Electronic Supplementary Information

N-heterocyclic carbenes which readily add ammonia, carbon monoxide and other small molecules

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Methods

Chemical syntheses

General

All reactions were carried out under N_2 in oven-dried glassware by applying standard Schlenk techniques. Solvents were dried and freshly distilled from the drying agent indicated prior to use (THF and hexanes: potassium, toluene: sodium). *N*-heterocyclic carbene **5-Np**[S1] and acyclic diaminocarbene **13-*i*Pr**[S2] were prepared according to the literature procedures. NMR: Varian MR 400 spectrometer operating at 399.87 MHz for ^{1}H. *In situ* NMR investigations: Bruker Avance 400 spectrometer utilising a modified 10 mm sapphire HP-NMR tube; gas feed, circulation, flow regulation, pressure adjustment *etc.* have been detailed elsewhere.[S3] Chemical shifts (^{15}N) are given relative to nitromethane (Ξ = 10.136767 MHz[S4]). IR: Bruker Alpha FT-IR spectrometer. Electrospray ionisation (ESI) mass spectra: Finnigan LCQ Deca. High-resolution mass spectra (HRMS): Bruker Daltonics micrOTOF. Melting points: Stuart Scientific smp 3 melting point apparatus. Elemental analyses were performed by the microanalytical laboratory of the University of Kassel.

Synthesis of 6-Np

Aniline (5.0 μl, 0.055 mmol) was added to a solution of **5-Np** (18.3 mg, 0.050 mmol) in THF (1 ml). The mixture was stirred for 10 min. Removal of volatile components in vacuo left the product in quantitative yield as a red oil, which was pure according to NMR spectroscopy. ^{1}H NMR (C_6D_6): δ 8.43 (br. s, 1H), 7.30–7.21 (m, 4H), 7.05–7.00 (m, 1H), 4.10 (br. s, 2H), 3.89 (m, 2H), 3.82 (m, 2H), 3.71 (br. s, 4H), 2.57 (d, *J* = 7.0 Hz, 2H), 2.16 (br. s, 1H), 0.96 (s, 9H), 0.84 (s, 9H); ^{13}C NMR (C_6D_6) δ 153.0, 152.9, 129.5, 123.2, 121.6, 113.2, 105.2, 64.8, 64.2, 61.8, 59.4, 58.2, 56.8, 34.3, 31.6, 28.9, 27.6; IR (KBr): 3388 (m), 3085 (m), 2954 (s), 2867 (s), 1749 (s), 1627 (s), 1590 (s), 1364 (s), 1191 (s) cm^{-1}; HRMS/ESI(+) *m/z* 459.234401 [M + H]$^{+}$, calcd. for $[C_{27}H_{37}FeN_3]^{+}$ 459.233142.

Synthesis of 7-Np

Ammonia (5 ml) was condensed on sodium metal (ca. 2 g) and subsequently recondensed into a stirred solution of **5-Np** (76.3 mg, 0.208 mmol) in THF (2 ml) kept in a separate flask at –80 °C. The mixture was stirred for 10 min and then allowed to warm to room temperature with evaporation of ammonia. Removal of volatile components in vacuo left the product in quantitative yield as a brownish oil, which was pure according to NMR spectroscopy. ^{1}H NMR (C_6D_6): δ 8.17 (d, *J* = 10.0 Hz, 1H), 6.76 (d, *J* = 11.7 Hz, 1H), 4.10 (s, 2H), 3.89 (s, 2H), 3.83 (s, 2H), 3.75 (s, 2H), 3.58 (s, 2H), 2.62 (d, *J* = 6.8 Hz, 2H), 2.44 (br. s, 1H), 0.93 (s, 18 H); ^{13}C NMR (C_6D_6) δ 157.8, 111.7, 103.9, 63.0, 62.5, 59.8, 58.1, 55.4, 33.0, 30.2, 27.5, 26.5; IR (KBr): 3381 (m), 3315 (m), 3091 (m), 2954 (s), 2867 (s), 1627 (s), 1615 (s), 1479 (s), 1365 (s) cm^{-1}; HRMS/ESI(+) *m/z* 384.210618 [M + H]$^{+}$, calcd. for $[C_{21}H_{33}FeN_3]$ 384.209667.

Synthesis of 8-Np

Methyl acrylate (14 μl, 0.154 mmol) was added to a solution of **5-Np** (31.6 mg, 0.086 mmol) in THF (1 ml). The mixture was stirred for 15 min. Volatile components were subsequently removed in vacuo and the oily, yellowish residue crystallised from hexanes affording the product as yellow crystals (20.1 mg, 52%). mp 140–142 °C; ^{1}H NMR (C_6D_6): δ 4.17 (m, 1H), 4.14 (m, 1H), 4.12 (m, 1H), 4.09 (m, 1H), 3.91 (m, 1H), 3.46 (m, 1H), 3.39 (s, 3H), 2.97 (d, *J* = 13.7 Hz, 1H), 2.84 (d, *J* = 13.8 Hz, 1H), 2.80 (d, *J* = 13.8 Hz, 1H), 2.65 (d, *J* = 13.7 Hz, 1H), 2.33 (dd, J_1 = 6.8 Hz, J_2 = 8.9 Hz, 1H), 1.94 (dd, J_1 = 4.7 Hz, J_2 = 6.8 Hz, 1H), 1.53 (dd, J_1 = 4.7 Hz, J_2 = 8.9 Hz, 1H), 1.07 (s, 9H), 0.83 (s, 9H); ^{13}C NMR (C_6D_6) δ 169.7, 102.9, 102.6, 82.3, 69.8, 69.5, 68.9, 68.8, 65.3, 65.1, 65.0, 62.4, 59.2, 58.8, 51.4, 37.4, 34.5, 33.8,

29.2, 28.9, 21.9; IR (KBr): 2952 (s), 1743 (s), 1470 (s) cm^{-1}; HRMS/ESI(+) *m/z* 453.220272 $[M + H]^+$, calcd. for $[C_{25}H_{37}FeN_2O_2]^+$ 453.219897; elemental analysis calcd. (%) for $C_{25}H_{36}FeN_2O_2$: C 66.37, H 8.02, N 6.19; found C 65.92, H 8.16, N 6.22.

Synthesis of 9-Np

tert-Butyl isocyanide (20 µl, 0.177 mmol) was added to a solution of **5-Np** (57.1 mg, 0.156 mmol) in toluene (1.5 ml). The mixture was stirred for 1 h. The solution was subsequently concentrated and stored at −40°C to afford the product as an orange, microcrystalline solid (50.3 mg, 72%). mp 118−120°C. Crystals suitable for an X-ray diffraction study were obtained from an oversaturated toluene solution at room temperature. ^{1}H NMR (C_6D_6, recorded at 46 °C): δ 4.09 (br. s, 4H), 3.97 (s, 4H), 3.00 (s, 4H), 1.27 (s, 9H), 0.99 (s, 18 H); ^{13}C NMR (C_6D_6) δ 192.9, 116.0, 105.1, 68.0, 59.3, 34.7, 31.0, 29.1; IR (KBr): 2017 (s) cm^{-1}; HRMS/ESI(+) *m/z* 450.256204 $[M + H]^+$, calcd. for $[C_{26}H_{40}FeN_3]^+$ 450.256617; elemental analysis calcd. (%) for $C_{26}H_{39}FeN_3$: C 69.49, H 8.75, N 9.35; found C 69.15, H 8.82, N 9.17.

Synthesis of 11-Np

5-Np (29.0 mg, 0.079 mmol) was placed in a one-necked 50 ml flask equipped with a balloon and dissolved in toluene (1.5 ml). The inert gas atmosphere was replaced by a slight overpressure of carbon monoxide. The reaction mixture was stirred for 3 d. The mixture was filtered and the filtrate concentrated to ca. 0.5 ml, whereupon crystallisation started. The product was isolated as yellow-brown crystals, which were suitable for an X-ray diffraction study (19.0 mg, 63%). mp 160 °C (dec.); ^{1}H NMR (C_6D_6): δ 5.21 (d, *J* = 13.7 Hz, 1H), 4.88 (d, *J* = 13.5 Hz, 1H), 4.60 (s, 1H), 4.51 (s, 1H), 4.44 (s, 1H), 4.40 (s, 1H), 4.25 (s, 1H), 4.20 (s, 1H), 4.17 (s, 1H), 4.11 (s, 1H), 4.03 (s, 1H), 3.98 (s, 1H), 3.97 (s, 1H), 3.94 (s, 1H), 3.89 (s, 1H), 3.86 (s 1H), 3.83 (s, 1H), 3.80 (s, 1H), 3.71 (d, *J* = 13.5 Hz, 1H), 3.40 (d, *J* = 13.7 Hz, 1H), 3.35 (d, *J* = 13.1 Hz, 1H), 3.27 (d, *J* = 13.7 Hz, 1H), 3.11 (d, *J* = 13.1 Hz, 1H), 3.08 (d, *J* = 13.7 Hz, 1H), 1.42 (s, 9H), 1.19 (s, 9H), 1.08 (s, 9H), 1.07 (s, 9H); ^{13}C NMR (C_6D_6) δ 176.9, 148.0, 136.3, 106.9, 105.6, 95.4, 94.5, 72.4, 72.1, 71.6, 71.4, 71.1, 70.3, 69.9, 69.3, 68.9, 68.8, 68.5, 67.7, 67.65, 67.6, 67.4, 67.1, 65.2, 63.3, 62.4, 60.3, 34.4, 33.6, 33.4, 33.0, 30.6, 30.1, 29.7, 21.6; IR (KBr): 1600 (s) cm^{-1}; MS/ESI(+) *m/z* 761.32 $[M + H]^+$ (100%); elemental analysis calcd. (%) for $C_{43}H_{60}Fe_2N_4O$: C 67.90, H 7.95, N 7.37; found C 67.61, H 8.03, N 7.13.

Synthesis of 16-*i*Pr

A 10 mm sapphire HP-NMR tube was charged with a solution of **13-*i*Pr** (57 mg, 0.27 mmol) in toluene-d_8 (2.4 ml). CO (1 bar) was bubbled through the solution at −50 °C. The solution was allowed to warm in 5 °C steps and was continuously monitored by NMR spectroscopy during this process. No reaction was observed below −20 °C. A slow progress in product formation was observed at −15 °C. The NMR data revealed no further species apart from the starting materials and the product. The reaction was completed by storing the solution under an atmosphere of CO (20 bar) at room temperature overnight. Volatile components were removed in vacuo, leaving the product as a light yellow oil in essentially quantitative yield. ^{1}H NMR (toluene-d_8): δ 3.64 (s, 1H), 3.22 (sept, J = 6.8 Hz, 1H, CH N-*i*Pr), 2.99 (m, 2H, CH N-*i*Pr$_2$), 1.09 and 0.85 (2 d, 6H each, Me N-*i*Pr$_2$), 1.08 and 1.07 (2 d, J = 6.8 Hz, 3H each, Me N-*i*Pr), 1.02 and 0.92 (2 s, 3H each, CMe$_2$); ^{13}C NMR (toluene-d_8) δ 167.4 (CO), 74.2 (CH), 62.5 (*C*Me$_2$), 47.7 (br., CH N-*i*Pr$_2$), 44.0 (CH N-*i*Pr), 25.2 and 22.5 (C*Me*$_2$), 23.9 and 21.9 (br., Me N-*i*Pr$_2$), 22.3 and 21.7 (Me N-*i*Pr); ^{15}N NMR (benzene-d_6) δ –218.5 (amide), –331.0 (amine); IR (KBr): 2964 (s), 1741 (s) cm^{-1}; HRMS/ESI(+) *m/z* 241.226792 $[M + H]^+$, calcd. for $[C_{14}H_{29}N_2O]^+$ 241.227440.

Single-crystal X-ray diffraction analyses

General

For each data collection a single crystal was mounted on a glass fibre and all geometric and intensity data were taken from this sample. Data collection using MoKα radiation (λ = 0.71073 Å) was made on a Stoe IPDS2 diffractometer equipped with a 2-circle goniometer and an area detector. Absorption correction was done by integration using X-red.[S5] The data sets were corrected for Lorentz and polarisation effects. The structures were solved by direct methods (SHELXS97) and refined using alternating cycles of least squares refinements against F^2 (SHELXL97).[S6] All non-H atoms were found in difference Fourier maps and were refined with anisotropic displacement parameters. H atoms were placed in constrained positions according to the riding model with the 1.2 fold isotropic displacement parameters.

Compound 8-Np

$C_{25}H_{36}FeN_2O_2$, M = 452.41, yellow (0.29 × 0.10 × 0.06 mm), T = 203(2) K, monoclinic, space group P $2_1/c$, a = 12.1007(16), b = 17.090(2), c = 11.5086(13) Å, β = 97.616(10)°, V = 2359.0(5) Å^3, Z = 4, μ = 0.662 mm^{-1}, ρ(calc.) = 1.274 Mg/m^3, 11142 measured refl., 2151 refl. observed (I>2σ(I)), 4155 unique refl. (R_{int} = 0.0755), 278 parameters refined, 0 restraints,

residual max./ min. electron densities after final Fourier synthesis 0.398/ –0.243 eÅ^{-3}, final *R* indices *R*1 ($I>2\sigma(I)$) = 0.0474, *wR*2 (all data) = 0.0719.

Compound 9-Np

$C_{26}H_{39}FeN_3$, *M* = 449.45, yellow (0.32 × 0.15 × 0.04 mm), *T* = 223(2) K, monoclinic, space group *P* $2_1/n$, *a* = 15.253(2), *b* = 9.8425(17), *c* = 16.706(2) Å, β = 95.195(11)°, *V* = 2497.8(7) Å^3, *Z* = 4, μ = 0.620 mm^{-1}, ρ(calc.) = 1.195 Mg/m^3, 13276 measured refl., 2277 refl. observed ($I>2\sigma(I)$), 4397 unique refl. (R_{int} = 0.0846), 280 parameters refined, 0 restraints, residual max./ min. electron densities after final Fourier synthesis 0.352/ –0.228 eÅ^{-3}, final *R* indices *R*1 ($I>2\sigma(I)$) = 0.0482, *wR*2 (all data) = 0.0858.

Compound 11-Np

$C_{43}H_{60}Fe_2N_4O$, *M* = 760.65, yellow (0.55 × 0.28 × 0.01 mm), *T* = 173(2) K, monoclinic, space group *P* $2_1/c$, *a* = 16.3194(13), *b* = 10.7454(5), *c* = 22.9601(17) Å, β = 97.397(6)°, *V* = 3992.7(5) Å^3, *Z* = 4, μ = 0.764 mm^{-1}, ρ(calc.) = 1.265 Mg/m^3, 25199 measured refl., 4350 refl. observed ($I>2\sigma(I)$), 7035 unique refl. (R_{int} = 0.0856), 459 parameters refined, 0 restraints, residual max./ min. electron densities after final Fourier synthesis 2.219/ –0.850 eÅ^{-3}, final *R* indices *R*1 ($I>2\sigma(I)$) = 0.0981, *wR*2 (all data) = 0.3049.

CCDC 782899–782901 contain the supplementary crystallographic data for this publication. This information can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Computational Details

The geometries of the molecules were optimised at the gradient corrected DFT level of theory using Becke's exchange functional[S7] in conjunction with Perdew's correlation functional[S8] with the *Gaussian03* program package.[S9] Ahlrich's def2-SVP basis set[S10] was used. This level of theory is denoted as BP86/def2-SVP. Stationary points were characterised with frequency calculations at BP86/def2-SVP. Thermodynamic corrections were taken from the frequency calculations. All relative energies given in this work include zero-point corrections. Intrinsic reaction coordinate (IRC) calculations were carried out to establish the transition states as the connections of reactants and products. For some molecules, singlepoint calculations at the

BP86/def2-TZVPP[S10] level were carried out using the geometries optimised at BP86/def2-SVP.

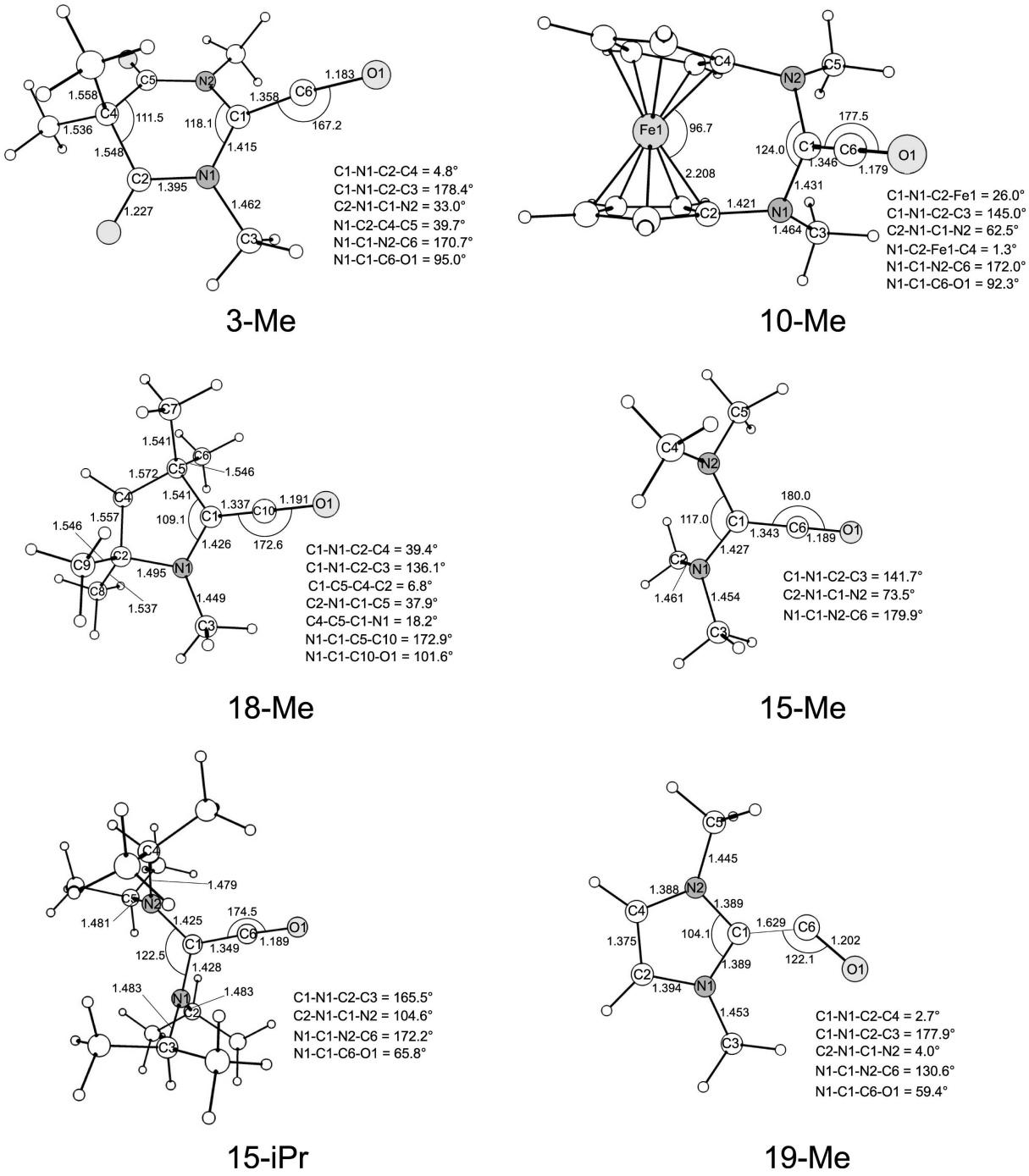

Fig. S1 Calculated geometries of ketenes and CO adducts at BP86/def2-SVP. Distances are given in Å, angles in degrees.

Table S1 Cartesian coordinates and energies at BP86/def2-SVP of the calculated molecules and transition states.

1-Me

1-Me, singlet carbene: E(BP86/def2-SVP)=-571.591208070 a.u.

N	1.421371	-0.524684	0.313130
C	1.555646	0.767488	-0.121576
N	0.423382	1.534417	-0.040945
C	-0.838288	1.149960	0.483836
C	-1.044004	-0.354786	0.679384
C	0.264641	-1.125380	0.875401
C	0.543217	2.954769	-0.416980
O	-1.712215	1.976536	0.694393
C	-2.008582	-0.621212	1.848146
C	-1.656184	-0.882102	-0.660520
O	0.321424	-2.218632	1.416600
C	2.635150	-1.361197	0.325388
H	-1.839985	-1.972020	-0.575502
H	-2.618498	-0.366073	-0.851822
H	-0.981549	-0.703387	-1.522562
H	-2.184952	-1.708763	1.947212
H	-1.587052	-0.252351	2.804698
H	-2.966173	-0.096875	1.669887
H	1.549563	3.089103	-0.849320
H	-0.242259	3.224248	-1.150792
H	0.415702	3.603748	0.472388
H	3.427015	-0.786321	-0.184677
H	2.936482	-1.592652	1.366571
H	2.444270	-2.320616	-0.195304

1-Me-trip, triplet carbene: E(BP86/def2-SVP)=-571.523928130 a.u.

N	1.380835	-0.585418	0.298641
C	1.286415	0.575352	-0.413218
N	0.332515	1.515032	-0.148424
C	-0.849171	1.160331	0.544807
C	-1.060342	-0.359543	0.697276
C	0.266645	-1.075364	1.020646
C	0.557772	2.914218	-0.526100
O	-1.639904	2.019396	0.937822
C	-2.080104	-0.631311	1.811693
C	-1.576732	-0.907917	-0.668285
O	0.378221	-2.024200	1.798445
C	2.660400	-1.298608	0.370613
H	-1.746136	-2.001533	-0.593972
H	-2.536482	-0.417962	-0.931032
H	-0.853392	-0.721579	-1.488943
H	-2.243028	-1.720975	1.915986
H	-1.720200	-0.244462	2.785241
H	-3.037755	-0.128672	1.577065
H	0.746917	2.989885	-1.615980
H	-0.357974	3.472074	-0.254367
H	1.424841	3.335039	0.023405
H	3.428055	-0.678598	0.877712
H	2.482725	-2.219511	0.957130
H	3.014000	-1.552456	-0.649126

TS-1-3-Me, transition state of ketene formation: E(BP86/def2-SVP)=-684.815301778 a.u.

C	-1.021913	-0.329846	0.723343
C	0.295560	-1.048097	1.026499
N	1.450581	-0.447844	0.461514
C	1.534086	0.825940	-0.028355
N	0.405942	1.594103	0.046084
C	-0.850748	1.185506	0.566397
O	0.372144	-2.093604	1.651347
C	2.694292	-1.233064	0.552035
C	2.144553	0.756444	-2.194761
O	3.262298	0.696107	-2.486600
C	0.540623	2.991419	-0.398545
O	-1.742971	1.984252	0.803067
C	-2.073385	-0.650969	1.796532
C	-1.485342	-0.851853	-0.678224
H	-1.632563	-1.949733	-0.631547
H	-2.448446	-0.373044	-0.947030
H	-0.744649	-0.625552	-1.472426

H	-2.213741	-1.745841	1.869459
H	-1.754789	-0.279070	2.790729
H	-3.032944	-0.164377	1.539918
H	0.934232	2.998312	-1.434934
H	-0.454445	3.469509	-0.359759
H	1.242134	3.540457	0.258431
H	3.014987	-1.327053	1.608821
H	2.529842	-2.252816	0.152800
H	3.470786	-0.705422	-0.028161

3-Me, ketene: E(BP86/def2-SVP)=-684.852199018 a.u.

C	-1.013632	-0.360324	0.608960
C	0.308491	-1.072912	0.985324
N	1.447685	-0.550033	0.373634
C	1.338063	0.610194	-0.429256
N	0.372306	1.580501	-0.070583
C	-0.825713	1.173862	0.516438
O	0.364233	-2.023702	1.758951
C	2.752656	-1.171689	0.589805
C	2.002046	0.698601	-1.610422
O	2.763211	0.897057	-2.494167
C	0.645738	3.000542	-0.282286
O	-1.657029	1.979657	0.922919
C	-2.083108	-0.680128	1.663501
C	-1.462534	-0.878816	-0.790237
H	-1.622669	-1.975393	-0.748256
H	-2.419437	-0.397383	-1.077362
H	-0.716015	-0.667241	-1.583008
H	-2.232781	-1.774449	1.727572
H	-1.778184	-0.317757	2.664511
H	-3.035105	-0.183883	1.396128
H	0.738886	3.238428	-1.364717
H	-0.213462	3.559715	0.133969
H	1.579786	3.301729	0.235439
H	3.468472	-0.441911	1.021424
H	2.597393	-2.009899	1.295117
H	3.172501	-1.572889	-0.358681

5-Me

5-Me, singlet carbene: E(BP86/def2-SVP)=-1876.62158360 a.u.

Fe	0.029935	0.012553	-0.040117
C	1.453427	0.042617	-1.397980
C	1.584984	1.211057	-0.544607
C	1.759828	0.753145	0.808647
C	1.780840	-0.689246	0.798642
C	1.619023	-1.133253	-0.560859
C	-1.398890	0.003304	-1.392669
C	-1.527539	-1.177801	-0.556458
C	-1.696907	-0.740246	0.804206
C	-1.717375	0.702140	0.815988
C	-1.560748	1.166499	-0.537308
N	1.202163	0.048992	-2.812921
N	-1.153190	0.018101	-2.808523
C	0.023137	0.038691	-3.497314
C	2.431257	0.071101	-3.618656
C	-2.385440	0.007966	-3.609663
H	-2.089081	0.020218	-4.674391
H	-2.990207	-0.901451	-3.398443
H	-3.014107	0.897590	-3.384407
H	2.130715	0.074730	-4.682276
H	3.036885	0.977278	-3.396270
H	3.060768	-0.821772	-3.409171
H	1.572867	-2.172638	-0.911494
H	1.906927	-1.336786	1.676447
H	1.867175	1.391853	1.695371
H	1.508508	2.253401	-0.880864
H	-1.452879	-2.214996	-0.908669
H	-1.801056	-1.392193	1.681628
H	-1.839720	1.336436	1.703934
H	-1.515477	2.211026	-0.872433

5-Me-trip, triplet carbene: E(BP86/def2-SVP)=-1876.56272112 a.u.

Fe	0.032084	-0.131449	0.034373
C	1.467766	0.069574	-1.372610
C	1.698456	1.229759	-0.546190
C	1.939921	0.758671	0.778827

C	2.046251	-0.678300	0.755639
C	1.754694	-1.125766	-0.567804
C	-1.413872	0.029501	-1.367242
C	-1.664434	-1.173334	-0.561463
C	-1.963409	-0.734117	0.763088
C	-1.897012	0.705255	0.785989
C	-1.673673	1.182841	-0.539881
N	1.202363	0.067520	-2.787446
N	-1.153783	0.034784	-2.783057
C	0.022889	0.060954	-3.464387
C	2.428093	0.061056	-3.599942
C	-2.381876	-0.005771	-3.590985
H	-2.078798	-0.006878	-4.654015
H	-2.973504	-0.920884	-3.367901
H	-3.024663	0.877370	-3.382875
H	2.121208	0.051453	-4.661837
H	3.046856	0.961736	-3.394196
H	3.045752	-0.837245	-3.379093
H	1.775561	-2.154601	-0.949474
H	2.272895	-1.312537	1.623120
H	2.088664	1.390322	1.665061
H	1.560358	2.273049	-0.856627
H	-1.658083	-2.202364	-0.943126
H	-2.169088	-1.374393	1.631357
H	-2.059977	1.332548	1.672817
H	-1.565814	2.229560	-0.850752

TS-5-10-Me, transition state of ketene formation: E(BP86/def2-SVP)=-1989.84428122 a.u.

C	3.506869	0.785359	-1.552996
C	2.147311	0.477173	-1.956951
C	1.247137	1.222104	-1.092578
C	2.049719	1.926269	-0.128149
C	3.439058	1.655938	-0.409364
Fe	2.407618	-0.106231	-0.096935
C	1.025464	-1.440819	0.547490
C	1.906630	-1.969411	-0.479291
C	3.262401	-1.940286	0.040483
C	3.217822	-1.340728	1.348090
C	1.842661	-1.034732	1.659607
N	1.503824	-2.425773	-1.777499
C	1.323364	-1.693473	-2.913391
C	-0.577461	-1.786650	-3.444589
O	-1.031760	-2.765431	-3.904342
N	1.761356	-0.407261	-3.017717
C	1.455532	0.264839	-4.286863
C	1.246036	-3.870970	-1.864241
H	0.397866	0.616796	-4.306861
H	2.198650	-4.443419	-1.823893
H	0.735974	-4.090195	-2.820395
H	1.606420	-0.442631	-5.123885
H	0.151010	1.196184	-1.147975
H	1.670249	2.565857	0.679900
H	4.297040	2.054920	0.147513
H	4.413783	0.373579	-2.014486
H	4.158821	-2.271104	-0.500087
H	4.081406	-1.156148	2.000460
H	1.481022	-0.577607	2.590224
H	-0.062491	-1.330451	0.451756
H	2.128278	1.135302	-4.416857
H	0.604756	-4.204252	-1.021184

10-Me, ketene: E(BP86/def2-SVP)=-1989.87639932 a.u.

C	3.187917	0.769168	-1.703202
C	1.776927	0.563550	-1.980889
C	1.026850	1.282727	-0.971942
C	1.963757	1.916732	-0.081978
C	3.295841	1.605701	-0.534427
Fe	2.246764	-0.118726	-0.130153
C	0.876065	-1.410814	0.650597
C	1.628532	-2.031542	-0.419735
C	3.030761	-1.997696	-0.042390
C	3.131112	-1.365777	1.249164
C	1.803442	-0.999991	1.672363
N	1.100047	-2.458996	-1.668696
C	0.507641	-1.424722	-2.462086
C	-0.829931	-1.434656	-2.608552
O	-1.995970	-1.468865	-2.781240
N	1.225904	-0.295701	-2.970083

C	1.997781	-0.471938	-4.201154
C	1.825475	-3.521657	-2.367340
H	2.254541	0.519519	-4.628305
H	2.823899	-3.206056	-2.758068
H	1.218540	-3.866780	-3.227488
H	1.379185	-1.018768	-4.939850
H	-0.067760	1.308514	-0.893921
H	1.704659	2.539737	0.784342
H	4.231876	1.956365	-0.079949
H	4.025889	0.355159	-2.278448
H	3.868694	-2.378049	-0.640649
H	4.058221	-1.204463	1.814847
H	1.540327	-0.506040	2.617051
H	-0.211587	-1.263580	0.658917
H	2.947676	-1.043448	-4.060523
H	1.981919	-4.381945	-1.684167

TS-10-11-Me, transition state of formation of final product: E(BP86/def2-SVP)=-3866.50017705 a.u.

C	5.836787	-2.619064	-0.250527
C	6.076180	-2.310424	1.138364
C	4.853250	-1.806868	1.706185
C	3.858107	-1.761913	0.649508
C	4.464283	-2.308556	-0.551821
Fe	5.388248	-0.641179	0.136720
C	4.926252	0.707362	-1.304387
C	4.281109	0.971812	-0.030536
C	5.323260	1.212425	0.952304
C	6.593182	1.027838	0.300680
C	6.348738	0.717707	-1.086959
N	2.864495	0.996022	0.211719
C	2.267083	2.318905	-0.019509
H	2.767586	3.087429	0.608409
N	2.511706	-1.271731	0.766640
C	1.544780	-2.311445	1.155683
H	1.551365	-3.144361	0.419404
C	2.030364	-0.020081	0.556947
C	-0.238336	0.139742	-1.115403
O	0.509355	0.175795	-2.034253
C	-1.300362	0.247912	-0.284120
N	-1.385862	-0.350859	1.014321
C	-1.144559	0.522800	2.163394
H	-1.113944	-0.085291	3.091098
C	-2.390753	-1.341663	1.158816
C	-2.468286	-2.591398	0.427548
C	-3.693212	-3.254836	0.793330
C	-4.382368	-2.429284	1.752833
C	-3.586564	-1.248325	1.978108
Fe	-4.059885	-1.396902	0.001463
C	-5.004010	-1.504443	-1.820192
C	-3.673798	-0.968923	-1.951232
C	-3.578826	0.215562	-1.122737
C	-4.871862	0.405120	-0.486457
C	-5.745319	-0.655730	-0.921903
N	-2.402864	0.964638	-0.869762
C	-2.576167	2.374886	-0.522241
H	-3.239203	2.868453	-1.263452
H	-5.133736	1.210109	0.212213
H	-6.796602	-0.782648	-0.631073
H	-5.388699	-2.398399	-2.328984
H	-2.853732	-1.390871	-2.546219
H	-3.843133	-0.415522	2.645469
H	-5.337843	-2.663729	2.240621
H	-4.034291	-4.227622	0.414466
H	-1.728936	-2.944620	-0.302701
H	-1.589695	2.878239	-0.552389
H	-3.011581	2.542079	0.493887
H	-1.914737	1.320991	2.299534
H	-0.148507	0.991440	2.028347
H	4.403270	0.487419	-2.244132
H	7.116879	0.532268	-1.849430
H	7.578899	1.119067	0.775773
H	5.156395	1.442119	2.012898
H	3.965199	-2.408284	-1.524478
H	6.572356	-3.030358	-0.954379
H	7.025303	-2.446326	1.673413
H	4.700306	-1.466649	2.738632
H	1.195300	2.265032	0.243477

H	2.367631	2.618496	-1.084932
H	0.539816	-1.847976	1.190153
H	1.802781	-2.733580	2.151388

11-Me, final product: E(BP86/def2-SVP)=-3866.54521508 a.u.

C	5.615419	-2.482774	0.240203
C	5.201223	-2.276256	1.606230
C	3.821316	-1.869316	1.606839
C	3.392647	-1.774157	0.222306
C	4.498383	-2.199598	-0.619220
Fe	4.896598	-0.558180	0.497203
C	4.891747	0.899753	-0.909065
C	3.821908	1.017347	0.067083
C	4.427647	1.207082	1.373729
C	5.853893	1.134715	1.208129
C	6.138545	0.943218	-0.192974
N	2.418367	0.998003	-0.199711
C	1.859462	2.326819	-0.520461
H	2.526078	3.094342	-0.086276
N	2.101479	-1.384627	-0.249976
C	1.210500	-2.526369	-0.501273
H	0.396697	-2.203630	-1.176557
C	1.646535	-0.110692	-0.419184
C	0.313580	0.144567	-1.127651
O	0.504608	0.573969	-2.318331
C	-0.860369	0.103440	-0.360009
N	-0.834686	-0.435319	0.989465
C	-0.671032	0.575772	2.042520
H	-0.554043	0.084723	3.031439
C	-1.828061	-1.408779	1.280472
C	-2.093693	-2.626377	0.534502
C	-3.244013	-3.276214	1.110407
C	-3.703484	-2.475893	2.215556
C	-2.836597	-1.329253	2.324862
Fe	-3.688519	-1.381904	0.471440
C	-5.054292	-1.378787	-1.072912
C	-3.741080	-1.003004	-1.521532
C	-3.306790	0.153492	-0.750216
C	-4.398279	0.495541	0.151062
C	-5.462425	-0.453281	-0.044031
N	-2.041016	0.777657	-0.781886
C	-1.905966	2.077989	-1.431606
H	-2.860173	2.344663	-1.927447
H	-4.385534	1.322170	0.873850
H	-6.422414	-0.466749	0.489327
H	-5.650522	-2.219263	-1.454028
H	-3.135451	-1.510017	-2.283854
H	-2.939806	-0.520774	3.059023
H	-4.549552	-2.705900	2.876757
H	-3.684336	-4.221688	0.766441
H	-1.553226	-2.963769	-0.356853
H	-1.101316	2.030473	-2.203759
H	-1.653717	2.889762	-0.705980
H	-1.529896	1.287720	2.103908
H	0.246041	1.164094	1.842732
H	4.753222	0.755173	-1.988299
H	7.137932	0.859037	-0.639939
H	6.598409	1.219568	2.010441
H	3.878478	1.331781	2.315995
H	4.482127	-2.240979	-1.716155
H	6.611006	-2.808601	-0.088263
H	5.828223	-2.418060	2.496242
H	3.206910	-1.621599	2.481966
H	0.844282	2.423782	-0.088368
H	1.765353	2.437385	-1.620061
H	0.766245	-2.895055	0.445566
H	1.799514	-3.339494	-0.970629

12-Me

12-Me, singlet carbene: E(BP86/def2-SVP)=-407.575801820 a.u.

C	1.207724	0.852251	-0.391373
C	-0.077274	0.196468	0.120244
N	0.241479	-0.401765	1.252739
C	1.689450	-0.327427	1.745473
C	2.250270	0.739262	0.773015
C	-0.734357	-1.170387	2.027700

C	2.365448	-1.704566	1.583043
C	1.749659	0.123100	3.215576
C	1.650097	0.075916	-1.656773
C	0.925999	2.320625	-0.772800
H	3.269545	0.478487	0.419801
H	2.333151	1.713792	1.298825
H	-1.681466	-1.169652	1.459281
H	-0.392972	-2.216625	2.177406
H	-0.903983	-0.714370	3.025729
H	3.427351	-1.647410	1.900534
H	1.876189	-2.479997	2.208734
H	2.340582	-2.046193	0.528822
H	2.803917	0.308844	3.509194
H	1.183060	1.064898	3.369316
H	1.348039	-0.645678	3.908365
H	0.844605	0.085854	-2.418931
H	2.559044	0.539184	-2.098049
H	1.882172	-0.986129	-1.432803
H	0.154649	2.375156	-1.567704
H	0.550305	2.898672	0.097669
H	1.849758	2.816990	-1.142760

12-Me-trip, triplet carbene: E(BP86/def2-SVP)=-407.501200753 a.u.

C	0.120476	-0.008602	0.103026
N	0.127095	-0.213588	1.477037
C	1.562445	-0.116002	1.908986
C	2.090767	0.957040	0.899058
C	1.204498	0.895577	-0.410479
C	-0.773631	-1.177932	2.074885
C	2.298062	-1.463708	1.747930
C	1.654439	0.381279	3.360087
H	3.166029	0.802132	0.673472
H	1.986253	1.963198	1.355125
C	1.967319	0.288201	-1.611666
C	0.690385	2.308117	-0.794287
H	-1.812064	-0.946675	1.758599
H	-0.562217	-2.237664	1.779451
H	-0.732120	-1.107372	3.180716
H	3.382990	-1.349503	1.952936
H	1.904339	-2.226507	2.452403
H	2.177075	-1.853665	0.716093
H	2.710682	0.597814	3.624632
H	1.061115	1.308685	3.494446
H	1.285099	-0.377881	4.081564
H	1.283393	0.144641	-2.474179
H	2.791869	0.957996	-1.940741
H	2.400610	-0.700756	-1.359881
H	0.021352	2.253831	-1.678448
H	0.115114	2.758870	0.040283
H	1.532559	2.990000	-1.047711

TS-12-18-Me, transition state of ketene formation: E(BP86/def2-SVP)=-520.801900428 a.u.

C	1.330907	0.054759	1.896074
C	2.291846	0.052402	0.707705
C	1.414173	0.435693	-0.529292
C	-0.059995	0.200000	-0.108193
N	0.105411	0.066372	1.402072
C	3.477511	1.017885	0.898894
C	2.842925	-1.395787	0.603252
C	-1.079707	0.034894	2.256263
C	1.595378	1.825669	3.332524
O	1.777359	1.645677	4.461923
C	-0.656122	-1.095547	-0.694369
H	1.564128	1.509376	-0.767562
H	-1.556807	1.036746	2.312634
H	-1.828698	-0.688111	1.871935
H	-0.767076	-0.271272	3.270563
H	4.169749	0.957194	0.031464
H	3.134096	2.066865	0.999900
H	4.050718	0.760129	1.813081
H	3.550000	-1.475018	-0.250218
H	3.381207	-1.675966	1.531411
H	2.035334	-2.140846	0.449644
H	1.678121	-0.138747	-1.441260
C	-0.961106	1.402092	-0.443829
H	-1.675092	-1.295784	-0.302192
H	-0.741270	-1.008674	-1.797213
H	-0.020875	-1.975146	-0.468116

H	-0.956228	1.580111	-1.539280
H	-2.016136	1.233056	-0.142978
H	-0.596327	2.324643	0.053536

18-Me, ketene: E(BP86/def2-SVP)=-520.846528702 a.u.

C	1.251684	0.201362	1.855424
C	2.323828	0.095651	0.754129
C	1.411229	-0.081639	-0.513988
C	-0.069175	0.110945	-0.071947
N	0.018575	-0.314525	1.358813
C	3.213370	1.350720	0.668966
C	3.197732	-1.160532	0.975086
C	-1.146052	-0.202713	2.213789
C	1.424755	0.821683	3.026992
O	1.636789	1.240311	4.121328
C	-1.018340	-0.816265	-0.848207
H	1.687397	0.630793	-1.318077
H	-1.421976	0.852408	2.476009
H	-2.021899	-0.676694	1.727790
H	-0.956554	-0.744091	3.164936
H	3.955804	1.247838	-0.150813
H	2.614296	2.264737	0.480670
H	3.780138	1.506980	1.611549
H	3.871288	-1.333160	0.107131
H	3.829246	-1.054259	1.881830
H	2.560679	-2.059270	1.103351
H	1.541203	-1.104529	-0.922955
C	-0.511197	1.584881	-0.220018
H	-2.077617	-0.670821	-0.549055
H	-0.955914	-0.607635	-1.936198
H	-0.749142	-1.878477	-0.675950
H	-0.455519	1.911228	-1.279282
H	-1.558993	1.729677	0.117775
H	0.136913	2.256157	0.381237

13-Me

13-Me, singlet carbene: E(BP86/def2-SVP)=-306.952192893 a.u.

C	0.405980	-1.034427	-0.948756
N	1.519151	-0.299802	-0.695616
N	-0.681762	-0.455673	-1.518642
C	1.734281	1.160187	-0.667550
C	2.692636	-1.051424	-0.250922
C	-1.885846	-1.283847	-1.582302
C	-0.843638	0.838004	-2.210634
H	-1.331946	1.618608	-1.582343
H	0.128031	1.220976	-2.568217
H	-1.488818	0.686587	-3.102930
H	-2.733362	-0.807760	-1.036958
H	-2.210908	-1.446180	-2.636972
H	-1.651846	-2.255565	-1.111316
H	3.552235	-0.907316	-0.945658
H	3.020671	-0.727275	0.764789
H	2.419154	-2.121740	-0.229646
H	2.245210	1.550451	-1.578146
H	0.780449	1.699236	-0.532246
H	2.381352	1.408434	0.201387

13-Me-trip, triplet carbene: E(BP86/def2-SVP)=-306.886893925 a.u.

C	0.410578	-0.796762	-1.006066
N	1.573607	-0.072932	-0.781674
N	-0.727146	-0.212668	-1.545816
C	1.562163	0.935173	0.283729
C	2.841408	-0.767565	-0.954187
C	-2.017926	-0.705520	-1.086927
C	-0.688270	0.198161	-2.953366
H	-1.492818	0.937506	-3.158116
H	0.291611	0.674031	-3.156945
H	-0.815280	-0.662071	-3.657033
H	-2.809805	0.045940	-1.298291
H	-2.317539	-1.662824	-1.583064
H	-1.971681	-0.887630	0.004746
H	3.662078	-0.031853	-1.101376
H	3.110136	-1.403961	-0.073768
H	2.778943	-1.425196	-1.843385
H	2.394982	1.656640	0.136251
H	0.602170	1.487003	0.239476

H	1.663813	0.486001	1.303135

TS-13-15-Me, transition state of ketene formation: E(BP86/def2-SVP)=-420.175511435 a.u.

H	-2.050991	1.522925	-1.803910
C	-1.104018	1.015854	-2.108711
N	-1.171833	0.398313	-3.435895
C	-1.529282	-0.867974	-3.768984
N	-1.901133	-1.788688	-2.837858
C	-2.568863	-1.594342	-1.541106
H	-1.920379	-1.861286	-0.674997
H	-0.303629	1.784971	-2.113956
C	-1.002277	1.322456	-4.552511
H	-1.942947	1.880930	-4.769309
H	-0.725866	0.750211	-5.457431
C	-1.878156	-3.184716	-3.275683
H	-2.893357	-3.641771	-3.232830
H	-1.505766	-3.229221	-4.315276
H	-3.466090	-2.251248	-1.498588
C	-2.916646	-0.868413	-5.174840
O	-2.996039	-1.758028	-5.936926
H	-0.836891	0.265086	-1.342926
H	-0.197328	2.053302	-4.326703
H	-1.203275	-3.789001	-2.627996
H	-2.917865	-0.554696	-1.424072

15-Me, ketene: E(BP86/def2-SVP)=-420.209998657 a.u.

H	-1.505761	2.025326	-2.340325
C	-0.832653	1.130066	-2.372011
N	-1.069934	0.270380	-3.528786
C	-2.191177	-0.604278	-3.412042
N	-2.048566	-1.726292	-2.541754
C	-3.223791	-2.176094	-1.812639
H	-2.911657	-2.837742	-0.975637
H	0.218982	1.490250	-2.375485
C	-0.832291	0.903211	-4.816634
H	-1.521278	1.759555	-5.040460
H	-0.944626	0.154329	-5.626539
C	-1.196617	-2.798637	-3.049356
H	-1.714626	-3.463136	-3.788108
H	-0.311276	-2.346671	-3.538424
H	-3.954040	-2.757419	-2.434705
C	-3.328312	-0.384118	-4.091804
O	-4.335041	-0.189196	-4.693608
H	-0.989416	0.535597	-1.450397
H	0.204186	1.303716	-4.848474
H	-0.840219	-3.431876	-2.208068
H	-3.757321	-1.301402	-1.388790

13-iPr

13-iPr, singlet carbene: E(BP86/def2-SVP)=-621.218464255 a.u.

C	1.891821	1.292667	-0.868263
N	1.489165	-0.119620	-0.556648
C	2.566299	-0.962756	0.063310
C	0.282961	-0.725645	-0.619081
N	-0.789885	-0.238334	-1.280583
C	-0.889693	0.831181	-2.329465
C	-2.062053	-0.994373	-1.024573
C	-1.669276	2.065200	-1.843847
H	0.149635	1.135112	-2.547186
C	-1.440928	0.294582	-3.665836
C	-2.476135	-0.888352	0.450377
H	-2.847093	-0.490259	-1.627563
C	-1.964727	-2.455332	-1.486624
H	3.488363	-0.343355	0.050858
C	2.247271	-1.320702	1.521915
C	2.840778	-2.213287	-0.784669
C	2.832730	1.385769	-2.081700
H	0.954498	1.825340	-1.108454
C	2.467603	2.024626	0.360726
H	-1.672048	2.864314	-2.616010
H	-2.728574	1.814096	-1.623969
H	-1.226761	2.483354	-0.916020
H	-1.362634	1.083372	-4.443544
H	-0.860985	-0.584369	-4.012379
H	-2.509181	0.001975	-3.605267
H	2.615645	3.098143	0.118259

H	1.773782	1.962576	1.223132
H	3.451753	1.624059	0.679230
H	3.061589	2.444830	-2.328363
H	3.799436	0.875792	-1.884434
H	2.383238	0.911840	-2.978856
H	-2.915109	-2.993945	-1.288835
H	-1.748581	-2.524571	-2.572433
H	-1.141478	-2.954988	-0.937666
H	-3.447456	-1.398083	0.624846
H	-1.701073	-1.359825	1.087943
H	-2.580504	0.171847	0.762322
H	3.678400	-2.803936	-0.356597
H	1.931259	-2.846754	-0.816409
H	3.106859	-1.940312	-1.827215
H	3.055499	-1.943565	1.959262
H	2.135167	-0.411956	2.148122
H	1.293471	-1.884442	1.556448

13-iPr-trip, triplet carbene: E(BP86/def2-SVP)=-621.158281972 a.u.

C	1.635964	1.287098	0.093138
N	1.528992	-0.024382	-0.610524
C	2.737383	-0.875031	-0.712434
C	0.292771	-0.646069	-0.662961
N	-0.805575	-0.136860	-1.335143
C	-0.738475	-0.020553	-2.821256
C	-2.134008	-0.270838	-0.693649
C	-1.430033	1.256514	-3.325493
H	0.349063	0.088378	-3.022687
C	-1.231218	-1.278609	-3.559216
C	-2.269108	0.715593	0.478923
H	-2.880936	0.013891	-1.466362
C	-2.441033	-1.714406	-0.246967
H	3.598725	-0.221304	-0.454001
C	2.724446	-2.055883	0.279079
C	2.933179	-1.363606	-2.157834
C	2.599883	2.244068	-0.626916
H	0.613668	1.713310	0.001302
C	1.959305	1.155674	1.592559
H	-1.240309	1.392403	-4.411123
H	-2.532186	1.219080	-3.190887
H	-1.049665	2.151756	-2.792711
H	-1.024942	-1.204083	-4.648438
H	-0.715733	-2.181916	-3.173075
H	-2.326302	-1.423563	-3.440008
H	1.882144	2.140441	2.101272
H	1.248788	0.459074	2.083177
H	2.990661	0.777857	1.759858
H	2.549936	3.254731	-0.169619
H	3.656510	1.908067	-0.556867
H	2.339959	2.336726	-1.701089
H	-3.462325	-1.785053	0.183436
H	-2.373055	-2.424106	-1.095467
H	-1.709269	-2.036362	0.522550
H	-3.264589	0.627829	0.962538
H	-1.493616	0.500508	1.244046
H	-2.138734	1.762748	0.137087
H	3.840751	-1.996895	-2.246310
H	2.057601	-1.969447	-2.473085
H	3.034627	-0.509297	-2.858012
H	3.665828	-2.640695	0.207876
H	2.612628	-1.705726	1.324608
H	1.871351	-2.729146	0.054941

TS-13-15-iPr, transition state of ketene formation: E(BP86/def2-SVP)=-734.433203566 a.u.

C	-1.491809	1.708238	-1.757761
C	-0.657250	0.560213	-2.349259
C	-1.206347	0.097661	-3.714797
N	-0.465741	-0.588517	-1.410029
C	-1.706528	-1.358705	-1.089551
C	-1.521104	-2.872816	-1.274086
C	0.735982	-1.107786	-1.044597
N	1.895113	-0.420490	-1.315230
C	3.125895	-1.242211	-1.512610
C	3.056431	-1.959351	-2.871790
C	2.122152	1.027119	-1.001299
C	2.894363	1.195557	0.321183
C	2.781357	1.808680	-2.151371
C	3.452499	-2.233953	-0.384245

C	-2.300400	-1.003563	0.288910
H	0.358775	0.937181	-2.553298
H	-2.451589	-1.028906	-1.844097
H	3.962229	-0.512586	-1.562449
H	1.115699	1.452636	-0.823735
H	-1.496733	2.576553	-2.450257
H	-2.549194	1.410038	-1.599110
H	-1.086329	2.049646	-0.783019
H	-1.167409	0.942979	-4.433262
H	-0.596117	-0.730682	-4.127476
H	-2.262825	-0.238863	-3.668054
H	2.911835	2.265032	0.619026
H	2.401128	0.615090	1.127749
H	3.949162	0.860063	0.234338
H	2.851397	2.887360	-1.897574
H	3.814280	1.453027	-2.349066
H	2.209974	1.715023	-3.098290
H	-2.503772	-3.379870	-1.171570
H	-1.115920	-3.101366	-2.280345
H	-0.829953	-3.295433	-0.520836
H	-3.294454	-1.485192	0.401693
H	-1.661240	-1.353662	1.121060
H	-2.439321	0.089731	0.403813
H	3.995448	-2.514900	-3.079344
H	2.216188	-2.685195	-2.871220
H	2.888238	-1.238897	-3.698637
H	4.430983	-2.716534	-0.590135
H	3.520264	-1.733892	0.601410
H	2.688035	-3.031574	-0.315726
C	0.764627	-1.615993	0.953290
O	0.623892	-2.708751	1.351548

15-iPr, ketene: E(BP86/def2-SVP)=-734.473189449 a.u.

C	-1.849010	1.553699	-1.593701
C	-0.838682	0.632009	-2.307593
C	-1.267892	0.324865	-3.753110
N	-0.488262	-0.594267	-1.554274
C	-1.526827	-1.630356	-1.366996
C	-0.962748	-3.043853	-1.588837
C	0.590332	-0.467084	-0.631270
N	1.931630	-0.211261	-1.048512
C	2.865137	-1.325333	-1.341307
C	2.590924	-1.959566	-2.718195
C	2.505871	1.144649	-0.875957
C	3.452870	1.264757	0.336938
C	3.180453	1.659500	-2.163055
C	2.911182	-2.382674	-0.224421
C	-2.311096	-1.565438	-0.035452
H	0.123307	1.183963	-2.381205
H	-2.263913	-1.443482	-2.177474
H	3.875653	-0.862603	-1.388253
H	1.627632	1.794955	-0.674067
H	-1.947700	2.523385	-2.126972
H	-2.860758	1.097255	-1.549863
H	-1.522181	1.772263	-0.555456
H	-1.356749	1.265555	-4.335472
H	-0.522684	-0.326869	-4.252260
H	-2.256554	-0.179466	-3.803836
H	3.799953	2.311991	0.463501
H	2.944970	0.960025	1.274484
H	4.358300	0.632687	0.213883
H	3.517181	2.709300	-2.032451
H	4.076464	1.058829	-2.427890
H	2.481202	1.623870	-3.023179
H	-1.755612	-3.809693	-1.458773
H	-0.540331	-3.152575	-2.607930
H	-0.159191	-3.265795	-0.855967
H	-3.187288	-2.247649	-0.071870
H	-1.688330	-1.884868	0.825611
H	-2.688366	-0.544922	0.173890
H	3.342437	-2.744350	-2.950019
H	1.586505	-2.425488	-2.744011
H	2.630126	-1.195135	-3.520327
H	3.679792	-3.152514	-0.445537
H	3.154249	-1.923478	0.755430
H	1.934955	-2.900171	-0.123193
C	0.440164	-0.422619	0.708120
O	0.374490	-0.474855	1.893697

14-Me

14-Me, singlet carbene: E(BP86/def2-SVP)=-304.575814617 a.u.

N	-1.055989	0.127900	0.022455
C	0.010985	1.000030	-0.001104
N	1.082113	0.132845	-0.019275
C	0.702125	-1.210447	-0.007674
C	-0.669639	-1.213635	0.018959
C	2.463160	0.591064	-0.047573
C	-2.439220	0.579664	0.048173
H	-1.379905	-2.048671	0.035777
H	1.416329	-2.042208	-0.019314
H	-2.995841	0.217621	-0.842092
H	-2.960274	0.223672	0.962097
H	-2.426817	1.684961	0.044293
H	3.021074	0.238035	0.845496
H	2.986347	0.231034	-0.958680
H	2.445544	1.696306	-0.051537

14-Me-trip, triplet carbene: E(BP86/def2-SVP)=-304.443022249 a.u.

C	-0.124790	0.035794	-0.083156
N	-0.023588	-0.226019	1.340385
C	1.289294	0.098449	1.663151
C	2.044321	0.104502	0.503159
N	1.219028	-0.214893	-0.568698
C	1.571629	-0.053430	-1.957584
H	3.108567	0.344800	0.381076
H	1.607250	0.333302	2.687355
C	-1.151113	-0.070683	2.226066
H	2.631029	-0.341495	-2.109855
H	0.933795	-0.712920	-2.582651
H	1.427871	0.996995	-2.316529
H	-0.861414	-0.365394	3.254533
H	-1.538004	0.979477	2.246663
H	-1.980430	-0.728484	1.891557

TS-14-19-Me, transition state of co adduct formation: E(BP86/def2-SVP)=-417.793470052 a.u.

C	-1.010165	0.688276	0.048779
N	0.296203	1.126232	-0.120610
C	1.185630	0.063951	-0.109038
N	0.370102	-1.050226	0.000347
C	-0.968785	-0.684276	0.126124
C	2.440903	0.189781	1.040645
O	3.257972	-0.678736	1.125345
C	0.893957	-2.405723	-0.052952
C	0.788086	2.485053	-0.036239
H	-1.863002	1.375129	0.086032
H	-1.776745	-1.414888	0.243190
H	1.245495	2.811855	-0.991577
H	-0.033314	3.174335	0.235790
H	1.578205	2.491691	0.757017
H	0.997264	-2.756596	-1.101315
H	1.899014	-2.413867	0.418691
H	0.220529	-3.092710	0.495907

19-Me, CO adduct: E(BP86/def2-SVP)=-417.793500475 a.u.

C	-1.008401	0.687989	0.026098
N	0.298863	1.130696	-0.120216
C	1.188522	0.064691	-0.073712
N	0.371828	-1.054624	0.016947
C	-0.968044	-0.683758	0.115982
C	2.410616	0.177934	0.997638
O	3.271455	-0.656936	1.074344
C	0.895684	-2.408830	-0.036608
C	0.793252	2.484874	-0.014608
H	-1.863150	1.373291	0.037737
H	-1.778883	-1.412810	0.221784
H	1.268796	2.822742	-0.957440
H	-0.028173	3.175351	0.254322
H	1.573774	2.474006	0.791109
H	1.001350	-2.760308	-1.084932
H	1.901429	-2.416719	0.434515
H	0.222674	-3.096945	0.511651

15-iPr

15-iPr, ketene: E(BP86/def2-SVP= -735.279 a.u.

C	0.16717600	-0.14522500	0.37722900
N	1.31102200	0.26106300	-0.37468800
N	-1.18165600	-0.05124600	-0.09326200
C	0.32708300	-0.57442500	1.64362700
O	0.47040600	-1.00452800	2.74168900
C	-1.80755100	-1.16687100	-0.84583600
C	-2.09663200	0.91972300	0.55475200
C	1.61102000	1.71153800	-0.52097300
C	2.48741600	-0.62788700	-0.54615700
C	0.78101600	2.34609400	-1.65213000
C	1.49697100	2.50797800	0.79024500
H	2.67689600	1.76155000	-0.83669400
H	2.98129100	-0.27496600	-1.48269900
C	3.53047800	-0.50818200	0.58894300
C	2.11354100	-2.09634700	-0.77201000
C	-1.37906200	-1.16401100	-2.32589100
C	-1.61349700	-2.54495400	-0.18760000
H	-2.90006300	-0.96078700	-0.82782300
C	-2.93400500	0.31968700	1.70472300
H	-1.42316600	1.68290500	1.00035500
C	-3.00211900	1.64589500	-0.45953200
H	1.81966600	3.55894700	0.63695500
H	0.45164000	2.53051200	1.16248700
H	2.12622100	2.06798100	1.59084100
H	1.08125500	3.40223400	-1.82206700
H	0.92010800	1.78736400	-2.59976300
H	-0.29972700	2.32846200	-1.40915900
H	4.43838200	-1.10375900	0.35444000
H	3.85504600	0.54163200	0.74086700
H	3.12121700	-0.88288300	1.55073000
H	3.02487500	-2.67387000	-1.03016300
H	1.67448400	-2.55518500	0.13707800
H	1.38935400	-2.20946500	-1.60195900
H	-2.18830800	-3.32162500	-0.73468400
H	-0.54890300	-2.85098400	-0.18971500
H	-1.96289300	-2.53874000	0.86514000
H	-1.89680100	-1.96678300	-2.89336300
H	-1.61798400	-0.19178600	-2.80222400
H	-0.28654600	-1.32184000	-2.42495300
H	-3.55037300	1.10282900	2.19531200
H	-3.63150900	-0.46312200	1.33638900
H	-2.28650700	-0.13557600	2.48140200
H	-3.57221400	2.45331000	0.04571700
H	-2.40855000	2.10122700	-1.27761700
H	-3.74671600	0.96184300	-0.91901500

TS-15-17-iPr, transition state of carbene formation: E(BP86/def2-SVP)=--735.252 a.u.

C	-3.38679500	-1.32222000	1.09113900
C	-2.21982600	-1.26012100	0.08828100
N	-1.54374700	0.07012900	0.09919000
C	-0.34951400	0.25074200	0.69490900
C	0.52403500	-0.24199500	1.60014100
N	1.26460000	-0.03270600	0.17386400
C	2.12150200	1.19057300	0.07032900
C	3.34575200	1.15917200	1.00783000
C	-2.65275400	-1.70036100	-1.32077100
C	-2.31712500	1.25755700	-0.36112800
C	-2.56706100	2.24882700	0.78623800
C	-1.64262300	1.93591600	-1.56314700
O	0.95939200	-0.64218600	2.66357900
C	1.59832800	-1.33314100	-0.47996500
C	2.99450000	-1.87710500	-0.13248800
C	1.32979000	-1.34970200	-1.99686300
C	2.50786800	1.58555200	-1.36313100
H	-1.43867500	-1.96652700	0.43988600
H	-3.30096000	0.86760200	-0.70013800
H	1.44163000	1.97880700	0.45882000
H	0.86464300	-2.03335100	-0.02094000
H	-3.05855300	-2.73335700	-1.29365100
H	-3.45140300	-1.04821900	-1.73373600
H	-1.79893200	-1.68772200	-2.02781100
H	-3.81346800	-2.34657100	1.12945300
H	-3.04591900	-1.05344700	2.11135100
H	-4.21060600	-0.63313900	0.80664700
H	-3.15202800	3.12404500	0.43397400

H	-3.12362600	1.77021800	1.61733700
H	-1.60053800	2.61414900	1.19187300
H	-2.25155400	2.78752300	-1.93230300
H	-0.64657000	2.33025400	-1.27237100
H	-1.50027600	1.22313500	-2.40130900
H	2.96309100	2.59816600	-1.34923200
H	3.26067200	0.89935000	-1.80290500
H	1.62816100	1.62033000	-2.03630800
H	3.75889400	2.18517300	1.10733700
H	3.05971400	0.80161300	2.01630100
H	4.16037700	0.51271200	0.62492600
H	3.08673000	-2.91933500	-0.50510300
H	3.80494900	-1.28707500	-0.60713900
H	3.15504900	-1.88758600	0.96321100
H	1.30403800	-2.39895300	-2.35925900
H	0.35340500	-0.88195100	-2.23314000
H	2.11418900	-0.82248100	-2.57401500

17, singlet carbene: E(BP86/def2-SVP)= -735.296 a.u.

C	0.67978500	0.25052300	-0.76572500
N	1.78139600	-0.01134600	-0.10936700
N	-1.67805000	-0.08165100	-0.15979600
C	-0.48726500	-0.63580300	-0.61638000
O	-0.40284700	-1.80292600	-1.05807800
C	-2.87632100	-0.94382000	-0.23185600
C	-1.63567900	1.31294600	0.31124400
C	1.93609100	-1.08243800	0.94276900
C	3.03723500	0.72854700	-0.50207500
C	2.70580100	-2.28591100	0.38008600
C	2.52669500	-0.53610100	2.25000200
H	0.89936600	-1.41816700	1.14293700
H	3.85750100	0.29019600	0.10407800
C	3.34506500	0.50054000	-1.98628000
C	2.90976300	2.21624400	-0.15343100
C	-3.73186800	-0.93035900	1.04361000
C	-3.71531200	-0.71218200	-1.50544200
H	-2.43211900	-1.95756800	-0.33757200
C	-1.55681000	1.45442000	1.84525000
H	-0.65544300	1.67103900	-0.10178700
C	-2.72061000	2.21803100	-0.29430200
H	2.49901600	-1.32890400	3.02614000
H	3.58597800	-0.22251200	2.14269000
H	1.94519300	0.32900500	2.62916600
H	2.73940400	-3.09784900	1.13648400
H	2.18781700	-2.67042100	-0.52006900
H	3.75547200	-2.03103000	0.12096600
H	4.28066900	1.02463300	-2.27123100
H	3.46648300	-0.57852000	-2.21040900
H	2.50866300	0.88654500	-2.60324600
H	3.84014600	2.75831900	-0.42058200
H	2.06583000	2.66038600	-0.72026600
H	2.72227900	2.36760100	0.92953200
H	-4.46966900	-1.52038200	-1.61347500
H	-4.26074300	0.25314600	-1.48993300
H	-3.06670100	-0.73550300	-2.40391200
H	-4.52343100	-1.70426900	0.96373400
H	-3.12625700	-1.16009300	1.94356500
H	-4.24377400	0.04115000	1.20753100
H	-1.29743600	2.49856400	2.12137500
H	-2.51754800	1.20820700	2.34137800
H	-0.77609500	0.78719100	2.26445300
H	-2.53175900	3.27145600	0.00005900
H	-2.71443000	2.16703500	-1.40113500
H	-3.73847400	1.95731300	0.06347800

TS-17-16-iPr, transition state of beta-lactam formation: E(BP86/def2-SVP)= -735.276 a.u.

C	-0.55812000	0.22337500	-0.37313400
N	-1.81042400	-0.10281800	-0.07541900
N	1.71751000	0.16657900	0.04772700
C	0.62922800	-0.63321700	-0.34155900
O	0.70741800	-1.81722600	-0.72863600
C	3.10866000	-0.16054500	-0.33314600
C	1.28741100	1.38829500	0.65210100
C	-2.92987500	0.74875700	-0.59477500
C	-2.26676100	-1.31622400	0.68612200
C	-3.21730800	1.89880100	0.38476000
C	-2.66875700	1.24488400	-2.01989800
H	-3.82106600	0.08344900	-0.62209600

H	-3.25543700	-1.03050600	1.11136600
C	-2.46646700	-2.49025700	-0.29026400
C	-1.35150300	-1.68471100	1.85623400
C	3.60955100	-1.39431300	0.44234100
C	3.26494300	-0.32976400	-1.85485200
H	3.71562600	0.71428100	-0.01496500
C	1.94629400	2.65940100	0.14176200
C	1.03622900	1.36843900	2.15367100
H	-3.56109500	1.78669300	-2.39650600
H	-1.79871600	1.92969600	-2.05440800
H	-2.45759200	0.39776100	-2.70295800
H	-4.09856700	2.48673500	0.05430800
H	-3.42394200	1.52124300	1.40770000
H	-2.34754600	2.58664000	0.43986000
H	-2.87101000	-3.37411500	0.24581600
H	-3.18192800	-2.22836500	-1.09752900
H	-1.49048000	-2.75109900	-0.74733000
H	-1.82935300	-2.49491800	2.44459800
H	-0.37093400	-2.05766400	1.50281300
H	-1.19443900	-0.82172800	2.53438500
H	4.32744900	-0.51399700	-2.11801000
H	2.65916200	-1.18825100	-2.20698300
H	2.92861900	0.57923000	-2.39470000
H	4.66941100	-1.60736000	0.18930000
H	3.54236900	-1.22962900	1.53745500
H	2.99480900	-2.27799400	0.18076400
H	1.39582400	3.55286400	0.50376000
H	2.99494100	2.76921400	0.50732700
H	1.96951700	2.69331700	-0.96703100
H	0.34061500	2.17915100	2.46201200
H	0.60905400	0.40060100	2.47899400
H	1.98445000	1.52379400	2.72273000
H	0.02015600	1.32489900	-0.03391500

16-iPr, beta-lactam: E(BP86/def2-SVP)= -735.325 a.u.

C	0.36564000	-0.24057900	-0.56934000
N	1.60655800	0.00617700	0.14463600
N	-1.71975100	-0.03783600	-0.18664800
C	-0.77758400	0.80562900	-0.74102900
O	-0.86825400	1.90957000	-1.26209700
C	-3.18877600	-0.02005100	-0.25557200
C	-0.78070200	-1.18079100	0.04789600
C	2.76404900	-0.70447800	-0.46655100
C	1.89924200	1.38300600	0.63408300
C	4.09371400	-0.44975700	0.26428200
C	2.52800800	-2.22530600	-0.51474500
H	2.89798100	-0.36116700	-1.52987800
H	2.83035500	1.27053500	1.22443000
C	2.18339500	2.41111100	-0.48355200
C	0.86179800	1.90293300	1.64290800
C	-3.81327900	-0.72253000	0.96134800
C	-3.71671100	1.41838800	-0.38425500
H	-3.49668400	-0.58399100	-1.17147700
C	-1.13723700	-2.40388500	-0.80801400
C	-0.57033200	-1.54705200	1.51698000
H	3.37663700	-2.72481300	-1.02606500
H	2.44827600	-2.64185900	0.51208800
H	1.61014900	-2.49785400	-1.06962600
H	4.87783400	-1.10043300	-0.17376100
H	4.45384400	0.59366300	0.17621900
H	4.00751300	-0.70464600	1.34228800
H	2.51907200	3.37568700	-0.04599300
H	2.98972100	2.06069400	-1.16223400
H	1.27317400	2.60042200	-1.08681700
H	1.24068900	2.84061600	2.10072900
H	-0.11321400	2.14666300	1.17891300
H	0.70133400	1.17018700	2.45962100
H	-4.81983800	1.39427900	-0.49992500
H	-3.47732600	2.00449100	0.52764800
H	-3.26888600	1.94548600	-1.24611200
H	-4.91946300	-0.69487400	0.87998600
H	-3.51252600	-1.78632400	1.03826900
H	-3.52331500	-0.21119500	1.90277400
H	-0.37749000	-3.20357700	-0.69207800
H	-2.11312300	-2.83836800	-0.50449000
H	-1.20266300	-2.14017300	-1.88481400
H	0.35008800	-2.15605900	1.62290600
H	-0.44231100	-0.64060700	2.13784300

H	-1.42059700	-2.13399200	1.91996600
H	0.58180400	-0.59756200	-1.60619500

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