773224 -0.713726
C -5.559313 -0.391774 -0.519150
C -4.480878 -1.325319 -0.416328
C -5.339926 0.942086 -0.380898
C -3.178894 -0.850942 -0.162528
C -4.642761 -2.718147 -0.558118
C -4.027690 1.451854 -0.124235
H -6.161656 1.651694 -0.463347
N -2.113007 -1.679452 -0.061691
C -2.947270 0.554832 -0.007545

C	-3.550108	-3.548225	-0.448137
H	-5.634795	-3.123263	-0.754077
C	-3.752659	2.825581	0.018438
C	-2.289918	-2.983283	-0.197609
N	-1.677472	0.979341	0.242087
H	-3.646057	-4.625462	-0.552587
C	-2.462301	3.238504	0.255977
H	-4.565761	3.545602	-0.065148
H	-1.398356	-3.603107	-0.104208
C	-1.445410	2.279003	0.360582
H	-2.214371	4.290652	0.364597
H	-0.410847	2.576678	0.539308
Pd	-0.275839	-0.593453	0.391538
C	3.532755	-1.216170	0.045810
C	3.891103	-2.465848	-0.484044
C	4.507376	-0.220279	0.212801
C	5.203449	-2.708511	-0.852598
H	3.125440	-3.230593	-0.596165
C	5.821344	-0.473923	-0.148221
H	4.232830	0.749081	0.626159
C	6.166515	-1.713168	-0.684401
H	5.483657	-3.673339	-1.269207
H	6.579908	0.293904	-0.015142
H	7.197934	-1.906807	-0.973045
C	1.542133	0.287681	0.920829
O	1.331963	-1.949296	0.541781
C	1.831217	1.513377	0.143448
C	2.058373	2.746617	0.771723
C	1.825347	1.476123	-1.261768
C	2.266986	3.901077	0.020595
H	2.083947	2.809270	1.858607
C	2.029392	2.626874	-2.007059
H	1.640900	0.529629	-1.772898
C	2.247868	3.847392	-1.368203
H	2.448291	4.846523	0.528548
H	2.017333	2.574591	-3.093986
H	2.407500	4.750359	-1.953815
C	1.498251	0.398171	2.434909
H	2.481318	0.700058	2.834511
H	0.758859	1.140195	2.762957
H	1.238623	-0.561875	2.895125

TS18-20

Zero-point correction= 0.406736 (Hartree/Particle)
Thermal correction to Energy= 0.432694
Thermal correction to Enthalpy= 0.433638
Thermal correction to Gibbs Free Energy= 0.349032
Sum of electronic and zero-point Energies= -1351.474159
Sum of electronic and thermal Energies= -1351.448202
Sum of electronic and thermal Enthalpies= -1351.447258

Sum of electronic and thermal Free Energies= -1351.531864
HF = -1351.8808959

Single Point Energy Calculations with extended basis set:
HF = -1354.6106247

Optimised Geometry:
Charge = 1 Multiplicity = 1

C	2.196505	0.643412	0.567421
H	-6.091097	1.412295	0.663242
C	-5.185295	0.881038	0.374894
C	-3.920720	1.457843	0.714162
C	-5.257332	-0.302911	-0.287350
C	-2.732604	0.791323	0.352012
C	-3.792553	2.677632	1.407212
C	-4.070311	-1.005140	-0.668053
H	-6.221589	-0.740989	-0.540385
N	-1.504553	1.279200	0.651592
C	-2.809172	-0.457078	-0.355150
C	-2.539981	3.165343	1.702106
H	-4.689182	3.220894	1.703397
C	-4.091786	-2.238410	-1.347670
C	-1.414458	2.428017	1.303693
N	-1.650767	-1.075125	-0.693699
H	-2.408793	4.102246	2.236563
C	-2.907330	-2.858995	-1.674361
H	-5.049250	-2.689976	-1.604697
H	-0.406928	2.781404	1.523440
C	-1.699517	-2.238287	-1.325981
H	-2.892248	-3.813002	-2.194195
H	-0.741169	-2.700511	-1.563795
Pd	0.151367	-0.023462	-0.064516
C	2.586676	1.905561	-0.095341
C	3.701506	2.588564	0.410990
C	1.849512	2.461503	-1.147020
C	4.080054	3.801537	-0.142475
H	4.253154	2.149383	1.240044
C	2.218130	3.687968	-1.684094
H	0.967707	1.937638	-1.525888
C	3.338711	4.350850	-1.188516
H	4.950810	4.327589	0.243073
H	1.639562	4.124186	-2.495560
H	3.637734	5.303687	-1.621262
C	1.809546	-0.936561	-0.572054
O	2.577924	0.317049	1.663016
C	2.132229	-2.158004	0.131872
C	2.936002	-3.165864	-0.446269
C	1.588933	-2.393984	1.415683
C	3.165182	-4.357803	0.217138
H	3.382046	-3.012952	-1.426766

C 1.814423 -3.591562 2.073363
H 0.996955 -1.615098 1.892286
C 2.604039 -4.572683 1.477149
H 3.783825 -5.125547 -0.242299
H 1.388140 -3.758422 3.059906
H 2.791015 -5.509285 1.999176
C 2.350968 -0.750904 -1.950674
H 3.452283 -0.779159 -1.961130
H 2.003974 -1.569919 -2.599014
H 2.045884 0.195424 -2.403884
Imaginary Vibrational Frequency = -287.2086 cm^{-1}

20
Zero-point correction= 0.407397 (Hartree/Particle)
Thermal correction to Energy= 0.434021
Thermal correction to Enthalpy= 0.434965
Thermal correction to Gibbs Free Energy= 0.347842
Sum of electronic and zero-point Energies= -1351.489184
Sum of electronic and thermal Energies= -1351.462560
Sum of electronic and thermal Enthalpies= -1351.461616
Sum of electronic and thermal Free Energies= -1351.548739
HF = -1351.8965807

Single Point Energy Calculations with extended basis set:
HF = -1354.6320741

Optimised Geometry:
Charge = 1 Multiplicity = 1
C 1.553350 -1.195734 -0.666817
H -6.122542 -0.627454 -0.849400
C -5.181504 -0.176155 -0.538753
C -3.968488 -0.887265 -0.800555
C -5.161937 1.032237 0.080067
C -2.732523 -0.331096 -0.409613
C -3.946627 -2.139807 -1.443974
C -3.926228 1.626353 0.485795
H -6.086477 1.572562 0.277379
N -1.552518 -0.965866 -0.632720
C -2.711641 0.949346 0.244735
C -2.744417 -2.769282 -1.666096
H -4.885047 -2.594521 -1.759054
C -3.857375 2.879490 1.124646
C -1.563969 -2.143890 -1.240674
N -1.512653 1.469021 0.606943
H -2.691667 -3.735103 -2.160817
C -2.633712 3.395911 1.483786
H -4.777440 3.427119 1.325347
H -0.597477 -2.621708 -1.398125
C -1.479483 2.651341 1.202509
H -2.547533 4.361241 1.975096

H -0.493756 3.033397 1.468795
Pd 0.206908 0.138396 0.079019
C 1.787470 -2.449521 0.096104
C 2.618048 -3.426110 -0.469318
C 1.196305 -2.675709 1.342066
C 2.854980 -4.610901 0.211789
H 3.068162 -3.229756 -1.440876
C 1.432439 -3.864522 2.020581
H 0.543942 -1.910465 1.769210
C 2.262743 -4.829692 1.455188
H 3.502921 -5.369032 -0.223589
H 0.971556 -4.041393 2.990293
H 2.450875 -5.760191 1.987734
C 1.794637 1.078049 0.801829
O 2.018686 -0.985360 -1.759845
C 2.621887 1.933882 0.013385
C 3.717752 2.659528 0.548756
C 2.351487 2.060906 -1.373038
C 4.491067 3.468180 -0.259201
H 3.965987 2.577692 1.604239
C 3.118822 2.886051 -2.175239
H 1.535977 1.478745 -1.798000
C 4.188228 3.585926 -1.619235
H 5.332025 4.015817 0.159907
H 2.898529 2.976092 -3.236124
H 4.799255 4.228410 -2.251040
C 2.028420 0.918167 2.258289
H 2.577332 -0.030073 2.394481
H 2.604875 1.711647 2.751180
H 1.081061 0.777438 2.795612

TS20-21
Zero-point correction= 0.403648 (Hartree/Particle)
Thermal correction to Energy= 0.429908
Thermal correction to Enthalpy= 0.430852
Thermal correction to Gibbs Free Energy= 0.343702
Sum of electronic and zero-point Energies= -1351.447562
Sum of electronic and thermal Energies= -1351.421302
Sum of electronic and thermal Enthalpies= -1351.420358
Sum of electronic and thermal Free Energies= -1351.507509
HF = -1351.8512101

Single Point Energy Calculations with extended basis set:
HF = -1354.5874817

Optimised Geometry:
Charge = 1 Multiplicity = 1
C 2.047588 -0.883795 0.936120
H -1.384759 5.838860 0.100764
C -1.467600 4.761116 -0.030478

C	-0.350402	3.945724	0.330524
C	-2.602663	4.204616	-0.523705
C	-0.420535	2.544222	0.171945
C	0.839458	4.490829	0.848659
C	-2.709990	2.789165	-0.690656
H	-3.454275	4.824780	-0.799256
N	0.622608	1.734898	0.497114
C	-1.626683	1.952168	-0.343808
C	1.881225	3.657701	1.180304
H	0.917848	5.569108	0.982156
C	-3.874218	2.176759	-1.193286
C	1.729734	2.278956	0.986275
N	-1.685365	0.602929	-0.474964
H	2.812257	4.043030	1.586412
C	-3.918599	0.809578	-1.324710
H	-4.725782	2.797156	-1.470370
H	2.541019	1.598837	1.240356
C	-2.795186	0.058279	-0.948283
H	-4.800468	0.303838	-1.708350
H	-2.805203	-1.028657	-1.032642
Pd	0.266972	-0.384057	0.191717
C	3.228429	-0.846018	0.030596
C	4.482339	-1.156164	0.575143
C	3.118985	-0.503174	-1.321217
C	5.611026	-1.126419	-0.230234
H	4.545116	-1.416339	1.630332
C	4.252201	-0.474687	-2.123748
H	2.137676	-0.256919	-1.732763
C	5.495715	-0.786526	-1.577734
H	6.585441	-1.368121	0.189276
H	4.169367	-0.207373	-3.175136
H	6.383192	-0.764045	-2.207483
C	-0.136541	-2.418029	-0.140129
O	2.114599	-1.140131	2.112859
C	-1.510795	-2.854661	0.171713
C	-2.263734	-3.576576	-0.763638
C	-2.097337	-2.489574	1.390109
C	-3.580045	-3.925473	-0.483378
H	-1.827138	-3.838236	-1.728309
C	-3.403093	-2.863536	1.677861
H	-1.514035	-1.912477	2.108682
C	-4.147997	-3.574716	0.738986
H	-4.163677	-4.474692	-1.219446
H	-3.845928	-2.592521	2.633963
H	-5.176390	-3.853886	0.959430
C	0.711749	-3.297411	-0.794698
H	0.407764	-4.311481	-1.082863
H	1.740041	-3.009591	-1.026951
H	0.741574	-2.872501	0.584084

Imaginary Vibrational Frequency = -1102.3406 cm^{-1}

21

Zero-point correction= 0.408408 (Hartree/Particle)
Thermal correction to Energy= 0.434669
Thermal correction to Enthalpy= 0.435613
Thermal correction to Gibbs Free Energy= 0.349327
Sum of electronic and zero-point Energies= -1351.519943
Sum of electronic and thermal Energies= -1351.493682
Sum of electronic and thermal Enthalpies= -1351.492738
Sum of electronic and thermal Free Energies= -1351.579024
HF = -1351.928351

Single Point Energy Calculations with extended basis set:
HF = -1354.664128

Optimised Geometry:
Charge = 1 Multiplicity = 1

C	2.025524	1.252855	-0.793166
H	-0.867208	-5.752172	-0.415521
C	-1.024557	-4.699922	-0.184187
C	0.006776	-3.769642	-0.522164
C	-2.170739	-4.280688	0.408765
C	-0.159502	-2.396587	-0.234560
C	1.203790	-4.173097	-1.143118
C	-2.375771	-2.898065	0.706510
H	-2.957074	-4.988549	0.666394
N	0.803979	-1.484074	-0.534148
C	-1.378467	-1.950370	0.387546
C	2.162366	-3.236119	-1.447461
H	1.353967	-5.226481	-1.376502
C	-3.556502	-2.426111	1.312723
C	1.920726	-1.896293	-1.121733
N	-1.532833	-0.627431	0.641781
H	3.096165	-3.510865	-1.929828
C	-3.697693	-1.083327	1.568549
H	-4.343739	-3.134300	1.568780
H	2.668870	-1.137654	-1.345834
C	-2.653310	-0.216991	1.212433
H	-4.595098	-0.682506	2.032135
H	-2.744645	0.855343	1.385559
Pd	0.311848	0.580023	-0.028060
C	3.251935	1.106964	0.023411
C	4.473718	1.447828	-0.574948
C	3.220955	0.642132	1.342269
C	5.650784	1.323582	0.147445
H	4.474757	1.810755	-1.601111
C	4.402693	0.520171	2.059861
H	2.265241	0.381361	1.800793
C	5.614702	0.860740	1.462133
H	6.600568	1.590275	-0.311196

H 4.382120 0.162675 3.087015
H 6.540074 0.766746 2.027265
C -0.529380 2.738086 -0.252936
O 1.982356 1.669949 -1.918963
C -1.987397 2.694653 -0.402586
C -2.832579 3.177542 0.605182
C -2.548648 2.185054 -1.580554
C -4.213086 3.118327 0.449918
H -2.403147 3.630164 1.498890
C -3.926842 2.108181 -1.724567
H -1.889134 1.831251 -2.374215
C -4.760821 2.570131 -0.707251
H -4.863185 3.513188 1.228249
H -4.355057 1.699154 -2.637343
H -5.841371 2.525057 -0.828375
C 0.142782 2.612818 0.942418
H 1.173152 2.950510 1.046192
H -0.401992 2.446524 1.874023
H 0.036096 3.018315 -1.145937

22

Zero-point correction= 0.273936 (Hartree/Particle)
Thermal correction to Energy= 0.292016
Thermal correction to Enthalpy= 0.292960
Thermal correction to Gibbs Free Energy= 0.225956
Sum of electronic and zero-point Energies= -1042.224279
Sum of electronic and thermal Energies= -1042.206199
Sum of electronic and thermal Enthalpies= -1042.205255
Sum of electronic and thermal Free Energies= -1042.272258
HF = -1042.4982148

Single Point Energy Calculations with extended basis set:
HF = -1044.8273152

Optimised Geometry:
Charge = 1 Multiplicity = 1
C -2.248487 -1.119473 -0.068032
H 4.567839 3.131074 0.040270
C 4.024171 2.187831 0.047460
C 2.599814 2.225061 -0.080377
C 4.683891 1.006835 0.169007
C 1.867770 1.019284 -0.058482
C 1.879734 3.424070 -0.241385
C 3.972600 -0.233658 0.160978
H 5.768286 0.982936 0.264070
N 0.510799 0.998758 -0.158958
C 2.568181 -0.229215 0.046186
C 0.511839 3.382631 -0.384197
H 2.416688 4.371485 -0.262758
C 4.610049 -1.487101 0.251869

C -0.138159 2.143043 -0.336039
N 1.839928 -1.370790 0.007487
H -0.071580 4.287457 -0.529732
C 3.858226 -2.638930 0.217215
H 5.694565 -1.529216 0.344645
H -1.218573 2.076943 -0.449513
C 2.464812 -2.535385 0.089826
H 4.321491 -3.619502 0.282020
H 1.838966 -3.425839 0.051458
Pd -0.322275 -0.958323 -0.081888
C -3.465682 -0.355158 0.053469
C -4.667271 -0.907017 -0.418983
C -3.444731 0.905747 0.663110
C -5.837718 -0.175525 -0.300145
H -4.661987 -1.893793 -0.877872
C -4.626359 1.617494 0.798342
H -2.508712 1.287656 1.069446
C -5.815677 1.080668 0.306447
H -6.773990 -0.585953 -0.670972
H -4.627780 2.587517 1.289736
H -6.740652 1.645431 0.404413
O -2.052128 -2.312041 -0.203208

23
Zero-point correction= 0.273115 (Hartree/Particle)
Thermal correction to Energy= 0.291495
Thermal correction to Enthalpy= 0.292439
Thermal correction to Gibbs Free Energy= 0.224834
Sum of electronic and zero-point Energies= -1042.230170
Sum of electronic and thermal Energies= -1042.211790
Sum of electronic and thermal Enthalpies= -1042.210846
Sum of electronic and thermal Free Energies= -1042.278451
HF = -1042.5032851

Single Point Energy Calculations with extended basis set:
HF = -1044.8286632

Optimised Geometry:
Charge = 1 Multiplicity = 1
C -2.096377 -1.811036 -0.168010
H 5.564843 -0.387574 0.253550
C 4.549195 -0.000582 0.188829
C 3.468831 -0.935270 0.116994
C 4.315385 1.337470 0.176831
C 2.144145 -0.461056 0.032570
C 3.661713 -2.331350 0.126087
C 2.982414 1.848710 0.091245
H 5.139920 2.046466 0.232085
N 1.088291 -1.311136 -0.036121
C 1.893915 0.955150 0.018220

C 2.576477 -3.174612 0.054348
H 4.674025 -2.728528 0.190141
C 2.691198 3.227115 0.075768
C 1.291289 -2.620161 -0.025927
N 0.610283 1.383410 -0.065356
H 2.695532 -4.254461 0.059070
C 1.383941 3.648885 -0.008227
H 3.508330 3.945440 0.130835
H 0.400747 -3.248522 -0.082799
C 0.367484 2.684744 -0.077686
H 1.129731 4.705169 -0.021427
H -0.680029 2.979171 -0.145058
Pd -0.822152 -0.347016 -0.151805
C -3.059601 -0.702498 -0.063877
C -3.694541 -0.433429 1.170969
C -3.105761 0.247190 -1.112646
C -4.419837 0.731353 1.315520
H -3.624016 -1.159915 1.978474
C -3.829735 1.430188 -0.930436
H -2.679303 0.005534 -2.086337
C -4.482498 1.663438 0.269294
H -4.945532 0.927402 2.247245
H -3.896593 2.149170 -1.743681
H -5.058336 2.577118 0.401391
O -2.015774 -2.990643 -0.152413

TS23-24
Zero-point correction= 0.271295 (Hartree/Particle)
Thermal correction to Energy= 0.289438
Thermal correction to Enthalpy= 0.290382
Thermal correction to Gibbs Free Energy= 0.223586
Sum of electronic and zero-point Energies= -1042.219133
Sum of electronic and thermal Energies= -1042.200990
Sum of electronic and thermal Enthalpies= -1042.200046
Sum of electronic and thermal Free Energies= -1042.266842
HF = -1042.4904284

Single Point Energy Calculations with extended basis set:
HF = -1044.8223253

Optimised Geometry:
Charge = 1 Multiplicity = 1
C -1.997931 -2.061628 -0.000164
H 5.621483 0.533517 -0.000589
C 4.543545 0.686717 -0.000372
C 3.693679 -0.464556 -0.000187
C 4.022366 1.941841 -0.000271
C 2.295794 -0.291915 -0.000024
C 4.182960 -1.785954 -0.000138
C 2.606685 2.148417 0.000030

H 4.674316 2.813848 -0.000412
N 1.434280 -1.342360 0.000083
C 1.746542 1.033306 0.000097
C 3.299207 -2.841080 0.000073
H 5.258547 -1.957972 -0.000243
C 2.007290 3.424102 0.000275
C 1.922628 -2.575379 0.000148
N 0.397183 1.159642 0.000317
H 3.646075 -3.870587 0.000167
C 0.634860 3.536751 0.000577
H 2.639591 4.311169 0.000233
H 1.196252 -3.386010 0.000275
C -0.142358 2.369306 0.000564
H 0.147959 4.507955 0.000798
H -1.232244 2.413581 0.000756
Pd -0.647517 -0.749344 -0.000027
C -2.684442 -0.288143 -0.000227
C -3.236489 0.117201 1.219420
C -3.235967 0.117825 -1.219860
C -4.331079 0.974531 1.211248
H -2.817145 -0.235398 2.160869
C -4.330552 0.975168 -1.211698
H -2.816232 -0.234274 -2.161280
C -4.871131 1.403129 -0.000254
H -4.769366 1.301697 2.151796
H -4.768445 1.302796 -2.152232
H -5.733045 2.067371 -0.000269
O -2.604480 -3.042083 0.000395
Imaginary Vibrational Frequency = -205.2024 cm^{-1}

24
Zero-point correction= 0.271574 (Hartree/Particle)
Thermal correction to Energy= 0.290457
Thermal correction to Enthalpy= 0.291402
Thermal correction to Gibbs Free Energy= 0.222635
Sum of electronic and zero-point Energies= -1042.228522
Sum of electronic and thermal Energies= -1042.209639
Sum of electronic and thermal Enthalpies= -1042.208695
Sum of electronic and thermal Free Energies= -1042.277461
HF = -1042.5000966

Single Point Energy Calculations with extended basis set:
HF = -1044.8388553

Optimised Geometry:
Charge = 1 Multiplicity = 1
C 1.557777 2.543635 -0.000301
H -5.496223 -0.975823 -0.000513
C -4.408465 -1.020888 -0.000338
C -3.675740 0.206888 -0.000124

C	-3.762776	-2.215922	-0.000316
C	-2.266433	0.176750	0.000100
C	-4.298253	1.470954	-0.000132
C	-2.334009	-2.278819	-0.000080
H	-4.321231	-3.150459	-0.000484
N	-1.519276	1.310694	0.000300
C	-1.584978	-1.085047	0.000122
C	-3.528782	2.611354	0.000093
H	-5.385874	1.530194	-0.000319
C	-1.622234	-3.494895	-0.000033
C	-2.132487	2.485644	0.000308
N	-0.223128	-1.090544	0.000338
H	-3.979522	3.599821	0.000114
C	-0.246866	-3.481147	0.000225
H	-2.172326	-4.435059	-0.000199
H	-1.496027	3.369298	0.000530
C	0.422882	-2.250317	0.000399
H	0.329554	-4.401872	0.000291
H	1.511173	-2.200934	0.000603
Pd	0.639741	0.859253	0.000101
C	2.518216	0.112942	-0.000037
C	3.108462	-0.211130	1.216131
C	3.108108	-0.211526	-1.216271
C	4.308340	-0.924102	1.206661
H	2.646427	0.069323	2.162393
C	4.307993	-0.924495	-1.206921
H	2.645792	0.068591	-2.162494
C	4.902067	-1.282511	-0.000159
H	4.779578	-1.192553	2.150574
H	4.778951	-1.193238	-2.150889
H	5.839644	-1.834486	-0.000199
O	2.106488	3.539539	-0.000563

CO

opt freq M06/gen pseudo=read scf=maxcycle=500 test
normal termination

Zero-point correction= 0.005062 (Hartree/Particle)
Thermal correction to Energy= 0.007423
Thermal correction to Enthalpy= 0.008367
Thermal correction to Gibbs Free Energy= -0.014075
Sum of electronic and zero-point Energies= -113.243570
Sum of electronic and thermal Energies= -113.241209
Sum of electronic and thermal Enthalpies= -113.240265
Sum of electronic and thermal Free Energies= -113.262707
HF = -113.2486321

Single Point Energy Calculations with extended basis set:
HF = -113.363238

Optimised Geometry:
Charge = 0 Multiplicity = 1
C -0.000000 0.000000 -0.649960
O 0.000000 -0.000000 0.487470

PhCHCH2
Zero-point correction= 0.132871 (Hartree/Particle)
Thermal correction to Energy= 0.139698
Thermal correction to Enthalpy= 0.140642
Thermal correction to Gibbs Free Energy= 0.101364
Sum of electronic and zero-point Energies= -309.249493
Sum of electronic and thermal Energies= -309.242666
Sum of electronic and thermal Enthalpies= -309.241721
Sum of electronic and thermal Free Energies= -309.281000
HF = -309.3823638

Single Point Energy Calculations with extended basis set:
HF = -309.7940662

Optimised Geometry:
Charge = 0 Multiplicity = 1
C 1.945330 -0.532983 0.000018
C 0.512571 -0.224652 0.000011
C 0.015477 1.085526 0.000016
C -0.407661 -1.279072 0.000002
C -1.350169 1.327567 0.000006
H 0.708121 1.926446 0.000032
C -1.776878 -1.039719 -0.000014
H -0.035048 -2.304285 0.000005
C -2.253926 0.266212 -0.000010
H -1.715663 2.353446 0.000015
H -2.472957 -1.877138 -0.000026
H -3.325375 0.459235 -0.000019
C 2.958564 0.335966 -0.000026
H 2.810148 1.415299 -0.000077
H 3.990917 -0.005199 -0.000016
H 2.180009 -1.600873 0.000065

PhCMe (carbene)
Zero-point correction= 0.130377 (Hartree/Particle)
Thermal correction to Energy= 0.137525
Thermal correction to Enthalpy= 0.138470
Thermal correction to Gibbs Free Energy= 0.099067
Sum of electronic and zero-point Energies= -309.152703
Sum of electronic and thermal Energies= -309.145554
Sum of electronic and thermal Enthalpies= -309.144610
Sum of electronic and thermal Free Energies= -309.184013
HF = -309.2830794

Single Point Energy Calculations with extended basis set:

HF = -309.6896205

Optimised Geometry:
Charge = 0 Multiplicity = 1

C	1.881786	-0.673227	-0.321116
C	0.507233	-0.272463	-0.155164
C	0.044622	1.062699	-0.143128
C	-0.450083	-1.304665	-0.053062
C	-1.309476	1.343392	-0.045227
H	0.757045	1.879554	-0.254262
C	-1.794124	-1.021610	0.129617
H	-0.085899	-2.329466	-0.108828
C	-2.225930	0.304466	0.116224
H	-1.658129	2.374742	-0.073300
H	-2.515882	-1.828860	0.241632
H	-3.286963	0.530073	0.214738
C	2.883453	0.245833	0.240118
H	3.818475	0.256035	-0.336332
H	2.591775	1.277416	0.522066
H	3.154699	-0.266054	1.184713

MePhC=C=O

Zero-point correction= 0.142878 (Hartree/Particle)
Thermal correction to Energy= 0.151750
Thermal correction to Enthalpy= 0.152695
Thermal correction to Gibbs Free Energy= 0.108389
Sum of electronic and zero-point Energies= -422.509045
Sum of electronic and thermal Energies= -422.500173
Sum of electronic and thermal Enthalpies= -422.499229
Sum of electronic and thermal Free Energies= -422.543534
HF = -422.6519232

Single Point Energy Calculations with extended basis set:
HF = -423.16952

Optimised Geometry:
Charge = 0 Multiplicity = 1

C	-2.222975	-0.592029	0.000121
C	-1.357996	0.409315	0.000129
C	0.087167	0.140481	-0.000012
C	0.594325	-1.168046	-0.000109
C	0.998797	1.202177	-0.000037
C	1.959985	-1.402690	-0.000244
H	-0.094107	-2.015077	-0.000078
C	2.369496	0.961768	-0.000166
H	0.637991	2.229493	0.000048
C	2.859716	-0.337950	-0.000273
H	2.326861	-2.428021	-0.000321
H	3.058162	1.805576	-0.000182
H	3.932160	-0.523123	-0.000374

O -2.994579 -1.470821 0.000128
C -1.911863 1.812043 0.000361
H -1.578304 2.365472 0.889313
H -1.578711 2.365603 -0.888661
H -3.007326 1.816222 0.000608

Solution phase (DMSO)

28a1
Zero-point correction= 0.409358 (Hartree/Particle)
Thermal correction to Energy= 0.445066
Thermal correction to Enthalpy= 0.446010
Thermal correction to Gibbs Free Energy= 0.336892
Sum of electronic and zero-point Energies= -2088.479204
Sum of electronic and thermal Energies= -2088.443497
Sum of electronic and thermal Enthalpies= -2088.442553
Sum of electronic and thermal Free Energies= -2088.551671
HF = -2088.8885624

Single Point Energy Calculations with extended basis set:
HF = -2091.8895052

Optimised Geometry:
Charge = 0 Multiplicity = 1
C 1.582365 -0.246526 -1.616580
Pd -1.042720 0.366720 -0.405711
C -0.794601 -1.595958 -0.264094
C -1.494012 -2.463683 -1.109547
C 0.152159 -2.114594 0.625615
C -1.240803 -3.840219 -1.078240
C 0.406280 -3.490485 0.672791
C -0.293710 -4.331365 -0.185743
H -1.771630 -4.525281 -1.734217
H 1.136553 -3.905355 1.362860
H -0.096800 -5.401739 -0.157182
O -2.412765 -1.885439 -1.929547
O 0.778523 -1.206124 1.428720
C 1.794064 -1.678299 2.292616
H 2.605469 -2.161871 1.727228
H 2.193868 -0.799074 2.804110
H 1.391493 -2.382604 3.035186
C -3.142124 -2.724196 -2.801218
H -3.815822 -2.071884 -3.361622
H -2.478816 -3.247672 -3.504247
H -3.735139 -3.464121 -2.245372
O -1.241186 2.524981 -0.632608
O -2.680948 0.383327 0.873949
C -0.221025 3.133365 -0.193558
O 0.793557 2.687117 0.340420

C -0.334633 4.661242 -0.388861
S -3.156916 -0.936396 1.566836
C -2.185997 -1.007260 3.082622
H -2.322944 -0.074494 3.640472
H -2.508772 -1.871190 3.673247
H -1.136929 -1.119091 2.785318
C -4.714737 -0.386644 2.278830
H -5.422616 -0.242121 1.458352
H -5.085219 -1.159802 2.959877
H -4.544909 0.555997 2.810093
F -1.406342 5.143050 0.254973
F 0.733202 5.317204 0.061911
F -0.478538 4.966281 -1.685450
C 2.618322 -1.009809 -1.365997
C 3.651377 -0.571901 -0.411886
C 3.513127 0.625081 0.308193
C 4.768768 -1.380140 -0.178758
C 4.471067 0.993035 1.241922
H 2.638572 1.263741 0.155389
C 5.721888 -1.006291 0.764906
H 4.895843 -2.311225 -0.728374
C 5.578070 0.177951 1.479290
H 4.348827 1.922053 1.796488
H 6.582586 -1.649722 0.939380
H 6.323503 0.467358 2.217625
O 0.623761 0.419836 -1.828602
C 2.636892 -2.370712 -2.020027
H 3.507672 -2.479725 -2.678902
H 2.679337 -3.147607 -1.243949
H 1.732805 -2.545319 -2.613664

28a2

Zero-point correction= 0.409288 (Hartree/Particle)
Thermal correction to Energy= 0.444686
Thermal correction to Enthalpy= 0.445630
Thermal correction to Gibbs Free Energy= 0.338626
Sum of electronic and zero-point Energies= -2088.501500
Sum of electronic and thermal Energies= -2088.466102
Sum of electronic and thermal Enthalpies= -2088.465158
Sum of electronic and thermal Free Energies= -2088.572162
HF = -2088.9107877

Single Point Energy Calculations with extended basis set:
HF = -2091.9079311

Optimised Geometry:
Charge = 0 Multiplicity = 1
C -0.615777 0.707814 2.019168
Pd 0.225227 -0.189382 -0.020407
C 2.033364 0.618894 0.240048

C	2.510287	1.524794	-0.712089
C	2.866737	0.245304	1.296694
C	3.791718	2.072667	-0.604597
C	4.157317	0.776893	1.414654
C	4.598077	1.688447	0.462301
H	4.167508	2.779513	-1.339953
H	4.812507	0.491499	2.233586
H	5.598849	2.107900	0.550810
O	1.652489	1.818903	-1.731719
O	2.354315	-0.673436	2.166682
C	3.128315	-1.022692	3.295006
H	3.364030	-0.142216	3.909018
H	2.520785	-1.717781	3.879507
H	4.065542	-1.520215	3.003126
C	2.004404	2.866481	-2.611109
H	1.155120	2.998488	-3.286715
H	2.181005	3.803358	-2.062152
H	2.898069	2.619817	-3.201433
O	-1.663420	-1.193508	-0.491950
O	1.058094	-1.777612	-1.204057
C	-2.485403	-1.319087	0.454192
O	-2.387362	-0.961248	1.632167
C	-3.811776	-1.963654	0.004481
S	2.577793	-1.837610	-1.524467
C	3.262303	-2.894542	-0.234781
H	2.740330	-3.857964	-0.240887
H	4.335143	-3.026806	-0.409463
H	3.090504	-2.379627	0.716938
C	2.614722	-3.029511	-2.872827
H	2.173848	-2.550745	-3.751373
H	3.655303	-3.301416	-3.078453
H	2.029431	-3.908633	-2.582009
F	-3.602180	-3.085045	-0.693066
F	-4.610956	-2.265734	1.025335
F	-4.471903	-1.111471	-0.791681
C	-0.718215	1.523298	0.904493
C	-2.013883	1.774052	0.199347
C	-3.234825	1.782015	0.877071
C	-1.981481	2.118245	-1.155695
C	-4.409974	2.092962	0.199637
H	-3.267475	1.532473	1.936327
C	-3.156257	2.432567	-1.828788
H	-1.024571	2.121333	-1.679959
C	-4.374979	2.415375	-1.153767
H	-5.356984	2.088534	0.736615
H	-3.119851	2.689766	-2.886007
H	-5.295430	2.658514	-1.681619
O	-0.372507	0.316498	3.084788
C	0.124970	2.791363	1.087135
H	1.024093	2.619477	1.688080

H 0.435146 3.164711 0.104606
H -0.493415 3.556699 1.575610

TS28a1-29a1
Zero-point correction= 0.409599 (Hartree/Particle)
Thermal correction to Energy= 0.444099
Thermal correction to Enthalpy= 0.445044
Thermal correction to Gibbs Free Energy= 0.340415
Sum of electronic and zero-point Energies= -2088.459476
Sum of electronic and thermal Energies= -2088.424976
Sum of electronic and thermal Enthalpies= -2088.424032
Sum of electronic and thermal Free Energies= -2088.528660
HF = -2088.8690756

Single Point Energy Calculations with extended basis set:
HF = -2091.8706084

Optimised Geometry:
Charge = 0 Multiplicity = 1
C 1.902117 0.325211 0.534534
Pd -0.637535 0.182156 -0.204522
C 0.531627 -1.423378 0.135921
C 1.036212 -2.142683 -0.971291
C 0.434650 -2.067511 1.389118
C 1.402682 -3.482528 -0.837056
C 0.827922 -3.402051 1.532861
C 1.286541 -4.086850 0.411898
H 1.775802 -4.055543 -1.681130
H 0.758526 -3.913551 2.488565
H 1.573663 -5.131515 0.517606
O 1.121735 -1.453081 -2.124002
O -0.088425 -1.329600 2.393130
C -0.173490 -1.915040 3.682346
H 0.817399 -2.213083 4.048708
H -0.587709 -1.145332 4.336285
H -0.841975 -2.787195 3.676400
C 1.673445 -2.103653 -3.256008
H 1.682162 -1.361992 -4.056940
H 2.700154 -2.440006 -3.057895
H 1.058664 -2.961094 -3.559934
O -1.827454 1.940559 -0.535163
O -2.148108 -0.909271 -1.141423
C -2.817107 2.032448 0.254248
O -3.138010 1.327498 1.206337
C -3.704196 3.247434 -0.097779
S -2.442317 -2.332801 -0.568072
C -3.218004 -2.032807 1.030838
H -3.952345 -1.227888 0.914938
H -3.677882 -2.961945 1.383856
H -2.428131 -1.712894 1.719536

C -3.918414 -2.765463 -1.499297
H -3.626408 -2.871501 -2.547526
H -4.310583 -3.715664 -1.123131
H -4.653352 -1.961771 -1.383861
F -4.162902 3.155818 -1.353348
F -4.758915 3.361804 0.707071
F -3.004794 4.386908 -0.011617
C 3.199093 0.058655 0.405231
C 4.081723 1.235412 0.190821
C 3.680289 2.552516 0.463020
C 5.378975 1.032269 -0.303258
C 4.541300 3.620166 0.245716
H 2.685698 2.748178 0.860942
C 6.238817 2.104946 -0.516674
H 5.723216 0.025618 -0.531691
C 5.827305 3.405424 -0.245287
H 4.203948 4.630851 0.470469
H 7.239854 1.916329 -0.901825
H 6.501145 4.243774 -0.411611
O 0.986355 1.110993 0.722795
C 3.787550 -1.318834 0.417091
H 4.049564 -1.666529 -0.593808
H 4.707075 -1.325216 1.016320
H 3.101744 -2.046060 0.858589
Imaginary Vibrational Frequency = -338.9697 cm^{-1}

TS28a2-29a2
Zero-point correction= 0.409199 (Hartree/Particle)
Thermal correction to Energy= 0.443954
Thermal correction to Enthalpy= 0.444898
Thermal correction to Gibbs Free Energy= 0.340204
Sum of electronic and zero-point Energies= -2088.491886
Sum of electronic and thermal Energies= -2088.457131
Sum of electronic and thermal Enthalpies= -2088.456187
Sum of electronic and thermal Free Energies= -2088.560881
HF = -2088.9010854

Single Point Energy Calculations with extended basis set:
HF = -2091.8940544

Optimised Geometry:
Charge = 0 Multiplicity = 1
C 1.449927 -2.072465 -0.746629
Pd 0.362375 0.291325 -0.235304
C 2.309572 -0.209228 0.069509
C 2.710289 -0.638578 1.349276
C 3.301077 0.168908 -0.854699
C 4.057956 -0.699908 1.701804
C 4.656087 0.105878 -0.516060

C	5.010085	-0.327059	0.756880
H	4.373493	-1.028726	2.688256
H	5.430442	0.391554	-1.222640
H	6.064744	-0.376149	1.022725
O	2.858102	0.569296	-2.072842
C	3.816606	0.868514	-3.069660
H	4.464608	0.005323	-3.274352
H	3.250528	1.117173	-3.970147
H	4.435981	1.729026	-2.782504
O	1.702597	-1.021187	2.173128
C	2.038969	-1.629649	3.405776
H	2.555026	-0.925712	4.072601
H	1.093327	-1.931212	3.863121
H	2.669527	-2.516410	3.252119
O	-1.700392	0.779435	-0.738733
O	0.704678	2.244691	0.700297
C	-2.559567	0.563316	0.166958
O	-2.406143	0.321687	1.363300
C	-4.005480	0.726195	-0.349179
S	-0.293224	3.365693	0.318276
C	-1.394160	3.497432	1.739458
H	-0.795934	3.661545	2.643054
H	-2.094072	4.324155	1.577751
H	-1.933922	2.546628	1.812411
C	0.665520	4.861771	0.613016
H	1.444362	4.914611	-0.152615
H	0.005387	5.731766	0.533661
H	1.114398	4.801379	1.610563
F	-4.184200	0.181736	-1.557601
F	-4.903845	0.182301	0.470378
F	-4.290366	2.034928	-0.453586
C	0.189303	-1.578240	-1.136591
C	-0.945194	-2.304368	-0.472181
C	-2.204849	-2.308705	-1.079686
C	-0.789985	-2.949890	0.761634
C	-3.285682	-2.924870	-0.456444
H	-2.355077	-1.809245	-2.033531
C	-1.867343	-3.580643	1.370151
H	0.175237	-2.937147	1.269636
C	-3.123636	-3.565597	0.767978
H	-4.262470	-2.896994	-0.937385
H	-1.724844	-4.077958	2.327972
H	-3.969927	-4.049561	1.251619
O	2.262582	-2.882375	-0.574250
C	0.112549	-1.315348	-2.641039
H	-0.701698	-0.613643	-2.850268
H	1.041337	-0.867974	-3.007471
H	-0.076077	-2.252316	-3.184542

Imaginary Vibrational Frequency = -378.3940 cm^{-1}

29a1

Zero-point correction= 0.412585 (Hartree/Particle)
Thermal correction to Energy= 0.446750
Thermal correction to Enthalpy= 0.447695
Thermal correction to Gibbs Free Energy= 0.344095
Sum of electronic and zero-point Energies= -2088.506657
Sum of electronic and thermal Energies= -2088.472492
Sum of electronic and thermal Enthalpies= -2088.471548
Sum of electronic and thermal Free Energies= -2088.575147
HF = -2088.9192422

Single Point Energy Calculations with extended basis set:
HF = -2091.9147924

Optimised Geometry:
Charge = 0 Multiplicity = 1

C	-1.916202	-0.264612	0.021623
Pd	0.636465	-0.090901	-0.009276
C	-1.004553	-1.443865	0.300377
C	-0.731235	-1.833990	1.656976
C	-0.689647	-2.376025	-0.748131
C	-0.068526	-3.027576	1.929358
C	-0.024243	-3.565085	-0.459521
C	0.273205	-3.860419	0.868002
H	0.167207	-3.323009	2.946799
H	0.238737	-4.269024	-1.243120
H	0.787437	-4.794690	1.087330
O	-1.101918	-2.017103	-1.965367
C	-0.669465	-2.789335	-3.077653
H	-1.079230	-3.805918	-3.034482
H	-1.050941	-2.279309	-3.963440
H	0.427416	-2.829808	-3.116661
O	-1.179206	-0.987328	2.585161
C	-0.856941	-1.241912	3.946435
H	0.230528	-1.271264	4.089405
H	-1.280289	-0.411948	4.514009
H	-1.304351	-2.184533	4.284763
O	1.869416	1.558518	-0.510206
O	2.385804	-1.193188	0.279561
C	2.131500	2.287147	0.503809
O	1.786734	2.161442	1.670603
C	3.016842	3.489909	0.109428
S	3.229687	-1.305081	-1.028683
C	4.717448	-0.364512	-0.659870
H	5.106732	-0.684249	0.313015
H	5.453536	-0.532794	-1.452808
H	4.426011	0.689494	-0.635060
C	3.905953	-2.965540	-0.889570
H	3.079177	-3.666109	-1.037857
H	4.664902	-3.110379	-1.665022

H 4.336012 -3.084760 0.110748
F 2.390261 4.263407 -0.783031
F 3.333913 4.246713 1.154469
F 4.161813 3.076072 -0.454487
C -3.272145 -0.338490 0.007592
C -4.149760 0.807552 -0.268517
C -3.668481 2.109390 -0.517042
C -5.547119 0.633983 -0.293065
C -4.535189 3.164161 -0.774490
H -2.597302 2.288323 -0.505968
C -6.411735 1.691856 -0.551468
H -5.974707 -0.349263 -0.107681
C -5.914389 2.968101 -0.795139
H -4.123708 4.155841 -0.961353
H -7.486337 1.512166 -0.561580
H -6.589877 3.797768 -0.997405
O -1.141749 0.795959 -0.196785
C -3.919704 -1.666961 0.286890
H -4.595994 -1.618139 1.153743
H -4.521949 -2.017604 -0.565203
H -3.185595 -2.452853 0.501022

29a2

Zero-point correction= 0.410992 (Hartree/Particle)
Thermal correction to Energy= 0.445048
Thermal correction to Enthalpy= 0.445992
Thermal correction to Gibbs Free Energy= 0.343979
Sum of electronic and zero-point Energies= -2088.533940
Sum of electronic and thermal Energies= -2088.499884
Sum of electronic and thermal Enthalpies= -2088.498939
Sum of electronic and thermal Free Energies= -2088.600953
HF = -2088.9449319

Single Point Energy Calculations with extended basis set:
HF = -2091.9297115

Optimised Geometry:
Charge = 0 Multiplicity = 1
C -0.965831 -2.379164 0.875075
Pd -0.364850 0.060770 0.097303
C -1.945747 -1.493065 0.111386
C -2.038719 -1.621011 -1.306277
C -2.949411 -0.740894 0.791879
C -2.999606 -0.909757 -2.020654
C -3.900860 -0.024044 0.068387
C -3.905978 -0.122092 -1.320710
H -3.053352 -0.979517 -3.103197
H -4.649940 0.579092 0.573221
H -4.661847 0.427473 -1.878953
O -2.911364 -0.818489 2.130316

C	-3.679231	0.112420	2.880109
H	-4.753764	-0.067155	2.752383
H	-3.406204	-0.044952	3.925240
H	-3.433366	1.141015	2.583524
O	-1.163815	-2.474401	-1.859761
C	-0.802433	-2.277906	-3.219408
H	-0.524482	-1.228274	-3.389957
H	0.062598	-2.921769	-3.397343
H	-1.615528	-2.565974	-3.896720
O	1.375780	1.238537	0.594470
O	-1.172038	1.822388	-1.073756
C	2.214921	1.270734	-0.359125
O	2.157903	0.781510	-1.482169
C	3.481639	2.060800	0.038212
S	-1.663376	2.902581	-0.091931
C	-0.301732	4.081864	0.013687
H	-0.020179	4.391285	-0.999742
H	-0.608148	4.943505	0.616144
H	0.529155	3.553994	0.492974
C	-2.784383	3.904729	-1.086567
H	-3.677117	3.304394	-1.285598
H	-3.057861	4.805892	-0.527984
H	-2.281493	4.162806	-2.025461
F	4.096771	1.480750	1.078271
F	4.364669	2.145887	-0.953884
F	3.169011	3.310967	0.409001
C	0.256322	-1.561176	1.199069
C	1.549407	-2.027607	0.632222
C	1.605421	-2.952374	-0.424321
C	2.761981	-1.502631	1.108447
C	2.819577	-3.310255	-0.998292
H	0.688793	-3.396220	-0.805152
C	3.973465	-1.858382	0.530640
H	2.759293	-0.778283	1.919009
C	4.010140	-2.760612	-0.530206
H	2.833233	-4.028111	-1.817317
H	4.896010	-1.422278	0.911056
H	4.960057	-3.038124	-0.983697
O	-1.164964	-3.542003	1.139340
C	0.262797	-1.134642	2.656752
H	0.576240	-1.979782	3.290697
H	0.953395	-0.301934	2.828272
H	-0.734876	-0.822184	2.983711

30a

Zero-point correction= 0.411398 (Hartree/Particle)
Thermal correction to Energy= 0.446287
Thermal correction to Enthalpy= 0.447232
Thermal correction to Gibbs Free Energy= 0.340828

Sum of electronic and zero-point Energies= -2088.528733
Sum of electronic and thermal Energies= -2088.493843
Sum of electronic and thermal Enthalpies= -2088.492899
Sum of electronic and thermal Free Energies= -2088.599303
HF = -2088.9401304

Single Point Energy Calculations with extended basis set:
HF = -2091.9288204

Optimised Geometry:
Charge = 0 Multiplicity = 1

C	-1.653815	0.079140	-0.664211
Pd	0.430789	0.148333	0.029718
C	-2.552659	-1.096259	-0.650067
C	-2.069469	-2.409098	-0.779592
C	-3.934517	-0.877426	-0.525829
C	-2.957665	-3.486883	-0.774563
C	-4.827588	-1.948950	-0.530694
C	-4.320045	-3.237303	-0.655387
H	-2.600073	-4.508397	-0.862507
H	-5.898430	-1.790568	-0.445640
H	-5.011355	-4.078093	-0.659758
O	-4.303064	0.420269	-0.426886
C	-5.678480	0.716403	-0.272129
H	-6.083842	0.258518	0.640194
H	-5.746997	1.803422	-0.193826
H	-6.257837	0.376959	-1.141172
O	-0.728454	-2.539624	-0.861690
C	-0.174477	-3.841891	-0.869264
H	-0.489617	-4.404553	-1.758085
H	0.909737	-3.708551	-0.892687
H	-0.454309	-4.398259	0.035546
O	2.407229	-0.548498	-0.591773
O	1.152584	0.074357	2.033473
C	3.050105	0.342943	-1.227382
O	2.711385	1.477253	-1.550203
C	4.470170	-0.135121	-1.601841
S	1.732753	-1.330093	2.374002
C	3.504917	-1.049568	2.513888
H	3.674900	-0.180036	3.158586
H	3.979335	-1.945142	2.928875
H	3.870438	-0.860036	1.500016
C	1.338060	-1.479643	4.122792
H	0.250838	-1.570864	4.202438
H	1.820384	-2.375953	4.525690
H	1.685229	-0.579205	4.641067
F	4.433380	-1.285234	-2.283439
F	5.131629	0.751778	-2.340171
F	5.194261	-0.353964	-0.490787
C	-1.472126	0.937833	0.499289

C -1.262254 2.394380 0.308512
C -1.816847 3.070349 -0.787404
C -0.543480 3.133525 1.260118
C -1.651494 4.442862 -0.928335
H -2.394701 2.514898 -1.523762
C -0.372617 4.504405 1.111979
H -0.093692 2.620851 2.110120
C -0.926849 5.164371 0.017505
H -2.097368 4.953546 -1.780127
H 0.196709 5.060116 1.854962
H -0.798186 6.239268 -0.095674
O -0.884829 0.308126 -1.659814
C -2.014320 0.495724 1.827524
H -1.420997 0.907767 2.651495
H -3.048311 0.852760 1.947348
H -2.011737 -0.597345 1.921073

28b1
Zero-point correction= 0.463195 (Hartree/Particle)
Thermal correction to Energy= 0.501702
Thermal correction to Enthalpy= 0.502647
Thermal correction to Gibbs Free Energy= 0.388396
Sum of electronic and zero-point Energies= -2280.011391
Sum of electronic and thermal Energies= -2279.972884
Sum of electronic and thermal Enthalpies= -2279.971939
Sum of electronic and thermal Free Energies= -2280.086190
HF = -2280.474586

Single Point Energy Calculations with extended basis set:
HF = -2283.7179276

Optimised Geometry:
Charge = 0 Multiplicity = 1
C 1.216733 0.971630 -1.003028
Pd -1.390082 -0.443562 -0.496092
C 0.003104 -1.675662 0.190033
C 0.297930 -2.877056 -0.464057
C 0.745929 -1.301680 1.315853
C 1.339393 -3.694236 -0.006696
C 1.783636 -2.115678 1.785605
C 2.064934 -3.299481 1.112756
H 1.585958 -4.625743 -0.509841
H 2.370843 -1.837057 2.656259
H 2.874903 -3.933234 1.469710
O -0.486012 -3.184543 -1.531555
O 0.388861 -0.122574 1.903389
C 1.048803 0.242233 3.100916
H 2.123031 0.404062 2.931388
H 0.593199 1.180186 3.427148
H 0.909104 -0.523553 3.878012

C	-0.175351	-4.353916	-2.260958
H	-0.902276	-4.410823	-3.074283
H	0.838508	-4.302700	-2.683084
H	-0.261031	-5.254406	-1.636976
O	-2.845039	0.979886	-1.269860
O	-2.937936	-1.553626	0.336489
C	-2.669403	2.130841	-0.769898
O	-1.853120	2.508838	0.069693
C	-3.668758	3.159826	-1.342436
S	-2.607291	-2.651162	1.402282
C	-2.427225	-1.727725	2.938123
H	-3.327219	-1.125740	3.104750
H	-2.265552	-2.431179	3.761526
H	-1.552940	-1.077295	2.815821
C	-4.248135	-3.329035	1.688398
H	-4.531504	-3.900068	0.800280
H	-4.209995	-3.989839	2.560453
H	-4.947000	-2.501985	1.852797
F	-4.928835	2.792348	-1.071972
F	-3.490653	4.382081	-0.844937
F	-3.555744	3.245674	-2.674832
C	2.410243	1.210201	-0.501899
C	2.548577	2.158640	0.622938
C	1.493104	3.011600	0.978003
C	3.721736	2.173676	1.384219
C	1.616053	3.858012	2.071616
H	0.562425	3.004664	0.405050
C	3.839712	3.030755	2.474374
H	4.541180	1.504271	1.127879
C	2.790150	3.874549	2.823453
H	0.787797	4.512794	2.336925
H	4.759325	3.031452	3.056970
H	2.884501	4.543695	3.676488
O	0.150875	0.767907	-1.474644
C	3.526729	0.438125	-1.113245
C	4.701348	1.085516	-1.514109
C	3.395925	-0.937846	-1.323431
C	5.730777	0.358940	-2.100683
H	4.803319	2.160358	-1.369025
C	4.423259	-1.657697	-1.924000
H	2.485572	-1.446656	-1.004929
C	5.594648	-1.013040	-2.309408
H	6.642530	0.869650	-2.405094
H	4.305940	-2.729652	-2.078537
H	6.402765	-1.575737	-2.773022

28b2

Zero-point correction= 0.464164 (Hartree/Particle)
Thermal correction to Energy= 0.501856
Thermal correction to Enthalpy= 0.502801

Thermal correction to Gibbs Free Energy= 0.393165
Sum of electronic and zero-point Energies= -2280.025855
Sum of electronic and thermal Energies= -2279.988162
Sum of electronic and thermal Enthalpies= -2279.987218
Sum of electronic and thermal Free Energies= -2280.096853
HF = -2280.4900182

Single Point Energy Calculations with extended basis set:
HF = -2283.7283358

Optimised Geometry:
Charge = 0 Multiplicity = 1

C	1.426231	0.874135	1.797258
Pd	0.169496	-0.339252	-0.083499
C	2.075295	-0.959065	-0.031548
C	3.042049	-0.437622	-0.895188
C	2.409076	-2.026376	0.806811
C	4.347926	-0.947945	-0.887354
C	3.702326	-2.556406	0.812108
C	4.657393	-1.999373	-0.033386
H	5.111227	-0.540263	-1.545457
H	3.971910	-3.385077	1.461554
H	5.669424	-2.400833	-0.028787
O	2.630176	0.552627	-1.730249
O	1.403090	-2.487102	1.611498
C	1.640267	-3.666447	2.352279
H	2.428755	-3.522439	3.103700
H	0.701815	-3.903236	2.861863
H	1.914397	-4.501297	1.690658
C	3.604925	1.225463	-2.496032
H	3.075266	2.013327	-3.039066
H	4.370315	1.684849	-1.852909
H	4.091211	0.553044	-3.217363
O	-1.968434	0.066056	-0.208626
O	-0.311260	-2.070507	-1.259436
C	-2.450591	0.259672	-1.361629
O	-1.909684	0.613511	-2.407322
C	-3.964031	-0.050288	-1.387309
S	-0.585005	-3.405448	-0.513950
C	-1.749227	-3.019893	0.811936
H	-2.506741	-2.331980	0.418269
H	-2.192480	-3.956257	1.168754
H	-1.180528	-2.540959	1.616008
C	-1.768378	-4.181256	-1.630581
H	-1.245813	-4.397690	-2.566351
H	-2.135664	-5.111149	-1.184353
H	-2.588219	-3.475022	-1.805140
F	-4.618875	0.573882	-0.402510
F	-4.547407	0.283975	-2.535512
F	-4.154726	-1.373875	-1.210934

C 0.483503 1.514287 1.027252
C 1.042092 2.554212 0.091654
C 2.166262 3.296746 0.458870
C 0.420987 2.805513 -1.135893
C 2.678217 4.269060 -0.396208
H 2.645219 3.126916 1.424027
C 0.924716 3.790165 -1.977145
H -0.443671 2.211357 -1.438760
C 2.056589 4.519811 -1.614326
H 3.557939 4.837718 -0.100786
H 0.435569 3.981975 -2.930737
H 2.450757 5.283273 -2.282586
O 2.192460 0.465864 2.558861
C -0.788530 1.771194 1.793395
C -1.550094 2.908554 1.525748
C -1.226488 0.871029 2.772008
C -2.744197 3.125487 2.207880
H -1.215501 3.622783 0.776025
C -2.408904 1.100281 3.461031
H -0.654295 -0.036240 2.978345
C -3.179631 2.225964 3.175024
H -3.334688 4.010910 1.978789
H -2.737013 0.388839 4.216613
H -4.114344 2.399377 3.704722

TS28b1-29b1
Zero-point correction= 0.380823 (Hartree/Particle)
Thermal correction to Energy= 0.411819
Thermal correction to Enthalpy= 0.412763
Thermal correction to Gibbs Free Energy= 0.315188
Sum of electronic and zero-point Energies= -1727.020490
Sum of electronic and thermal Energies= -1726.989494
Sum of electronic and thermal Enthalpies= -1726.988549
Sum of electronic and thermal Free Energies= -1727.086125
HF = -1727.4013128

Single Point Energy Calculations with extended basis set:
HF = -1730.3628082

Optimised Geometry:
Charge = 0 Multiplicity = 1
C -1.499604 0.329893 1.465444
Pd 0.400287 -0.366371 -0.079231
C -1.226208 -1.527281 0.234842
C -1.200875 -2.457344 1.295167
C -2.228440 -1.641701 -0.750923
C -2.197550 -3.421212 1.423451
C -3.236632 -2.605583 -0.619841
C -3.205648 -3.473338 0.462805
H -2.195552 -4.127914 2.248825

H	-4.023479	-2.697877	-1.362801
H	-3.987187	-4.224839	0.560183
O	-0.191353	-2.299452	2.181152
O	-2.141304	-0.801301	-1.800299
C	-3.221537	-0.745964	-2.713162
H	-4.167668	-0.537743	-2.194439
H	-2.996277	0.078218	-3.394694
H	-3.311471	-1.681908	-3.280882
C	-0.274977	-2.995529	3.411363
H	0.573324	-2.658621	4.010977
H	-1.213055	-2.756110	3.931862
H	-0.204017	-4.081288	3.264541
O	1.976501	-1.698621	-0.953779
C	2.753514	-0.712455	-1.030462
O	2.467282	0.456772	-0.693301
C	4.163412	-1.014080	-1.556250
F	4.100742	-1.654569	-2.724984
F	4.887067	0.087304	-1.722990
F	4.804918	-1.806190	-0.691575
C	-0.785986	1.208706	0.628503
C	0.159702	2.075692	1.427424
C	0.847676	1.563587	2.538162
C	0.359695	3.412515	1.069136
C	1.710163	2.369704	3.267800
H	0.718252	0.520294	2.828612
C	1.232399	4.212941	1.800190
H	-0.174810	3.837587	0.223088
C	1.910303	3.698744	2.899699
H	2.233613	1.952855	4.125958
H	1.374717	5.251036	1.505775
H	2.590234	4.328461	3.469868
O	-2.034110	0.007725	2.445612
C	-1.541758	1.801169	-0.521565
C	-2.925659	1.972793	-0.456435
C	-0.851356	2.228125	-1.661462
C	-3.612897	2.550110	-1.520233
H	-3.476505	1.661069	0.431987
C	-1.538072	2.812331	-2.717756
H	0.229677	2.092897	-1.714610
C	-2.921772	2.973092	-2.651081
H	-4.692182	2.675664	-1.458330
H	-0.990895	3.140571	-3.599385
H	-3.457951	3.431329	-3.479918

Imaginary Vibrational Frequency = -343.8939 cm^{-1}

TS28b2-29b2

Zero-point correction= 0.463078 (Hartree/Particle)
Thermal correction to Energy= 0.500353
Thermal correction to Enthalpy= 0.501298
Thermal correction to Gibbs Free Energy= 0.391951

Sum of electronic and zero-point Energies= -2280.023243
Sum of electronic and thermal Energies= -2279.985968
Sum of electronic and thermal Enthalpies= -2279.985024
Sum of electronic and thermal Free Energies= -2280.094370
HF = -2280.4863215

Single Point Energy Calculations with extended basis set:
HF = -2283.7219256

Optimised Geometry:
Charge = 0 Multiplicity = 1

C	-1.051379	-1.883304	-0.925455
Pd	-0.281825	0.440124	-0.251807
C	-2.218020	-0.000940	-0.667427
C	-2.710122	0.124393	-1.980508
C	-3.141075	-0.094459	0.392442
C	-4.076286	0.066299	-2.247126
C	-4.516281	-0.163313	0.134262
C	-4.958945	-0.085696	-1.179378
H	-4.460638	0.144196	-3.260579
H	-5.236415	-0.256469	0.942518
H	-6.027855	-0.133820	-1.380556
O	-2.622566	-0.094612	1.640510
C	-3.478593	-0.403709	2.722513
H	-3.974427	-1.373404	2.572744
H	-2.840537	-0.459364	3.608114
H	-4.239621	0.375760	2.866948
O	-1.764682	0.248195	-2.943946
C	-2.152326	0.017147	-4.284645
H	-2.829436	0.800166	-4.651722
H	-1.234021	0.032186	-4.876370
H	-2.639410	-0.963481	-4.386120
O	1.706011	0.923255	0.490922
O	-0.695728	2.575310	-0.371602
C	2.640060	1.038865	-0.361506
O	2.589382	1.170172	-1.579081
C	4.025541	1.071170	0.321152
S	-0.607228	3.226503	1.031781
C	0.957533	4.121474	1.026882
H	1.027327	4.706074	0.102478
H	1.001102	4.772273	1.906729
H	1.752114	3.370833	1.072046
C	-1.709243	4.642732	0.882047
H	-2.728768	4.256619	0.796168
H	-1.619499	5.265769	1.777634
H	-1.437741	5.206884	-0.017058
F	4.135319	0.161745	1.295300
F	5.023908	0.864212	-0.535867
F	4.216853	2.278501	0.883185
C	0.038415	-1.637964	-0.069734

C 1.349572 -1.957567 -0.746386
C 2.461558 -2.337143 0.010244
C 1.494348 -1.843636 -2.136395
C 3.689009 -2.569133 -0.603550
H 2.376982 -2.439968 1.089436
C 2.712969 -2.102541 -2.746987
H 0.656762 -1.516753 -2.753482
C 3.822090 -2.456943 -1.983114
H 4.545053 -2.847820 0.008853
H 2.799510 -2.007394 -3.827866
H 4.782410 -2.642398 -2.460549
C -0.192850 -1.990266 1.373480
C 0.533024 -1.351085 2.387069
C -1.129214 -2.967943 1.720837
C 0.316884 -1.687823 3.717965
H 1.261218 -0.585298 2.118693
C -1.351579 -3.292367 3.055747
H -1.694029 -3.487056 0.945120
C -0.628565 -2.653988 4.058323
H 0.887059 -1.185363 4.497527
H -2.088987 -4.052000 3.308900
H -0.798739 -2.909092 5.102739
O -1.625373 -2.484134 -1.741276
Imaginary Vibrational Frequency = -340.3734 cm^{-1}

29b1
Zero-point correction= 0.465907 (Hartree/Particle)
Thermal correction to Energy= 0.503108
Thermal correction to Enthalpy= 0.504052
Thermal correction to Gibbs Free Energy= 0.393933
Sum of electronic and zero-point Energies= -2280.042851
Sum of electronic and thermal Energies= -2280.005650
Sum of electronic and thermal Enthalpies= -2280.004706
Sum of electronic and thermal Free Energies= -2280.114825
HF = -2280.508758

Single Point Energy Calculations with extended basis set:
HF = -2283.7461549

Optimised Geometry:
Charge = 0 Multiplicity = 1
C -1.323899 0.641624 0.100750
Pd 1.125845 -0.044359 0.029658
C -0.851299 -0.780249 0.338428
C -0.678722 -1.258422 1.684436
C -0.965139 -1.752991 -0.716510
C -0.519998 -2.618539 1.937904
C -0.836812 -3.109234 -0.441879
C -0.606926 -3.508396 0.873751
H -0.361711 -2.992077 2.944280

H	-0.908127	-3.855420	-1.227080
H	-0.496372	-4.572068	1.078089
O	-1.190403	-1.247510	-1.929183
C	-1.354112	-2.147937	-3.015173
H	-2.195179	-2.828308	-2.829358
H	-1.568505	-1.529684	-3.888249
H	-0.435680	-2.724462	-3.185651
O	-0.719959	-0.315586	2.627215
C	-0.548784	-0.705863	3.983995
H	0.427175	-1.184103	4.132342
H	-0.599871	0.213899	4.568185
H	-1.351986	-1.386436	4.294059
O	2.847314	1.093032	-0.460462
O	2.326119	-1.749854	0.131370
C	3.424033	1.568388	0.572911
O	3.129458	1.459152	1.755289
C	4.671737	2.392032	0.184078
S	2.931499	-2.110824	-1.262003
C	4.674539	-1.694886	-1.104830
H	5.062742	-2.134190	-0.179327
H	5.212217	-2.078445	-1.978333
H	4.736651	-0.603493	-1.071134
C	3.062412	-3.900506	-1.156690
H	2.047062	-4.304940	-1.190008
H	3.640169	-4.263272	-2.012772
H	3.551312	-4.162013	-0.212057
F	4.338603	3.412185	-0.612999
F	5.297652	2.889915	1.245051
F	5.551054	1.631613	-0.485071
C	-2.641501	0.960802	-0.019790
C	-3.152494	2.302185	-0.326144
C	-2.312648	3.377414	-0.675547
C	-4.535320	2.555858	-0.274130
C	-2.835859	4.633499	-0.957592
H	-1.239150	3.214833	-0.728538
C	-5.054300	3.813665	-0.556603
H	-5.213258	1.747363	-0.003260
C	-4.208724	4.864657	-0.901214
H	-2.158956	5.443422	-1.228233
H	-6.130868	3.972413	-0.504028
H	-4.613575	5.851046	-1.121662
C	-3.592747	-0.181183	0.102226
C	-3.823891	-0.811664	1.329405
C	-4.218928	-0.702609	-1.038456
C	-4.615744	-1.955468	1.410823
H	-3.361606	-0.404204	2.229370
C	-5.013881	-1.840580	-0.961226
H	-4.051252	-0.216595	-2.000866
C	-5.204587	-2.478407	0.264084
H	-4.769336	-2.438556	2.374840

H -5.477995 -2.239283 -1.862397
H -5.817651 -3.376297 0.322796
O -0.257942 1.421015 -0.003989

29b2
Zero-point correction= 0.465082 (Hartree/Particle)
Thermal correction to Energy= 0.502598
Thermal correction to Enthalpy= 0.503543
Thermal correction to Gibbs Free Energy= 0.394532
Sum of electronic and zero-point Energies= -2280.067162
Sum of electronic and thermal Energies= -2280.029646
Sum of electronic and thermal Enthalpies= -2280.028702
Sum of electronic and thermal Free Energies= -2280.137712
HF = -2280.5322441

Single Point Energy Calculations with extended basis set:
HF = -2283.7589595

Optimised Geometry:
Charge = 0 Multiplicity = 1
C 1.156730 -2.096780 0.811864
Pd 0.386558 0.316606 0.200823
C 2.107393 -0.912711 0.813396
C 2.467228 -0.284675 2.050604
C 2.868063 -0.598825 -0.354154
C 3.440002 0.707618 2.071473
C 3.821761 0.421680 -0.325796
C 4.089494 1.046922 0.884278
H 3.700882 1.216767 2.994027
H 4.381839 0.684805 -1.218804
H 4.853797 1.821747 0.915527
O 2.651402 -1.398975 -1.403988
C 2.974030 -0.914402 -2.699470
H 4.059862 -0.854660 -2.843972
H 2.550181 -1.634491 -3.403415
H 2.518586 0.072926 -2.859773
O 1.794491 -0.714547 3.125269
C 1.980077 -0.033143 4.357172
H 1.724539 1.029393 4.256201
H 1.301074 -0.507642 5.067593
H 3.012986 -0.135954 4.712164
O -1.485501 1.074522 -0.576171
O 1.083008 2.457066 0.309513
C -2.307325 1.500761 0.294580
O -2.184971 1.639064 1.505546
C -3.655570 1.877126 -0.362046
S 1.224060 3.004235 -1.124354
C -0.168477 4.130492 -1.335205
H -0.209767 4.807818 -0.474336
H -0.044292 4.690089 -2.268424

H -1.071203 3.514133 -1.383034
C 2.523496 4.244071 -0.972514
H 3.459282 3.712102 -0.776905
H 2.601168 4.807940 -1.907827
H 2.279594 4.905544 -0.133543
F -4.254982 0.787887 -0.860658
F -4.502485 2.448173 0.491192
F -3.473923 2.731377 -1.381351
C -0.110869 -1.688803 0.098102
C -1.365245 -1.847485 0.886811
C -2.612900 -1.831536 0.244596
C -1.345516 -1.942358 2.289483
C -3.793057 -1.888015 0.974616
H -2.657846 -1.760632 -0.840785
C -2.527786 -2.012622 3.015499
H -0.395034 -1.956398 2.819638
C -3.758873 -1.981103 2.363695
H -4.747219 -1.857521 0.450649
H -2.485721 -2.090352 4.100757
H -4.684302 -2.030907 2.934732
C -0.151242 -2.156450 -1.335835
C -0.605546 -1.349575 -2.385674
C 0.251522 -3.466242 -1.623911
C -0.637355 -1.838413 -3.689209
H -0.947369 -0.337789 -2.172559
C 0.218211 -3.952501 -2.926110
H 0.597403 -4.108347 -0.814246
C -0.222091 -3.137563 -3.966626
H -0.991093 -1.195129 -4.493586
H 0.537407 -4.973682 -3.128532
H -0.246557 -3.515748 -4.987169
O 1.366666 -3.134049 1.400711

30b

Zero-point correction= 0.465553 (Hartree/Particle)
Thermal correction to Energy= 0.502941
Thermal correction to Enthalpy= 0.503885
Thermal correction to Gibbs Free Energy= 0.393408
Sum of electronic and zero-point Energies= -2280.063364
Sum of electronic and thermal Energies= -2280.025976
Sum of electronic and thermal Enthalpies= -2280.025032
Sum of electronic and thermal Free Energies= -2280.135509
HF = -2280.5289168

Single Point Energy Calculations with extended basis set:
HF = -2283.7609016

Optimised Geometry:
Charge = 0 Multiplicity = 1
C 1.132988 -0.154883 -1.295258

Pd	-0.774636	-0.108714	-0.151779
C	2.062446	0.961594	-1.550974
C	1.601879	2.285267	-1.632777
C	3.441678	0.701626	-1.581413
C	2.512524	3.340075	-1.706885
C	4.356985	1.749478	-1.670496
C	3.873200	3.052783	-1.726971
H	2.172681	4.371024	-1.747167
H	5.426373	1.563008	-1.700293
H	4.583652	3.874737	-1.793702
O	3.778379	-0.604799	-1.514133
C	5.139611	-0.931762	-1.305052
H	5.536357	-0.420596	-0.416580
H	5.172764	-2.012477	-1.148345
H	5.750258	-0.671383	-2.179987
O	0.263561	2.446617	-1.555485
C	-0.246975	3.723647	-1.218278
H	-0.095928	4.447234	-2.029914
H	-1.318582	3.582343	-1.054297
H	0.218517	4.101825	-0.297014
O	-2.812270	0.596895	-0.482239
O	-1.127203	0.028921	1.944624
C	-3.564274	-0.361498	-0.842327
O	-3.296639	-1.547433	-1.009886
C	-5.017071	0.108004	-1.071824
S	-1.574327	1.452339	2.389011
C	-3.332499	1.282493	2.734538
H	-3.484371	0.413919	3.384934
H	-3.693271	2.199221	3.212783
H	-3.827887	1.137493	1.769817
C	-0.969700	1.520131	4.081838
H	0.123247	1.547210	4.035884
H	-1.349049	2.426920	4.563588
H	-1.307500	0.622235	4.610719
F	-5.068642	1.090928	-1.977900
F	-5.811039	-0.872402	-1.492272
F	-5.538703	0.588387	0.068686
C	1.181945	-0.927858	-0.049870
C	2.048983	-0.445412	1.056137
C	2.008047	0.884755	1.501420
C	2.997447	-1.304782	1.624004
C	2.891429	1.340139	2.471102
H	1.279137	1.575750	1.075725
C	3.883518	-0.849276	2.595497
H	3.063158	-2.334869	1.275699
C	3.834971	0.473809	3.021853
H	2.842448	2.377236	2.798977
H	4.619169	-1.533617	3.014486
H	4.528865	0.831887	3.780208
O	0.145473	-0.396467	-2.063806

C 0.867313 -2.378887 -0.102185
C 1.162528 -3.149378 -1.233816
C 0.301398 -3.009698 1.016400
C 0.882619 -4.511298 -1.251538
H 1.628737 -2.677947 -2.097162
C 0.018215 -4.368923 0.993622
H 0.075088 -2.414782 1.901551
C 0.305907 -5.124168 -0.142226
H 1.125443 -5.098639 -2.135382
H -0.429394 -4.842000 1.865891
H 0.086970 -6.190235 -0.159121

MePhC=C=O (in DMSO)
Zero-point correction= 0.142663 (Hartree/Particle)
Thermal correction to Energy= 0.151559
Thermal correction to Enthalpy= 0.152503
Thermal correction to Gibbs Free Energy= 0.108098
Sum of electronic and zero-point Energies= -422.513541
Sum of electronic and thermal Energies= -422.504645
Sum of electronic and thermal Enthalpies= -422.503700
Sum of electronic and thermal Free Energies= -422.548105
HF = -422.6562038

Single Point Energy Calculations with extended basis set:
HF = -423.1736406

Optimised Geometry:
Charge = 0 Multiplicity = 1
C -2.223884 -0.591470 -0.000261
C -1.358544 0.408415 -0.000210
C 0.086931 0.138914 -0.000100
C 0.595971 -1.170023 0.000033
C 0.997631 1.202859 -0.000119
C 1.962974 -1.403241 0.000096
H -0.089938 -2.018896 0.000096
C 2.369560 0.963702 -0.000042
H 0.636024 2.229756 -0.000200
C 2.861884 -0.336477 0.000060
H 2.331017 -2.428092 0.000191
H 3.056909 1.808474 -0.000061
H 3.934543 -0.520376 0.000121
O -2.997278 -1.470609 0.000091
C -1.913282 1.812266 0.000228
H -1.578602 2.364251 0.888949
H -1.579079 2.364607 -0.888451
H -3.008090 1.815475 0.000517

Ph2CCO (in DMSO)
Zero-point correction= 0.195089 (Hartree/Particle)
Thermal correction to Energy= 0.207137

Thermal correction to Enthalpy= 0.208081
Thermal correction to Gibbs Free Energy= 0.155352
Sum of electronic and zero-point Energies= -614.046840
Sum of electronic and thermal Energies= -614.034793
Sum of electronic and thermal Enthalpies= -614.033849
Sum of electronic and thermal Free Energies= -614.086577
HF = -614.2419297

Single Point Energy Calculations with extended basis set:
HF = -615.0006962

Optimised Geometry:
Charge = 0 Multiplicity = 1

C	0.000203	2.157596	-0.000013
C	-0.000045	0.830183	-0.000092
C	-1.308425	0.137017	-0.029883
C	-2.433692	0.684847	0.598608
C	-1.446077	-1.075021	-0.718334
C	-3.666635	0.046343	0.526367
H	-2.337628	1.616396	1.157642
C	-2.675934	-1.720339	-0.771720
H	-0.579642	-1.509016	-1.215993
C	-3.792954	-1.161421	-0.154384
H	-4.530108	0.489862	1.019440
H	-2.763239	-2.664065	-1.307703
H	-4.755764	-1.666824	-0.200907
O	0.000515	3.326373	0.000051
C	1.308332	0.136902	0.029825
C	1.445902	-1.075144	0.718286
C	2.433647	0.684666	-0.598621
C	2.675731	-1.720520	0.771735
H	0.579444	-1.509172	1.215867
C	3.666558	0.046106	-0.526317
H	2.337696	1.616218	-1.157660
C	3.792803	-1.161655	0.154457
H	2.762942	-2.664234	1.307754
H	4.530081	0.489555	-1.019364
H	4.755607	-1.667063	0.201041

Reference

1 Joshi BS, Dabholkar KDM, Gawad DH. Reaction of furanopyrones with aluminium chloride in benzene. *Indian J Chem* **1972**; 10(6): 567–570.