The Stabilities of Carbenes: Independent Measures for Singlets and Triplets

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Table S1. G3MP2 enthalpies and free energies of carbocations and related species (hartrees).^a Point groups^b and selected geometric data

Carbocation and Precursors (Point Group)	H (298K, 1 atm.) ^c	G (298K, 1 atm.) ^c	Geometric Feature(s) ^d
water (C _{2v})	-76.338150	-76.359525	d = 0.967, Φ = 104.0
dihydrogen hydride ⁻	-1.166608 333.1 kcal/mol ^e	-1.181367	d = 0.738
methyl ⁺ (D _{3h})	-39.389408	-39.410565	d(CH) = 1.088
methanol (C _s)	-115.546805	-115.573786	
¹ CH ₂ (C _{2v})	-39.062446	-39.083873	d = 1.109, Φ = 102.1 ^f
³ CH ₂ (C _{2v})	-39.077421	-39.099613	d = 1.077, Φ = 131.6 ^f
ethyl ⁺ (C _{2v}) ^g	-78.685172	-78.712034	
ethane (D _{3d})	-79.645106	-79.670991	
¹ methylcarbene (C _s)	-78.309638	-78.335971	Φ = 104.4
³ methylcarbene (C _s)	-78.314313	-78.342715	Φ = 131.5
isopropyl ⁺ (C ₁ /C ₂)	-117.947741	-117.977014	
propane (C ₁ /C _{2v})	-118.877260	-118.908473	
¹ dimethylcarbene (C _{2v})	-117.555846	-117.584265	Φ = 110.1
³ dimethylcarbene ((C ₁ /C _{2v}))	-117.552875	-117.585962	Φ = 130.5
allyl ⁺ (C _{2v})	-116.726685	-116.755305	Φ (CCC) = 117.6, d(C1C3) = 2.365
propene (C ₁ /C _s)	-117.665968	-117.696070	d(C=C) = 1.337
¹ vinylcarbene (C ₁)	-116.339787	-116.369397	d(C=C) = 1.363
³ vinylcarbene (C ₁ /C _s)	-116.352932	-116.383133	d(C=C) = 1.369
propargyl ⁺ (C _{2v})	-115.472843	-115.500946	d(C≡C) = 1.232
propyne ((C _{3v}))	-116.438306	-116.466220	d(C≡C) = 1.218
¹ ethynylcarbene (C ₁ /C _s)	-115.118567	-115.146896	d(C≡C) = 1.237
³ ethynylcarbene (C ₁ /C ₂)	-115.136804	-115.166782	d(C≡C) = 1.266

Table S1. G3MP2 enthalpies and free energies of carbocations and related species (hartrees).^a Point groups^b and selected geometric data.

Carbocation and Precursors (Point Group)	H (298K, 1 atm.) ^c	G (298K, 1 atm.) ^c	Geometric Feature(s) ^d
diethynylCH ⁺ (C _{2v})	-191.522795	-191.556352	d(C-C) = 1.229, 1.379, Φ = 122.6
diethynylmethane (C _{2v})	-192.455962	-192.489501	d(C-C) = 1.219, 1.466, Φ = 112.6
carbene, singlet (C _{2v})	-191.164154	-191.197553	d(C-C) = 1.233, 1.375, Φ = 120.7
carbene, triplet (C _{2v} /D _{∞h})	-191.184226	-191.214080	d(C-C) = 1.219, 1.315, Φ = 179.9
cyclopropyl ⁺ (C _{2v}) ^h	-116.671950	-116.700693	d(C-C) = 1.529, 1.423, 1.423
cyclopropane (D _{3h})	-117.651296	-117.678193	d(C-C) = 1.501
¹ cyclopropylidene (C _{2v})	-116.329949	-116.357737	d(CH ₂ -CH ₂) = 1.482
³ cyclopropylidene (C _{2v})	-116.303364	-116.331868	d(CH ₂ -CH ₂) = 1.595
cyclopropylcarbiny ⁺ , bisected (C ₁ /C _s)	-155.971663	-156.004676	d(CH-CH ₂) = 1.646
methylcyclopropane (C ₁ /C _s)	-156.886817	-156.918983	d(CH-CH ₂) = 1.502
¹ cyclopropylcarbene, anti (C ₁ /C _s)	-155.568634	-155.600468	d(CH-CH ₂) = 1.566
³ cyclopropylcarbene (C ₁)	-155.558226	-155.591165	d(CH-CH ₂) = 1.513
cyclobutyl ⁺ (C ₁ /C _s)	-155.973935	-156.006101	d(C1-C3) = 1.649
cyclobutane (D _{2d})	-156.886113	-156.916095	d(C1-C3) = 2.14, Θ (CCCC) = 21.7
¹ cyclobutylidene (C ₁ /C _s)	-155.573496	-155.604680	d(C1-C3) = 1.711
³ cyclobutylidene (C ₁ /C _{2c})	-155.556857	-155.589091	d(C1-C3) = 2.06, flat ring
isobutyl ⁺	NA	NA	rearranges to <i>t</i> -butyl ⁺
isobutane (C _{3v})	-158.112675	-158.146020	d(C-C)=1.526
¹ 2-methylpropylidene (C ₁)	-156.778872	-156.813984	d(C1-C2) = 1.455, d(C2-CH ₃) = 1.515, 1.577, Φ (C1CC) = 80.5, 117.7
³ 2-methylpropylidene (C ₁)	-156.779857	-156.815193	d(C1-C2) = 1.481, Φ (HC1C2) = 131.5
cyclopentany ⁺ (C ₁ /C ₂)	-195.230433	-195.264036	d(C2-H) = 1.094, 1.126
cyclopentane (C ₂)	-196.149476	-196.185264	d(C-H) = 1.094-1.097

¹ cyclopentylidene (C ₁ /C ₂)	-194.838704	-194.872042	d(C2-H) = 1.094, 1.113
³ cyclopentylidene (C ₁ /C ₂)	-194.822892	-194.857226	d(C2-H) = 1.094, 1.100

Table S1. G3MP2 enthalpies and free energies of carbocations and related species (hartrees).^a Point groups^b and selected geometric data.

Carbocation and Precursors (Point Group)	H (298K, 1 atm.) ^c	G (298K, 1 atm.) ^c	Geometric Feature(s) ^d
cyclohexadienyl ⁺ (C _{2v})	-232.103032	-232.136479	d(HC-H) = 1.109, Φ (HCH) = 100.6
cyclohexa-1,3-diene (C ₂)	-232.976477	-233.011170	d(C=C) 1.353
cyclohexa-1,4-diene (D _{2h})	-232.976695	-232.010494	d(C=C) 1.343
¹ cyclohexa-2,4-dienylidene (C ₁ /C _s)	-231.677009	-231.710628	d(C=C) = 1.382, 1.357
³ cyclohexa-2,4-dienylidene (C ₁ /C _s)	-231.680697	-231.715976	d(C=C) = 1.409, 1.341
¹ cyclohexa-2,5-dienylidene (C _{2v})	-231.673546	-2231.707632	d(C=C) = 1.363
6,6-dimethylcyclohexa-2,4-dienyl ⁺ (C _{2v})	-310.577328	-310.617208	d(C-Me) = 1.569, Φ (MeCMe)=107.3
6,6-dimethyl-1,3-cyclohexadiene (C ₁)	-311.450117	-311.490462	d(C-Me) = 1.527, 1.535
¹ 6,6-dimethylcyclohexa-2,4-dien-1-ylidene (C _s)	-310.144203	-310.185296	d(C-Me) = 1.550
³ 6,6-dimethylcyclohexa-2,4-dien-1-ylidene (C _s)	-310.152664	-310.194298	d(C-Me) = 1.539
phenonium ⁺ (C _s /C _{2v})	-309.383355	-309.421655	d(C1-C3) = d(C2-C3) = 1.625
spiro[2.5]octa-4,6-diene (C ₁)	-310.225925	-310.264568	d(C1-C3)=1.504, d(C2-C3)=1.516
¹ spiro[2.5]octa-4,6-dien-8-ylidene (C _s)	-308.945403	-308.983587	d(C1-C3)=d(C2-C3) = 1.594
³ spiro[2.5]octa-4,6-dien-8-ylidene (C _s)	-308.933579	-308.973014	d(C1-C3)=d(C2-C3) = 1.527
spiro[2.5]octa-4,7-diene (C ₁ C _{2v})	-310.227307	-310.266052	d(C1-C3) = d(C2-C3) = 1.517
¹ spiro[2.5]octa-4,7-dien-6-ylidene (C _{2v})	-308.931445	-308.969189	d(C1-C3) = d(C2-C3) = 1.555
³ spiro[2.5]octa-4,7-dien-6-ylidene (C _{2v})	-308.932797	-308.971599	d(C1-C3) = d(C2-C3) = 1.528

^aOne hartree = 627.51 kcal/mol. GAUSSIAN 03, Revision B.04, Frisch, M. J, et al., Gaussian, Inc., Pittsburgh PA, 2003. The G3 method uses a composite "...recipe involving a variety of different models with the purpose of providing accurate thermochemical data." See Hehre, W. J. *A Guide to Molecular Mechanics and Quantum Chemical Calculations*; Wavefunction, Inc.: Irvine, CA, 2003, p 252. Results are estimated to be accurate within about 2 kcal/mol. ^bA slash indicates the species has virtually the higher symmetry. ^cA scaling factor of 0.9135 was used for vibrations. ^dDistances (d) are in Å; angles (Φ) and dihedrals (Θ) are in degrees. ^eThis is the experimental electronic energy of the hydride ion. ^fThe experimental values for the angles are ~102° for the singlet and ~137° for the triplet. See (a) Hoffmann, R.; Zeiss, G. D.; Van Dine, G. W. *J. Am. Chem. Soc.* **1968**, 90, 1485. (b) Shavitt, I. *Tetrahedron* **1985**, 41, 1531. Also See Moss, R. A.; Platz,

M. S.; Jones, M., Jr., Eds., *Reactive Intermediate Chemistry*; Wiley-Interscience: New York, 2004, p 277. This volume has five chapters covering various aspects of carbene chemistry. ^gThe ethyl cation is a symmetrical hydrogen-bridged structure. Some of the data listed here were reported by Keeffe, J. R.; More O'Ferrall, R. A. *ARKIVOC* **2008**, 183, and in Gronert, S.; Keeffe, J. R.; More O'Ferrall, R. A. *J. Org. Chem.* **2009**, *74*, 5250. ^hCyclopropyl⁺ is calculated to be a stable species at HF/6-31G*. At HF/6-311+G** it is a transition state, $\nu = 284\text{ cm}^{-1}$. At MP2/6-31G* and at MP2/6-311+G** it is also a transition state, $\nu = 543\text{ cm}^{-1}$, shown by an irc calculation in the latter case to correspond to disrotatory ring opening leading to allyl⁺. ⁱSpiro[2.5]octa-4,6-dienyl⁺, the conjugate acid of the C8 carbene.

Table S2. Calculated G3MP2 enthalpies and free energies for singlet and triplet substituted arylcarbenes, benzylic cations, and toluenes, 298K.^a

Substituent (point group) ^{b, c}	Enthalpy	Free Energy
<i>meta</i> -substituents		
NH ₂ ^d		
singlet carbene (C1)	-325.016804	-325.055682
triplet carbene (C1)	-325.019243	-325.059673
cation (C1)	-325.441365	-325.480079
toluene (C1)	-326.341067	-326.382783
OH		
singlet carbene, syn (Cs)	-344.883001	-344.921265
triplet carbene, syn (Cs)	-344.885711	-344.925546
cation, syn (Cs)	-345.297740	-345.336303
toluene, syn (C1)	-346.207573	-346.248307
SH		
singlet carbene, syn (C1/Cs)	-667.491099	-667.531105
triplet carbene, gauche (C1)	-667.493694	-667.536125
cation, anti (C1/Cs)	-667.904223	-667.944852
toluene, gauche (C1)	-668.816601	-668.860424
CH ₃		
singlet carbene (Cs)	-308.971987	-309.009895
triplet carbene (Cs)	-308.974587	-309.014026
cation (Cs)	-309.390434	-309.428700
toluene (Cs)	-310.297361	-310.335106
H		
singlet carbene (C1/Cs)	-269.733859	-269.769278
triplet carbene (Cs)	-269.737248	-269.774168
cation (C1/C2v)	-270.148084	-270.183853
toluene (Cs)	-271.058922	-271.097378
Cl		
singlet carbene (Cs)	-728.893955	-728.932818
triplet carbene (Cs)	-728.897886	-728.938297
cation (Cs)	-729.301667	-729.340830
toluene (C1)	-730.221177	-730.263382

Table S2. Calculated G3MP2 enthalpies and free energies for singlet and triplet substituted arylcarbenes, benzylic cations, and toluenes, 298K.^a

Substituent (point group)^{b, c}		Enthalpy	Free Energy
F	singlet carbene (Cs)	-368.893713	-368.931277
	triplet carbene (Cs)	-368.898044	-368.937103
	cation (Cs)	-369.300176	-369.338025
	toluene (C1)	-370.220844	-370.261652
CHO	singlet carbene (C1/Cs)	-382.920172	-382.960662
	triplet carbene C1/Cs)	-382.923739	-382.965726
	cation (Cs)	-383.324922	-383.365857
	toluene (C1)	-384.247069	-384.291173
CF ₃	singlet carbene (C1/Cs)	-606.474676	-606.521184
	triplet carbene (C1/Cs)	-606.479487	-606.527324
	cation (C1/Cs)	-606.877086	-606.922894
	toluene (C1)	-607.802891	-607.852198
CN	singlet carbene (C1Cs)	-361.859893	-361.899855
	triplet carbene (C1Cs)	-361.864759	-361.906302
	cation (C1Cs)	-362.256674	-362.297040
	toluene (C1)	-363.189248	-363.232025
NO ₂	singlet carbene (C1/Cs)	-474.021024	-474.063302
	triplet carbene (Cs)	-474.026409	-474.070345
	cation (C1/Cs)	-474.417238	-474.459727
	toluene (C1)	-475.350737	-475.395962
<u><i>para</i>-substituents</u>			
NH ₂ ^d	singlet carbene (C1)	-325.026133	-325.064051
	triplet carbene (C1)	-325.019682	-325.060163
	cation (C1/C2v)	-325.473764	-325.512243
	toluene (C1/Cs)	-326.340208	-326.382712

Table S2. Calculated G3MP2 enthalpies and free energies for singlet and triplet substituted arylcarbenes, benzylic cations, and toluenes, 298K.^a

Substituent (point group)^{b, c}		Enthalpy	Free Energy
OH	singlet carbene, anti (C1/Cs)	-344.887961	-344.925854
	triplet carbene, anti (Cs)	-344.885256	-344.925206
	cation (Cs)	-345.317642	-345.355767
	toluene (C1)	-346.206695	-346.247340
SH	singlet carbene, anti (C1/Cs)	-667.494670	-667.534761
	triplet carbene, gauche (C1)	-667.494602	-667.537070
	cation (C1/Cs)	-667.924423	-667.964242
	toluene, gauche (C1)	-668.817201	-668.857514
CH ₃	singlet carbene (C1)	-308.972498	-309.013834
	triplet carbene ((C1)	-308.973748	-309.016508
	cation (C1/Cs)	-309.395811	-309.436744
	toluene (C1/C2v)	-310.295312	-310.338750
CH ₂ F	singlet carbene, syn (C1/Cs)	-408.125396	-408.167374
	triplet carbene, gauche (C1)	-408.127774	-408.171544
	cation, syn (Cs)	-408.542081	-408.583810
	toluene, gauche (C1)	-409.449969	-409.495981
H	singlet carbene (C1/Cs)	-269.733859	-269.769278
	triplet carbene (Cs)	-269.737248	-269.774168
	cation (C1/C2v)	-270.148084	-270.183853
	toluene (Cs)	-271.058922	-271.097378
Cl	singlet carbene (Cs)	-728.895960	-728.934772
	triplet carbene (Cs)	-728.898186	-728.938625
	cation (Cs/C2v)	-729.311071	-729.350189
	toluene (C1/Cs)	-730.220808	-730.263099
F	singlet carbene (C1/Cs)	-368.897063	-368.934525
	triplet carbene (Cs)	-368.897421	-368.938625
	cation (Cs/C2v)	-369.310824	-369.348669
	toluene (C1/Cs)	-370.220126	-370.261662

Table S2. Calculated G3MP2 enthalpies and free energies for singlet and triplet substituted arylcarbenes, benzylic cations, and toluenes, 298K.^a

Substituent (point group)^{b, c}	Enthalpy	Free Energy
CHO		
singlet carbene, syn (C1/Cs)	-382.918336	-382.959036
triplet carbene, syn (C1/Cs)	-382.925543	-382.967482
cation (C1/Cs)	-383.323626	-383.364817
toluene (C1)	-384.247410	-384.290470
CF ₃		
singlet carbene (C1/Cs)	-606.473877	-606.520520
triplet carbene (C1)	-606.479914	-606.527560
cation (C1/Cs)	-606.876315	-606.919153
toluene (C1Cs)	-607.803920	-607.849109
CN		
singlet carbene (C1/Cs)	-361.859551	-361.899589
triplet carbene (Cs)	-361.866549	-361.908096
cation (Cs/C2v)	-362.258230	-362.298644
toluene (C1/Cs)	-363.189357	-363.232975
NO ₂		
singlet carbene (Cs)	-474.020145	-474.062878
triplet carbene (Cs)	-474.028074	-474.071911
cation (Cs/C2v)	-474.416035	-474.456412
toluene (C1/Cs)	-475.350963	-475.396554
<u>miscellaneous arylcarbenes, arylcarbenium ions, and hydrogen adducts</u>		
¹ methylphenylcarbene (C ₁)	-308.976428	-309.016947
³ methylphenylcarbene (C _s)	-308.977731	-309.019702
1-phenylethyl ⁺ (C ₁ /C _s)	-309.398541	-309.438369
ethylbenzene (C ₁)	-310.291540	-310.332061
¹ diphenylcarbene (C ₁ /C ₂)	-500.401930	-500.449636
³ diphenylcarbene (C ₁ /C ₂)	-500.397719	-500.447984
diphenylmethyl ⁺ (C ₁ /C ₂)	-500.828936	-500.876368
diphenylmethane (C ₁ /C ₂)	-501.706233	-501.755817
¹ cycloheptatrienylCH ⁺ (C ₁ /C _s) ^e	-308.063758	-308.102283
³ cycloheptatrienylCH ⁺ (C ₁ /C _s) ^e	-308.078349	-308.117701
cycloheptatrienyl-CH ₂ ²⁺ (C ₁ /C _{2v})	-308.282367	-308.320943
Tr ⁺ -CH ₃ (C ₁ /C _s)	-309.402742	-308.444426

Table S2. Calculated G3MP2 enthalpies and free energies for singlet and triplet substituted arylcarbenes, arylcarbenium ions, and hydrogen adducts, 298K.^a

Substituent (point group) ^{b, c}	Enthalpy	Free Energy
¹ cyclopentadienyl-CH ⁻ (C1/Cs) ^f	-231.152477	-231.186034
³ cyclopentadienyl-CH ⁻ (C1/Cs) ^f	-231.110355	-231.145881
cyclopentadienyl-CH ₃ ⁻ (C1/Cs)	-232.414305	-232.450668
cyclopentadienyl-CH ₂ (fulvene), (C _{2v})	-231.771867	-231.805762
¹ cyclopropenyl-CH ⁺ (C _{2v}) ^g	-153.474208	-153.504721
³ cyclopropenyl-CH ⁺ (Cs) ^g	-153.441209	-153.472758
cyclopropenyl-CH ₂ ²⁺ , bisected (C _{2v})	-153.559305	-153.589789
cyclopropenyl ⁺ -CH ₃ (C1/Cs)	-154.773389	-154.806584
¹ cyclopropenyliene (C _{2v}) ^h	-115.155559	-115.182369
³ cyclopropenyliene (C _{2v}) ^h	-115.041309	-115.069307
cyclopropenyl ⁺ (D _{3h})	-115.514741	-115.541773
cyclopropene (C _{2v})	-116.400192	-116.428330

^aIn hartrees; 1 hartree = 627.51 kcal/mol. See also Gronert, S.; Keeffe, J. R.; More O'Ferrall, R. A. *J. Org. Chem.* **2009**, 74, 5250. ^bA slash indicates the structure has virtually the higher symmetry. In all the carbenes the carbenic C-H bond is coplanar with the ring to within 0.5 degree, usually to within 0.1 degree. ^cThe term syn indicates that the substituent group is coplanar with the ring, and oriented *toward* the CH hydrogen in the most stable structure as is the case for singlet and triplet *m*-CH=O (C=O bond), and the C-F bond in *m*-CH₂F singlet and cation, and for *p*-O-H (triplet and singlet) and S-H (singlet). The term anti indicates the substituent's orientation is coplanar with the ring and oriented preferentially *away* from the CH hydrogen as for singlet and triplet *m*-OH, singlet *m*-SH, and *m*-CH₂F, cation, and for singlet and triplet *p*-CH=O (C=O) bond). *Gauche* indicates neither syn nor anti as, for example, the triplet *m*-SH, the *m*-C-F bond in CH₂F, toluene, and for the S-H bond in the *p*-triplet. ^dThe NH₂ group is pyramidal except in the cations where it is coplanar with the ring. ^eThe carbenic C-H unit is perpendicular to the ring in the singlet, and in the ring plane in the triplet. ^fThe carbenic C-H unit is bent and in the ring plane in the singlet, and perpendicular to the ring in the triplet. ^gThe carbenic C-C-H unit is linear in the singlet, and is bent and in the ring plane in the triplet. ^hBond lengths in the singlet are 1.329, 1.427, 1.427 Å, averaging 1.394 ± 0.043. In the triplet they are 1.337, 1.457, 1.457, averaging 1.417 ± 0.053 Å. In the triplet, there is a dramatic drop in the population of the beta spin electron on one of the carbons pi p-orbital. A node bisects the carbenic carbon and the shorter bond, with the unpaired electron of the pi-system localized on two of the carbons.

Table S3. Calculated G3MP2 enthalpies and free energies for acyclic heteroatom- and cyano-substituted carbenes (X-CH, X₂C), their conjugate acid carbocations (X-CH₂⁺, X₂C⁺), and the hydrogenation products of the singlet carbenes, 298K.^a

Heteroatom substituent, X or X ₂ (point group) ^b	Enthalpy	Free Energy
amino		
carbene, singlet (C _s)	-94.418137	-94.444005
carbene, triplet (C ₁ /C _s) ^c	-94.363160	-94.390627
cation (C _{2v})	-94.803643	-95.829102
aminomethane (C _s)	-95.680373	-95.707627
diamino		
carbene, singlet (C _{2v})	-149.735223	-149.764784
carbene, triplet (C ₁)	-149.643828	-149.675665
cation (C _{2v})	-150.132983	-150.161555
diaminomethane (C ₁)	-150.957875	-150.988365
hydroxy		
carbene, singlet, anti (C _s)	-114.265735	-114.291250
carbene, singlet, syn (C _s)	-114.258381	-114.283931
carbene, triplet (C ₁)	-114.224891	-114.251949
cation (C _s)	-114.617745	-114.643599
methanol (C _s)	-115.546803	-115.573787
methoxy		
carbene, singlet (C ₁ /C _s)	-153.486245	-153.516175
carbene, triplet (C ₁)	-153.441506	-153.473048
cation (C ₁ /C _s)	-153.856324	-153.886692
methoxymethane (C ₁ /C _{2v})	-154.764705	-154.795430
methoxy, methyl ^d		
carbene, singlet (C ₁ /C _s)	-192.732530	-192.767564
carbene, triplet (C ₁)	-192.680467	-192.716627
cation (C ₁ /C _s)	-193.118961	-193.153791
methoxyethane (C ₁)	-194.002110	-194.036497
dimethoxy		
carbene, singlet (C ₁ /C _{2v})	-267.898677	-267.936473
carbene, triplet (C ₁)	-267.803324	-267.842607
cation (C ₁ /C _s)	-268.274132	-268.312094
dimethoxymethane (C ₁)	-269.130363	-269.168036
fluoro		
carbene, singlet (C _s)	-138.255744	-138.281045
carbene, triplet (C _s)	-138.232451	-138.258692
cation (C _{2v})	-138.573018	-138.598051
fluoromethane (C _{3v})	-139.565138	-139.590375

Table S3. Calculated G3MP2 enthalpies and free energies for acyclic heteroatom- and cyano-substituted carbenes (X-CH, X₂C), their conjugate acid carbocations (X-CH₂⁺, X₂C⁺), and the hydrogenation products of the singlet carbenes, 298K.^a

Heteroatom substituent, X or X ₂ (point group) ^b	Enthalpy	Free Energy
difluoro		
carbene, singlet (C _{2v})	-237.472104	-237.499393
carbene, triplet (C _{2v})	-237.382459	-237.410931
cation (C _{2v})	-237.752071	-2237.779496
difluoromethane (C _{2v})	-238.733471	-238.761428
phosphino		
carbene, singlet (C ₁ /C _s)	-380.621801	-380.650027
carbene, triplet (C ₁ /C _s) ^c	-380.600403	-380.630063
cation (C ₁ /C _{2v})	-380.993967	-381.022489
phosphinomethane (C _s)	-381.922034	-381.951323
sulfhydryl (thio)		
carbene, singlet, anti (C _s)	-436.878179	-436.905308
carbene, singlet, syn (C _s)	-436.876251	-436.903405
carbene, triplet (C ₁)	-436.845312	-436.874047
cation (C _s)	-437.239391	-437.266785
methanethiol (C _s)	-438.164939	-438.193701
methylthio		
carbene, singlet (C ₁ /C _s)	-476.117188	-476.149135
carbene, triplet (C ₁)	-476.077456	-476.110665
cation (C ₁ /C _s)	-476.491272	-476.524014
methylthiomethane (C ₁ /C _{2v})	-477.394868	-477.427742
chloro		
carbene, singlet (C _s)	-498.252971	-498.279628
carbene, triplet (C _s)	-498.241909	-498.269415
cation (C _{2v})	-498.592261	-498.618544
chloromethane (C _{3v})	-499.568852	-499.595425
dichloro		
carbene, singlet (C _{2v})	-957.437542	-957.467576
carbene, triplet (C _{2v})	-957.402860	-957.433884
cation (C _{2v})	-957.767645	-957.797600
dichloromethane (C _{2v})	-958.722710	-958.753338
silylmethyl (H ₃ SiCH ₂)		
carbene, singlet ^c	NA	NA
carbene, triplet (C ₁)	-368.571863	-368.606655
silylethene (C ₁ /C _s) ^c	-368.689821	-368.723016

cation (C_1/C_s) ^e	-368.983056	-369.015720
silylethane (C_1/C_s)	-369.899776	-369.933734

Table S3. Calculated G3MP2 enthalpies and free energies for acyclic heteroatom- and cyano-substituted carbenes (X-CH, X_2C), their conjugate acid carbocations ($X-CH_2^+$, X_2C^+), and the hydrogenation products of the singlet carbenes, 298K.^a

Heteroatom substituent, X or X_2 (point group) ^b	Enthalpy	Free Energy
silyl (H_3Si)		
carbene, singlet (C_1)	-329.318535	-329.348210
carbene, singlet ts (C_1) ^f	-329.319669	-329.348245
carbene, triplet (C_1/C_s)	-329.347351	-329.378466
cation (C_1/C_s) ^g	-329.756741	-329.787215
silylmethane (C_{3v})	-330.672257	-330.702415
disilyl (H_3Si) ₂		
carbene, singlet (C_1/C_s)	-619.583421	-619.620268
carbene, triplet (C_1/D_{3h})	-619.618423	-619.658157
cation ^h (C_{2v})	-620.039501	-620.073111
disilylmethane (C_1/C_{2v})	-620.931153	-620.968131
nitroso ($O=N$) ⁱ		
carbene, singlet ($C_{\infty v}$)	-168.361078	-168.386568
carbene, triplet, syn (C_s)	-168.264792	-168.293841
cation (C_{2v})	-168.623743	-168.651761
nitrosomethane (C_1/C_s)	-169.562238	-169.591776
diaminomethyl ⁺		
carbene, singlet (C_1)	-188.025054	-188.058079
carbene, singlet, ts (C_2) ^j	-188.013890	-188.046179
carbene, triplet (C_1/C_s)	-188.044379	-188.077590
dication (C_1/C_{2v})	-188.169612	-188.204254
1,1-diaminoethyl ⁺ (C_1/C_s)	-189.383023	-189.416879
imino ($HN=$) ^k		
carbene, singlet ($C_{\infty v}$)	-93.272356	-93.295578
carbene, triplet (C_s)	-93.102080	-93.127896
cation ($C_{\infty v}$)	-93.564035	-93.587267
formaldimine (C_s)	-94.475420	-94.501158
oxo ($O=$) ^l		
carbene, singlet ($C_{\infty v}$)	-113.185455	-113.207857
carbene, triplet ($C_{\infty v}$)	-112.965319	-112.988898
cation ($C_{\infty v}$)	-113.409011	-113.431831
formaldehyde (C_{2v})	-114.348622	-114.373393
cyano		
carbene, singlet (C_s)	-131.204112	-131.231848

carbene, triplet (C_s)	-131.219901	-131.248381
cation (C_{2v})	-131.510055	-131.537901
acetonitrile (C_s/C_{3v})	-132.540533	-132.569076

Table S3. Calculated G3MP2 enthalpies and free energies for acyclic heteroatom- and cyano-substituted carbenes ($X-CH$, X_2C), their conjugate acid carbocations ($X-CH_2^+$, X_2C^+), and the hydrogenation products of the singlet carbenes, 298K.^a

Heteroatom substituent, X or X_2 (point group) ^b	Enthalpy	Free Energy
dicyano		
carbene, singlet (C_{2v})	-223.334049	-223.366463
carbene, triplet ($C_{2v}/D_{\infty h}$)	-223.352783	-223.383524
cation (C_s/C_{2v})	-223.618017	-223.651786
dicyanomethane (C_{2v})	-224.651325	-224.684100
nitro		
carbene, singlet ^m		
carbene, triplet (C_1C_s)	-243.360457	-243.391741
cation (C_1C_s) ⁿ	-243.700451	-243.730423
nitromethane (C_1C_s)	-244.699114	-244.732671
dinitro		
carbene, singlet (C_1) ⁿ	-447.655041	-447.694872
carbene, triplet (C_1/C_2)	-447.623663	-447.662894
cation (C_1) ⁿ	-447.946742	-447.984000
dinitromethane (C_1/C_s)	-448.970014	-449.009531
amino, cyano		
carbene, singlet (C_1/C_s)	-186.553559	-186.584431
carbene, triplet (C_1/C_s)	-186.501973	-186.535445
cation (C_s)	-186.900293	-186.931462
aminocyanomethane (C_1)	-187.804322	-187.836384
amino, nitro		
carbene, singlet (C_1)	-298.719662	-298.753902
carbene, triplet (C_1)	-298.653582	-298.689412
cation (C_1/C_s)	-299.056169	-299.089655
aminonitromethane (C_1/C_s)	-299.978719	-300.013659

^aIn hartrees; 1 hartree = 627.51 kcal/mol. ^bA slash indicates the structure has virtually the higher symmetry. ^cThese triplets have pyramidal NH_2 (PH_2) group. The C-H bond is perpendicular and *anti* to the NH_2 (PH_2) plane. ^dThese species have *two* substituents, methoxy and methyl. ^esinglet silylmethylcarbene rearranges to silylethene upon optimization at the MP2 level. The silylethyl cation is a symmetrical, silyl-bridged structure. ^fThis is the transition state for rotation about the Si-C bond. $\Delta H^\ddagger = -0.7$ kcal/mol and $\Delta G^\ddagger = 0.0$ kcal/mol. ^gThe silylmethyl cation, $H_3SiCH_2^+$, rearranges to the methylsilyl cation, $CH_3SiH_2^+$, upon optimization. ^hThe cation rearranges to a symmetrical (C_{2v}) bridged structure, a hydrogen bridging the two silicons. A second cation, $H_3Si-CH_2-SiH_2^+$, is 10.6 kcal/mol less stable. ⁱThe singlet carbene is hydrogen cyanide-*N*-oxide,

O-N≡C-H. The cation is O=N=CH₂⁺. ^jThis ts has a linear CCH structure, and corresponds to 2,2-diaminovinyl cation, $\nu = 623\text{ cm}^{-1}$ (CCH bending). ^kThe singlet carbene is hydrogen isocyanide, HN≡C. The cation is protonated hydrogen cyanide, HN≡CH⁺. ^lThe singlet carbene is carbon monoxide. See also Gronert, S.; Keeffe, J. R.; More O'Ferrall, R. A. *J. Org. Chem.* **2009**, *74*, 5250. ^mThis structure is that of nitrosocarbaldehyde (C₁). The C-N-O angle is 110.0°, and the O-C-N-O dihedral is 25.7°. ⁿAn oxygen from a nitro group partially bridges to the carbon in the cations, and in the dinitro singlet.

Table S4. Calculated G3MP2 enthalpies and free energies for miscellaneous 1,3-diheterocyclic carbenes,, their C2 conjugate acids (carbene-CH⁺), the C2 hydrogenation products of the carbenes (carbene-CH₂), and their 4,5-dihydro analogs (carbeneH₂) 298K.^a

Carbene, (point group) ^b	Enthalpy	Free Energy
Set 1, X = Y = NH		
1. imidazol-2-ylidene, singlet (C _{2v})	-225.820192	-225.850622
1. triplet, cis (C ₁ C _s) ^c	-225.683581	-225.716425
triplet ts (C _{2v}) ^c	-225.653707	-225.687258
imidazole (C _s)	-225.861555	-225.892512
1-CH ⁺ (imidazolium+) (C _{2v}) ^{c, d}	-226.218697	-226.249074
1-CH ₂ cis-1,3-diazacyclopent-4-ene) (C ₁ /C _s) ^d	-227.010068	-227.042386
1-CH ₂ trans-1,3-diaza-cyclopent-4-ene) (C ₁) ^d	-227.010676	-227.042947
1H ₂ . 4,5-dihydroimidazol-2-ylidene, singlet (C ₁ /C ₂) ^e	-227.000781	-227.033920
1H ₂ triplet (C ₁)	-226.885642	-226.919711
triplet ts (C ₁ /C ₂) ^f	-227.001779	-227.033594
1H ₂ -CH ⁺ (C ₂)	-227.403599	-227.436440
1H ₂ -NH ⁺ (C ₁)	-227.325872	-227.358944
1H ₂ -CH ₂ , (cis-1,3-diazacyclopentane) (C _s) ^g	-228.216362	-228.250115
1H ₂ -CH ₂ , (trans-1,3-diazacyclopentane) (C ₁ /C ₂) ^g	-228.215533	-228.249829
Set 2, X = Y = O		
2. 1,3-dioxol-2-ylidene, singlet (C _{2v})	-265.519783	-265.549762
2. triplet (C ₁)	-265.381822	-265.415100
2-CH ⁺ (C _{2v})	-265.871359	-265.901403
2-OH ⁺ (C ₁ /C _s) ^h	-265.778152	-265.811179
2-CH ₂ (1,3-dioxole) (C ₁ /C _s) ⁱ	-266.740024	-266.772172
2-CH ₂ , ts (C _{2v}) ⁱ	-266.739573	-267.769771
2H ₂ . 4,5-dihydro-1,3-dioxol-2-ylidene (C ₂ /C _{2v})	-266.720970	-266.753058
2H ₂ -CH ⁺ (C ₁ /C _{2v})	-267.085185	-267.117807
2H ₂ -CH ₂ (1,3-dioxolane) (C ₂) ^j	-267.948326	-267.982335
2H ₂ -OH ⁺	NA ^k	NA ^k
Set 3, X = O, Y = NH		
3. 1-oxa-3-azacyclopent-4-ene-2-ylidene, singlet (C ₁ /C _s)	-245.668231	-245.699084
3. triplet (C ₁)	-245.529957	-245.563568
3-CH ⁺ (C ₁ /C _s)	-246.046399	-246.077237
3-OH ⁺ (C ₁ /C _s) ^l	-245.934554	-245.966623
3-CH ₂ (1-oxa-3-aza-cyclopent-4-ene) (C ₁) ^m	-246.876764	-246.908697

Table S4. Calculated G3MP2 enthalpies and free energies for miscellaneous 1,3-diheterocyclic carbenes,, their C2 conjugate acids (carbene-CH⁺), the C2 hydrogenation products of the carbenes (carbene-CH₂), and their 4,5-dihydro analogs (carbeneH₂) 298K.^a

Carbene, (point group) ^b	Enthalpy	Free Energy
3H₂ , 1-oxa-3-azacyclopentane-2-ylidene (C ₁) ⁿ	-246.860054	-246.893580
3H₂-CH⁺ (C ₁ /C _s)	-247.246818	-247.279694
3H₂-OH⁺ (C ₁) ^o	-247.152554	-247.185718
3H₂-CH₂ (1-oxa-3-azacyclopentane) (C ₁) ^p	-248.084336	-248.117893
Set 4, X = Y = PH		
4 , 1,3-diphosphol-2-ylidene, singlet, cis (C ₁ /C _s) ^q	-798.232022	-798.267028
4 , triplet, cis (C ₁ /C _s) ^q	-798.195012	-798.231277
4 , singlet, trans (C ₁ /C ₂) ^q	-798.237437	-798.272789
4 , triplet, trans (C ₁ /C ₂) ^q	-798.195832	-798.232195
4-CH⁺ , trans (C ₁ /C ₂) ^q	-798.624664	-798.659885
4-CH⁺ , cis, ts (C _s) ^q	-798.618174	-798.652924
4-CH₂ , cis (C _s) ^q	-799.515194	-799.551134
4-CH₂ , trans (C ₁) ^q	-799.515650	-799.549970
4H₂ 4,5-dihydro-1,3-diphospholane-2-ylidene, singlet, cis (C ₁) ^{q, r}	-799.429888	-799.466193
4H₂ , triplet, cis (C ₁) ^{q, r}	-799.403330	-799.440624
4H₂ , singlet, trans (C ₁ /C ₂) ^q	-799.427012	-799.472891
4H₂ , triplet, trans (C ₁ /C ₂) ^q	-799.401923	-799.439494
4H₂-CH⁺ , cis (C ₁) ^{q, r}	-799.821593	-799.858274
4H₂-CH⁺ , trans (C ₁ /C ₂) ^q	-799.827474	-799.864200
4H₂-CH₂ , cis (C ₁) ^{q, r}	-800.723018	-800.760129
4H₂-CH₂ , trans (C ₁) ^{q, r}	-800.719621	-800.756648
Set 5, X = Y = S		
5 , 1,3-dithiol-2-ylidene, singlet (C _{2v})	-910.768219	-910.801497
5 , triplet (C _s)	-910.677468	-910.714564
5-CH⁺ (C _{2v})	-911.141533	-911.174828
5-CH₂ (C _s)	-911.991562	-912.026526
5H₂ 1,3-dithiolan-2-ylidene, singlet (C ₂)	-911.955024	-911.989273
4H₂ triplet (C ₁)	-911.879860	-911.917052
4H₂-CH⁺ (C ₂)	-912.329966	-912.364793
4H₂-CH₂ (C ₂)	-913.196354	-913.233456

Table S4. Calculated G3MP2 enthalpies and free energies for miscellaneous 1,3-diheterocyclic carbenes,, their C2 conjugate acids (carbene-CH⁺), the C2 hydrogenation products of the carbenes (carbene-CH₂), and their 4,5-dihydro analogs (carbeneH₂) 298K.^a

Carbene, (point group) ^b	Enthalpy	Free Energy
Set 6, X = Y = NCH ₃		
6. <i>N,N'</i> -dimethyl-2-imidazol-2-ylidene singlet (C ₁ /C _{2v})	-304.276053	-304.315097
6. triplet (C ₁ C _s)	-304.136531	-304.176819
6-CH ⁺ (C ₁ /C _{2v})	-304.687816	=304.727437
6-CH ₂ cis (C ₁ /C _s)	-305.466380	-305.505389
Set 7, 4,5-dimethyl, X = Y = NH		
7. 4,5-dimethylimidazol-2-ylidene, singlet (C ₁ /C _{2v})	-304.297092	-304.336101
7. triplet (C ₁ C _s)	-304.163859	-304.204163
7-CH ⁺ (C ₁ /C _{2v})	-304.707585	-304.746958
7-CH ₂ (C ₁ /C _s)	-305.490261	-305.529965
Set 8, 4,5-difluoro, X = Y = NH		
8. 4,5-difluoroimidazol-2-ylidene, singlet (C _{2v})	-424.115589	-424.150520
8. triplet, trans C-F bonds (C ₁ /C ₂)	-424.010714	-424.048324
8. triplet, ts (C _{2v}) ^s	-423.965863	-424.003280
8-CH ⁺ (C _{2v})	-424.496013	-424.530746
8-CH ₂ cis (C ₁ /C _s) ^t	-425.321175	-425.357596
Set 9, 4,5-dimethyl, X = Y = NCH ₃		
9. 4,5, <i>N,N'</i> -tetramethylimidazol-2-ylidene, singlet (C ₁ //C _{2v})	-382.753558	-382.799488
9. triplet, trans, twisted ring (C ₁ /C _s) ^t	-382.616075	-382.663618
8-CH ⁺ (C ₁ //C _{2v})	-383.175874	-383.222420
8-CH ₂ , trans, twisted ring (C ₁) ^t	-383.943265	-383.989279
Set 10, 4,5-disilyl, X = Y = SiH ₃		
10. 4,5, <i>N,N'</i> -tetrasilylimidazol-2-ylidene, singlet (C ₁ //C _{2v})	-1386.894560	-1386.950521
10. triplet, trans, twisted ring (C ₁) ^t	-1386.762263	-1386.822519
10-CH ⁺ (C ₁)	-1387.306083	-1387.361728
10-CH ₂ , cis (C ₁) ^t	-1388.088095	-1389.147253

Table S4. Calculated G3MP2 enthalpies and free energies for miscellaneous 1,3-diheterocyclic carbenes,, their C2 conjugate acids (carbene-CH⁺), the C2 hydrogenation products of the carbenes (carbene-CH₂), and their 4,5-dihydro analogs (carbeneH₂) 298K.^a

Carbene, (point group) ^b	Enthalpy	Free Energy
Set 11 , 3-membered ring, X = Y = NH		
11 . 1,2-diaziridin-3-ylidene, singlet, trans (C ₂) ^t	-148.432232	-148.459403
11 . singlet, ts (C _{2v}) ^u	-148.372102	-148.399243
11 . triplet, trans (C ₂) ^t	-148.344558	-148.372626
11-CH⁺ , trans (C ₁ /C ₂) ^t	-148.755714	-148.784703
11-CH⁺ , cis (C _s) ^t	-148.747795	-148.776897
11-CH⁺ , open form, exo, exo (C _{2v}) ^v	-148.713598	-148.741614
11-CH₂ , trans (C ₂) ^t	-149.701610	-149.729031
Set 12 , 4-membered ring, X = Y = NH		
12 . 1,3,13-diazetid-2-ylidene, singlet, trans (C ₁ /C ₂) ^t	-187.720838	-187.751699
12 . singlet, cis, ts (C ₁ /C _s) ^{t,w}	-187.720976	-187.751203
12 . triplet, trans (C ₂) ^t	-187.620713	-187.651523
12-CH⁺ , trans (C ₁ C ₂) ^t	-188.113494	-188.144773
12-CH₂ , cis, (C _s) ^{t,x}	-188.949105	-188.979806
Set 13 , 4-membered ring, X = NH, Y = CH or CH ₂		
13 . azet-2-ylidene, singlet (C ₁) ^y	-170.423677	-170.453310
13 . triplet (C ₁ /C _s)	-170.361113	-170.392383
13-CH⁺ (C ₁ /C _s)	-170.787658	-170.817874
13-CH₂ (C ₁) ^y	-171.703968	-171.733986
13H₂ . azetid-2-ylidene, singlet (C ₁ /C _s)	-171.665555	-171.695976
13H₂ triplet (C ₁) ^y	-171.590799	-171.622536
13H₂-CH⁺ (C ₁ /C _s)	-172.063261	-172.093642
13H₂-CH₂ (C ₁) ^y	-172.917912	-172.948878
Set 14 , 5-membered ring, X = NH, Y = CH		
14 . imidazole-5-ylidene, singlet (C _s)	-225.789219	-225.820249
14 . triplet (C ₁)	-225.685194	-225.718225
14-CH⁺ (imidazolium ⁺) (C _{2v})	-226.218697	-226.249074
14-CH₂ (C ₁)	-226.961892	-226.994637

^aIn hartrees; 1 hartree = 627.51 kcal/mol. ^bA slash indicates the structure has virtually the higher symmetry. ^cThe descriptors cis and trans refer to the two N-H bonds. The triplet ts has $\nu = 285$ cm⁻¹ corresponding to planarization of the ring (wobbling about the H-N-C-N-H moiety).

^dProtonation at C2 of the carbene gives the same conjugate acid as protonation at N1 of imidazole, namely, the imidazolium ion. The descriptors cis and trans refer to the two N-H

bonds. The ring skeletons have an envelope shape. ^cThe torsional angle about the C4-C5 bond is 21.5°. ^fThis ts, $\nu = 98\text{ cm}^{-1}$, involves torsion about the C4-C5 bond. ^gThe descriptors cis and trans refer to the two N-H bonds. The ring skeleton of the cis isomer has an envelope shape. The torsional angle about the C4-C5 bond in the trans isomer is 38.4°. ^hProtonation at oxygen results in C-O cleavage giving $(\text{HO-CH=CH-C}\equiv\text{O})^+$ in which the separated C and O are 2.600 Å apart. ⁱThe stable form has an envelope-shaped ring skeleton. The ts is planar, $\nu = 110\text{ cm}^{-1}$. ^jThe torsional angle about C4-C5 is 40.5°. ^kThe oxygen-protonated conjugate acid did not converge. It was undergoing fragmentation to a complex between protonated acetaldehyde and carbon monoxide. ^lThe C2-O bond is somewhat elongated at 1.481 Å while the C2=N bond is short at 1.323 Å. ^mThe ring skeleton has an envelope shape with the CH₂ unit out of the plane. ⁿThe torsional angle about C4-C5 is 12.8°. ^oThe ring skeleton has the envelope shape with C5 out of the plane. The C2-O bond is elongated to 1.520 Å and the C2=N is short at 1.299 Å. ^pThe ring is completely buckled. The torsional angle about C4-C5 is 15.4°. ^qThe descriptors cis and trans refer to the two P-H bonds. In series **4** and **4H₂** the phosphorus atoms are pyramidal, more so in the triplet than the singlet carbenes. The carbenium ions also have pyramidal phosphorus atoms, and those in the hydrogenation products are most pyramidal of all with bond angles less than 100°. The cis carbenium ion, **4-CH⁺**, is a transition state (ts), $\nu = 360\text{ cm}^{-1}$, inversion about phosphorus, $\Delta H^\ddagger = 4.1\text{ kcal/mol}$ (from the trans isomer). ^rThe two phosphorus atoms in these species are not identical. For the singlet, cis carbene and the cis carbenium ion (ts) one phosphorus is virtually planar, the other decisively pyramidal. In the others both phosphorus atoms are pyramidal. ^sThis triplet is a second-order saddle point, $\nu = 310\text{ and }226\text{ cm}^{-1}$, corresponding, respectively, to symmetric and asymmetric, pyramidalization at the nitrogens. Its C4-N and C5-N bonds are short at 1.318 Å, and the C2-N bonds long at 1.598 Å. ^tThe nitrogens are pyramidal in these species; cis and trans refer to the orientation of the N-H bonds. In the singlet the carbenic angle is 65.8°, and the N-N distance is 1.508 Å. In the triplet these values are 71.6° and 1.629 Å. ^uTransition state for flattening the nitrogen valences; $\nu = 1313, 1099\text{ cm}^{-1}$, corresponding to asymmetric and symmetric inversion at the nitrogens, respectively. ^vA stable structure at HF/6-31G*, but a transition state for disrotatory ring opening/closing at the MP2 level of theory. The term exo, exo indicates that the coplanar N-H bonds are directed away from each other. ^wTransition state for inversion at one nitrogen, $\nu = 260\text{ cm}^{-1}$. The ring is folded. ^xThe ring is folded, and the N-H hydrogens are in pseudo-equatorial positions. ^yThe ring is folded and the nitrogen is pyramidal.

Table S5. G3MP2 cartesian coordinates for compounds in this study: 91 sets of singlet and triplet carbenes, their conjugate acid carbenium ions, and their hydrogenation products.

miscellaneous carbene sets

carbene, singlet

H	0.000000	0.862238	-0.523024
C	0.000000	0.000000	0.174341
H	0.000000	-0.862238	-0.523024

carbene, triplet

H	0.000000	0.982420	-0.331211
C	0.000000	0.000000	0.110404
H	0.000000	-0.982420	-0.331211

methyl+

H	0.000000	1.088256	0.000000
C	0.000000	0.000000	0.000000
H	0.942457	-0.544128	0.000000
H	-0.942457	-0.544128	0.000000

methane

H	0.628989	0.628989	0.628989
C	0.000000	0.000000	0.000000
H	-0.628989	-0.628989	0.628989
H	0.628989	-0.628989	-0.628989
H	-0.628989	0.628989	-0.628989

methylcarbene, singlet

H	0.642644	0.084212	1.088060
C	0.594625	0.021248	-0.026953
H	1.028370	0.953400	-0.407828
C	-0.854314	-0.190034	-0.035579
H	1.192475	-0.847522	-0.305958
H	-1.305352	0.822627	0.000922

methylcarbene, triplet

H	0.453670	-1.023029	0.885452
C	-0.049474	-0.615418	0.000000
H	0.453670	-1.023029	-0.885452
C	-0.049474	0.859926	0.000000
H	-1.073573	-0.997648	0.000000
H	0.759921	1.576657	0.000000

ethyl+, symmetrically H-bridged ion

H	0.000002	0.000000	1.044690
C	-0.690209	0.000000	-0.062470

H	-1.244834	-0.935696	-0.073763
C	0.690208	0.000000	-0.062469
H	-1.244834	0.935696	-0.073763
H	1.244834	-0.935696	-0.073764
H	1.244834	0.935696	-0.073764

ethane

H	0.000000	1.018689	1.157275
C	0.000000	0.000000	0.762189
H	0.882211	-0.509345	1.157275
C	0.000000	0.000000	-0.762189
H	-0.882211	-0.509345	1.157275
H	0.882211	0.509345	-1.157275
H	-0.882211	0.509345	-1.157275
H	0.000000	-1.018689	-1.157275

dimethylcarbene, singlet

H	-0.876222	1.214375	-0.816643
C	0.000000	1.220860	-0.149777
H	0.876222	1.214375	-0.816643
C	0.000000	0.000000	0.703596
H	0.000000	2.150168	0.421162
C	0.000000	-1.220860	-0.149777
H	0.876222	-1.214375	-0.816643
H	-0.876222	-1.214375	-0.816643
H	0.000000	-2.150168	0.421162

dimethylcarbene, triplet

H	1.496391	-0.744967	-0.885353
C	1.341346	-0.113076	0.000000
H	1.496391	-0.744967	0.885353
C	0.000000	0.505866	0.000000
H	2.123105	0.650792	0.000000
C	-1.341346	-0.113076	0.000000
H	-1.496391	-0.744966	0.885354
H	-1.496391	-0.744968	-0.885353
H	-2.123105	0.650792	-0.000001

isopropyl+

H	2.035511	0.348745	-0.591284
C	1.277159	-0.196331	-0.021389
H	1.241144	-1.263120	-0.238951
C	0.000002	0.462386	-0.000038
H	1.596946	-0.072394	1.042106
C	-1.277180	-0.196286	0.021396
H	0.000066	1.555072	-0.000030
H	-1.241120	-1.263047	0.239162
H	-1.596964	-0.072717	-1.042125

H	-2.035472	0.348844	0.591308
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propane

H	-1.303387	-0.904599	0.883524
C	-1.266727	-0.260173	0.000000
H	-1.303321	-0.904699	-0.883454
C	0.000000	0.587968	0.000000
H	-2.166508	0.361265	-0.000069
C	1.266727	-0.260173	0.000000
H	0.000000	1.245164	0.876738
H	0.000000	1.245167	-0.876737
H	1.303320	-0.904701	-0.883452
H	1.303388	-0.904597	0.883525
H	2.166508	0.361265	-0.000071

isopropylcarbene, singlet, (2-methylpropylidene)

C	-0.124061	-0.184920	0.429721
C	0.739663	-1.088262	-0.316389
H	1.547355	-1.392571	0.377703
C	-1.506809	0.086264	-0.126348
C	0.965313	0.843751	-0.062807
H	-0.113954	-0.208386	1.524952
H	0.487005	1.587855	-0.696427
H	1.717886	0.359808	-0.728306
H	1.484793	1.279773	0.787763
H	-2.194427	-0.712375	0.165367
H	-1.461869	0.110375	-1.217714
H	-1.911426	1.034525	0.241599

isopropylcarbene, triplet, (2-methylpropylidene)

C	0.010431	0.128874	-0.346649
C	0.373358	1.470006	0.167274
H	1.296144	2.035075	0.110550
C	-1.401057	-0.259951	0.099481
C	1.032463	-0.927800	0.092901
H	0.016276	0.164119	-1.448166
H	1.042910	-1.013801	1.182930
H	2.041215	-0.666957	-0.238800
H	0.777141	-1.905147	-0.328367
H	-2.136337	0.477568	-0.231363
H	-1.450161	-0.324173	1.190044
H	-1.678362	-1.233451	-0.314866

isobutyl+, NA, structure rearranges to t-butyl+

isobutane

H	-0.885472	1.984741	0.261334
C	0.000000	1.450293	-0.096216

H	0.000000	1.494137	-1.190832
C	0.000000	0.000000	0.376871
H	0.885472	1.984741	0.261334
C	-1.255990	-0.725146	-0.096216
H	0.000000	0.000000	1.475163
C	1.255990	-0.725146	-0.096216
H	-1.293960	-0.747068	-1.190832
H	-2.161572	-0.225529	0.261334
H	-1.276100	-1.759212	0.261334
H	1.293960	-0.747068	-1.190832
H	1.276100	-1.759212	0.261334
H	2.161572	-0.225529	0.261334

cyclopropanylcarbene, singlet, anti

H	-0.639338	1.247946	-1.057633
C	-0.845480	0.724720	-0.133530
C	-0.846369	-0.723962	-0.134221
C	0.394724	-0.000949	0.487663
H	-1.437864	1.258215	0.601071
H	-0.640946	-1.246469	-1.058898
H	-1.439727	-1.257333	0.599685
C	1.517839	-0.000053	-0.372951
H	0.401706	-0.001357	1.578584
H	2.431883	0.000463	0.255426

cyclopropanylcarbene, singlet, syn

H	-0.094785	1.517542	-0.698598
C	-0.476403	0.864144	0.077989
C	-1.006708	-0.471562	-0.294331
C	0.309268	-0.463793	0.440409
H	-0.847992	1.378264	0.955896
H	-0.980108	-0.733700	-1.347339
H	-1.864505	-0.846742	0.255892
C	1.534147	-0.039856	-0.131636
H	0.268325	-0.683936	1.505103
H	1.357239	0.034976	-1.225536

cyclopropanylcarbene, singlet, rot. Ts

H	-0.731103	1.315666	-1.027223
C	-0.826835	0.785742	-0.083754
C	-0.880887	-0.733425	-0.141874
C	0.338424	-0.037959	0.375492
H	-1.446582	1.290146	0.650908
H	-0.806932	-1.197592	-1.120337
H	-1.533719	-1.251318	0.552634
C	1.695024	-0.166870	-0.179199
H	0.502003	-0.112294	1.461991
H	2.061982	0.870460	-0.341961

cyclopropanylcarbene, triplet

H	-0.572226	1.322255	-1.030708
C	-0.788925	0.788272	-0.112369
C	-0.887375	-0.700990	-0.173393
C	0.327005	-0.065746	0.467447
H	-1.422254	1.322939	0.587499
H	-0.738545	-1.180153	-1.134375
H	-1.594479	-1.201506	0.478838
C	1.610290	-0.142253	-0.205113
H	0.350323	-0.117574	1.556242
H	2.411210	0.578336	-0.316932

cyclopropylcarbinyl+, bisected

H	1.451712	1.259082	0.641677
C	0.945183	0.707569	-0.145089
C	0.945303	-0.707284	-0.145738
C	-0.375335	-0.000488	0.535973
H	0.714559	1.258720	-1.049986
H	1.452184	-1.259352	0.640407
H	0.714899	-1.257581	-1.051205
H	-0.393402	-0.001006	1.618841
C	-1.509796	0.000115	-0.206528
H	-1.481250	0.000710	-1.294107
H	-2.490833	-0.000038	0.262660

cyclopropylcarbinyl+, perp ts

H	1.419593	1.236784	0.819703
C	0.930029	0.778519	-0.034179
C	1.000871	-0.739268	-0.113946
C	-0.282062	-0.020070	0.206171
H	0.968362	1.350535	-0.956011
H	1.506951	-1.261205	0.690274
H	1.035424	-1.224616	-1.084199
H	-0.703481	-0.241866	1.266646
C	-1.624262	0.000637	-0.120639
H	-2.213718	-0.916318	-0.077914
H	-2.160588	0.937776	-0.282942

methylcyclopropane

H	0.745647	-1.258665	-1.079421
C	0.950079	-0.752582	-0.140984
C	0.950074	0.752585	-0.140982
C	-0.179383	-0.000003	0.501601
H	1.662291	-1.266500	0.495719
H	0.745637	1.258670	-1.079417
H	1.662283	1.266506	0.495722
H	-0.184313	-0.000006	1.589208

C	-1.544296	0.000000	-0.136256
H	-2.117818	-0.886251	0.152567
H	-1.454821	-0.000085	-1.227087
H	-2.117755	0.886334	0.152436

cyclohexa-2,4-dienylidene, singlet

C	1.163881	-0.761271	0.000093
C	-0.095707	-1.556688	-0.000025
C	-1.254937	-0.718596	-0.000118
C	-1.215611	0.662440	0.000097
H	-2.237679	-1.189812	-0.000262
H	-2.149938	1.225582	0.000382
C	0.009862	1.403217	-0.000002
C	1.183470	0.721883	-0.000147
H	-0.018537	2.489144	-0.000030
H	2.137201	1.247876	-0.000180
H	1.761359	-1.139195	0.850561
H	1.761846	-1.139513	-0.849860

cyclohexa-2,4-dienylidene-to-benzene, singlet, ts

C	1.098249	-0.835783	0.020484
C	-0.193878	-1.547305	-0.092626
C	-1.287059	-0.617515	-0.026475
C	-1.151575	0.757609	0.033277
H	-2.298599	-1.020236	-0.073466
H	-2.040740	1.385768	0.087878
C	0.122105	1.391408	0.004372
C	1.245393	0.618091	-0.059938
H	0.185469	2.475962	-0.013477
H	2.234193	1.067593	-0.126064
H	0.938858	-1.096854	1.115790
H	1.981411	-1.411261	-0.265227

cyclohexa-2,4-dienylidene, triplet

H	-1.975935	-0.887827	0.872969
C	-1.356748	-0.625949	0.000005
H	-1.975957	-0.887837	-0.872940
C	-0.092043	-1.393933	-0.000006
C	1.161552	-0.909340	-0.000001
C	1.340794	0.488063	0.000002
H	2.022613	-1.571947	0.000001
C	0.193784	1.336783	0.000000
H	2.337493	0.915218	0.000005
C	-1.055418	0.853080	-0.000005
H	0.347782	2.412576	0.000005
H	-1.907524	1.527594	-0.000011

cyclohexa-2,5-dienylidene, singlet

C	0.000000	0.000000	1.588386
C	0.000000	1.208191	0.784522
C	0.000000	1.242927	-0.578007
H	0.000000	2.162480	1.311476
H	0.000000	2.188652	-1.120614
C	0.000000	0.000000	-1.378229
H	0.866603	0.000000	-2.060420
H	-0.866603	0.000000	-2.060420
C	0.000000	-1.242927	-0.578007
C	0.000000	-1.208191	0.784522
H	0.000000	-2.188652	-1.120614
H	0.000000	-2.162480	1.311476

cyclohexa-2,5-dienylidene, triplet

C	0.000000	0.000000	1.459911
C	0.000000	1.241963	0.796252
C	0.000000	1.257142	-0.547611
H	0.000000	2.167630	1.364327
H	0.000000	2.202718	-1.083394
C	0.000000	0.000000	-1.367965
H	0.868240	0.000000	-2.048619
H	-0.868240	0.000000	-2.048619
C	0.000000	-1.257142	-0.547611
C	0.000000	-1.241963	0.796252
H	0.000000	-2.202718	-1.083394
H	0.000000	-2.167630	1.364327

benzenonium+

H	0.853560	0.000000	-2.102107
C	0.000000	0.000000	-1.393602
H	-0.853560	0.000000	-2.102107
C	0.000000	1.250301	-0.632191
C	0.000000	-1.250301	-0.632191
H	0.000000	-2.189348	-1.180801
C	0.000000	-1.237553	0.742519
H	0.000000	-2.161791	1.311027
C	0.000000	0.000000	1.413244
C	0.000000	1.237553	0.742519
H	0.000000	0.000000	2.501959
H	0.000000	2.189348	-1.180801
H	0.000000	2.161791	1.311027

cyclohexa-1,3-diene

H	0.019551	1.268477	-2.048796
C	0.341311	0.682964	-1.181330
H	1.429650	0.545383	-1.278942
C	-0.341311	-0.682964	-1.181330

C	0.055589	1.417795	0.100698
H	-0.019551	-1.268477	-2.048796
H	-1.429650	-0.545383	-1.278942
C	-0.055589	-1.417795	0.100698
H	0.011201	2.504418	0.095651
C	0.055589	-0.728849	1.253342
H	-0.011201	-2.504418	0.095651
C	-0.055589	0.728849	1.253342
H	0.219629	-1.245752	2.195830
H	-0.219629	1.245752	2.195830

cyclohexa-1,4-diene

C	0.000009	-0.669330	1.248521
C	-0.000016	-1.500332	0.000000
H	0.000027	-1.203071	2.197416
H	0.871259	-2.172454	0.000000
H	-0.871331	-2.172403	0.000000
C	0.000009	0.669330	-1.248521
C	0.000009	-0.669330	-1.248521
H	0.000027	1.203071	-2.197416
H	0.000027	-1.203071	-2.197416
C	-0.000016	1.500332	0.000000
C	0.000009	0.669330	1.248521
H	0.000027	1.203071	2.197416
H	-0.871331	2.172403	0.000000
H	0.871259	2.172454	0.000000

6,6-dimethylcyclohexa-2,4-dienylidene, singlet

C	-1.656446	-0.039433	-1.251767
C	-0.742311	-0.034033	-0.000070
C	0.036629	1.233215	-0.000444
C	-0.042509	-1.355875	0.000010
C	-1.655417	-0.039077	1.252419
H	-2.291132	0.852932	1.255581
H	-1.059669	-0.046016	2.169320
H	-2.277732	-0.935203	1.233121
H	-1.061475	-0.046687	-2.169171
H	-2.292111	0.852613	-1.254674
H	-2.278819	-0.935500	-1.231701
C	1.392911	1.218266	-0.000154
H	-0.505158	2.180684	-0.000900
H	1.974076	2.136361	-0.000229
C	2.063981	-0.045886	0.000047
C	1.380218	-1.245994	-0.000262
H	3.155112	-0.046160	0.000359
H	1.974566	-2.160123	-0.000380

6,6-dimethylcyclohexa-2,4-dienylidene, triplet

C	-1.707309	-0.078198	-1.254964
C	-0.816115	-0.058395	-0.000002
C	0.025097	1.198547	-0.000009
C	0.103509	-1.223926	-0.000007
C	-1.707283	-0.078196	1.254980
H	-2.365960	0.796692	1.262481
H	-1.094917	-0.062550	2.159412
H	-2.327180	-0.979820	1.266142
H	-1.094962	-0.062553	-2.159409
H	-2.365987	0.796689	-1.262452
H	-2.327205	-0.979822	-1.266112
C	1.362578	1.203890	-0.000003
H	-0.530017	2.135793	-0.000012
H	1.894088	2.152153	0.000002
C	2.125906	-0.003095	0.000000
C	1.446791	-1.237001	-0.000005
H	3.209774	0.032099	0.000005
H	2.003320	-2.170449	-0.000003

6,6-dimethylcyclohexadienyl+

H	0.000000	0.000000	3.179408
C	0.000000	0.000000	2.090656
C	0.000000	1.232697	1.413907
C	0.000000	-1.232697	1.413907
C	0.000000	-1.233181	0.039266
H	0.000000	-2.161089	1.976103
H	0.000000	2.161089	1.976103
C	0.000000	1.233181	0.039266
H	0.000000	2.175870	-0.507002
C	0.000000	0.000000	-0.750649
H	0.000000	-2.175870	-0.507002
C	-1.263423	0.000000	-1.679804
C	1.263423	0.000000	-1.679804
H	1.237983	0.888888	-2.313490
H	1.237983	-0.888888	-2.313490
H	2.183216	0.000000	-1.092059
H	-1.237983	0.888888	-2.313490
H	-2.183216	0.000000	-1.092059
H	-1.237983	-0.888888	-2.313490

6,6-dimethylcyclohexa-2,4-diene

C	-2.140120	0.105714	-0.738146
C	-0.806446	0.012667	-0.000263
C	-0.005557	1.278040	-0.194562
C	-1.064287	-0.164921	1.501534
H	-1.607344	0.696957	1.902115
H	-0.120919	-0.261351	2.045662

H	-1.666250	-1.063189	1.682928
H	-1.983672	0.257786	-1.810702
H	-2.737616	0.941656	-0.358564
H	-2.721000	-0.813126	-0.602839
C	1.340931	1.270722	-0.130601
H	-0.548383	2.217320	-0.300277
H	1.902617	2.198552	-0.213239
C	2.066049	0.018805	0.066186
C	1.431763	-1.158552	-0.095014
H	3.117250	0.053222	0.342247
H	1.964692	-2.099400	0.023808
C	-0.002451	-1.174980	-0.544509
H	-0.023277	-1.142543	-1.646550
H	-0.495391	-2.110855	-0.252332

spiro[2.5]octa-4,6-dien-8-ylidene, singlet

C	-1.346558	0.006843	0.000000
C	-0.041451	0.611724	0.000000
C	-1.241732	-1.415381	0.000000
C	-0.040619	-2.112144	0.000000
H	-2.158814	-2.006215	0.000000
C	1.210091	-1.444431	0.000000
H	-0.045620	-3.202869	0.000000
C	1.223997	-0.075470	0.000000
H	2.135303	-2.014339	0.000000
H	2.164291	0.477593	0.000000
C	-0.040619	2.034459	0.718460
C	-0.040619	2.034459	-0.718460
H	-0.971080	2.206442	1.243378
H	0.876031	2.246300	1.257440
H	-0.971080	2.206442	-1.243378
H	0.876031	2.246300	-1.257440

spiro[2.5]octa-4,6-dien-8-ylidene, triplet

C	-0.130470	-1.227687	-0.000001
C	0.718927	-0.047606	-0.000001
C	-1.475480	-1.245874	0.000000
C	-2.159450	-0.015917	0.000001
H	-2.027185	-2.181807	0.000000
C	-1.411330	1.194883	0.000000
H	-3.243540	0.009953	0.000002
C	-0.069105	1.203335	-0.000002
H	-1.949476	2.138948	0.000003
H	0.483466	2.141080	-0.000003
C	2.053018	-0.078097	-0.743864
C	2.053017	-0.078096	0.743866
H	2.294746	-0.999617	-1.262542
H	2.336246	0.830703	-1.265312

H	2.294743	-0.999616	1.262545
H	2.336243	0.830704	1.265314

spiro[2.5]octa-4,6-dienyl+ (phenonium+)

C	-0.000001	0.080730	1.231681
C	0.000001	-0.623597	0.000000
C	-0.000001	1.465043	1.222816
C	-0.000001	2.149706	0.000000
H	-0.000002	2.017852	2.157105
C	-0.000001	1.465043	-1.222816
H	0.000000	3.237131	0.000000
C	-0.000001	0.080730	-1.231681
H	-0.000002	2.017852	-2.157105
H	-0.000002	-0.469462	-2.170942
C	-0.713259	-2.083564	0.000000
C	0.713264	-2.083560	0.000000
H	-1.260312	-2.259276	0.919958
H	-1.260312	-2.259276	-0.919958
H	1.260317	-2.259271	0.919958
H	1.260317	-2.259271	-0.919958
H	-0.000002	-0.469462	2.170942

spiro[2.5]octa-4,6-diene

C	0.715180	0.028429	-0.135903
C	-1.446355	-1.178470	0.107839
C	-2.077003	0.002586	0.260299
H	-1.948773	-2.112994	0.347326
C	-1.404741	1.254007	-0.076085
H	-3.092498	0.040343	0.647502
C	-0.069373	1.277026	-0.270862
H	-1.988425	2.169040	-0.140956
H	0.452674	2.212182	-0.470161
C	2.191686	0.052368	-0.418906
C	1.716823	-0.038321	1.000752
H	2.631147	-0.831055	-0.873155
H	2.626013	0.989938	-0.754024
H	1.816053	-0.988487	1.517371
H	1.820276	0.834952	1.637085
C	-0.067008	-1.217135	-0.492970
H	0.481919	-2.108370	-0.165900
H	-0.153635	-1.288485	-1.590077

spiro[2.5]octa-4,7-dien-6-ylidene, singlet

H	1.261639	0.915554	-2.229412
C	0.730582	0.000000	-1.994345
C	0.000000	0.000000	-0.621596
C	-0.730582	0.000000	-1.994345
H	1.261639	-0.915554	-2.229412

C	0.000000	1.231337	0.129774
C	0.000000	-1.231337	0.129774
H	-1.261639	0.915554	-2.229412
H	-1.261639	-0.915554	-2.229412
H	0.000000	-2.172768	-0.424416
C	0.000000	-1.199192	1.500625
H	0.000000	2.172768	-0.424416
C	0.000000	1.199192	1.500625
H	0.000000	-2.159641	2.017972
C	0.000000	0.000000	2.304577
H	0.000000	2.159641	2.017972

spiro[2.5]octa-4,7-dien-6-ylidene, triplet

H	1.265246	0.913752	-2.230004
C	0.743374	0.000000	-1.963623
C	0.000000	0.000000	-0.627488
C	-0.743374	0.000000	-1.963623
H	1.265246	-0.913752	-2.230004
C	0.000000	1.248065	0.156069
C	0.000000	-1.248065	0.156069
H	-1.265246	0.913752	-2.230004
H	-1.265246	-0.913752	-2.230004
H	0.000000	-2.188410	-0.391744
C	0.000000	-1.238562	1.502466
H	0.000000	2.188410	-0.391744
C	0.000000	1.238562	1.502466
H	0.000000	-2.167396	2.065259
C	0.000000	0.000000	2.166495
H	0.000000	2.167396	2.065259

spiro[2.5]octa-4,7-diene

H	2.355886	-0.913054	-1.264842
C	2.078131	0.000001	-0.747036
C	0.756786	0.000000	-0.000003
C	2.078072	-0.000001	0.747149
H	2.355885	0.913058	-1.264839
C	-0.039996	-1.242979	-0.000072
C	-0.039996	1.242979	-0.000072
H	2.355775	-0.913059	1.264978
H	2.355778	0.913055	1.264981
H	0.507490	-2.185715	-0.000168
C	-1.380613	-1.248742	-0.000067
H	0.507490	2.185716	-0.000167
C	-1.380613	1.248742	-0.000066
C	-2.212846	0.000000	0.000129
H	-1.910269	-2.199710	-0.000147
H	-1.910269	2.199709	-0.000147
H	-2.885453	0.000000	0.871596

H -2.885866 0.000000 -0.871014

vinylcarbene, singlet, anti

H -1.077205 -1.281730 -0.111567

C -1.093479 -0.205915 0.023792

C 0.073914 0.484789 -0.107881

H -2.023971 0.263884 0.334094

C 1.188882 -0.394634 -0.031676

H 0.078351 1.573291 -0.019971

H 2.006925 0.139116 0.492035

vinylcarbene, singlet, rotational ts

H 1.362268 -1.245210 -0.068062

C 1.186877 -0.179082 0.012364

C -0.054123 0.334989 0.012225

H 2.052261 0.468311 0.060150

C -1.370586 -0.188876 -0.166184

H -0.180699 1.431117 0.041761

H -1.806836 -0.456409 0.815719

vinylcarbene, triplet, anti

H -1.299176 -1.255713 0.000000

C -1.173304 -0.180045 0.000000

C 0.072259 0.386486 -0.000001

H -2.068013 0.428263 0.000001

C 1.256224 -0.311817 0.000000

H 0.141030 1.476587 0.000001

H 2.295090 -0.016887 0.000002

vinylcarbene, triplet, syn

H -1.128553 -1.325169 -0.000005

C -1.116526 -0.241623 -0.000001

C 0.060569 0.459974 0.000001

H -2.073126 0.264838 0.000005

C 1.311292 -0.110398 -0.000003

H 0.011516 1.547335 0.000001

H 1.658155 -1.134723 0.000015

allyl+

H 0.000000 1.178997 -1.301599

C 0.000000 1.182481 -0.213387

C 0.000000 0.000000 0.502648

H 0.000000 2.151277 0.280141

C 0.000000 -1.182481 -0.213387

H 0.000000 0.000000 1.587668

H 0.000000 -2.151277 0.280141

H 0.000000 -1.178997 -1.301599

propene

H	1.805488	0.142331	-0.879917
C	1.230458	-0.164128	0.000000
H	1.159716	-1.254923	-0.000912
C	-0.130219	0.461369	-0.000010
H	1.804793	0.140898	0.880875
C	-1.278865	-0.222075	0.000001
H	-0.164239	1.550111	-0.000014
H	-1.293126	-1.308306	-0.000018
H	-2.240879	0.278891	0.000039

ethynylcarbene, singlet

H	2.306162	0.142479	0.000030
C	1.251814	-0.026425	0.000007
C	0.016171	0.039806	-0.000015
C	-1.337797	-0.168152	-0.000005
H	-1.887288	0.786145	0.000052

ethynylcarbene, triplet

H	2.297084	0.166347	0.129566
C	1.263854	-0.037212	-0.039232
C	0.000006	0.019048	0.000033
C	-1.263865	-0.037375	0.039119
H	-2.297055	0.166890	-0.129089

ethynylCH₂⁺ (propargyl⁺)

H	0.000000	0.000000	2.418196
C	0.000000	0.000000	1.340013
C	0.000000	0.000000	0.108023
C	0.000000	0.000000	-1.248665
H	0.000000	0.936921	-1.807213
H	0.000000	-0.936921	-1.807213

propyne

H	0.000000	0.000000	2.498858
C	0.000000	0.000000	1.432831
C	0.000000	0.000000	0.214800
C	0.000000	0.000000	-1.246063
H	0.000000	1.021388	-1.636088
H	-0.884548	-0.510694	-1.636088
H	0.884548	-0.510694	-1.636088

cyclopropanylidene, singlet

C	0.000000	0.000000	0.991622
C	0.000000	0.740401	-0.313137
H	-0.909176	1.289322	-0.548022
C	0.000000	-0.740401	-0.313137
H	0.909176	1.289322	-0.548022

H	-0.909176	-1.289322	-0.548022
H	0.909176	-1.289322	-0.548022

cyclopropanylidene, triplet

C	0.000000	0.000000	0.938530
C	0.000000	0.797518	-0.264916
H	-0.913768	1.276696	-0.613045
C	0.000000	-0.797518	-0.264916
H	0.913768	1.276696	-0.613045
H	-0.913768	-1.276696	-0.613045
H	0.913768	-1.276696	-0.613045

cyclopropyl+

H	-0.000480	-1.301611	1.178409
C	-0.000032	-0.213415	1.182348
C	-0.000032	-0.213415	-1.182348
C	-0.000032	0.502812	0.000000
H	0.000601	0.279774	2.151284
H	-0.000480	-1.301611	-1.178409
H	0.000601	0.279774	-2.151284
H	0.000330	1.587783	0.000000

cyclopropane

C	0.000000	0.866820	0.000000
H	0.000000	1.455591	0.910104
C	-0.750688	-0.433410	0.000000
H	0.000000	1.455591	-0.910104
H	-1.260579	-0.727796	0.910104
H	-1.260579	-0.727796	-0.910104
C	0.750688	-0.433410	0.000000
H	1.260579	-0.727796	0.910104
H	1.260579	-0.727796	-0.910104

cyclobutanylidene, singlet

C	0.000000	-0.812718	-0.481257
C	1.122027	-0.213450	0.206680
H	1.205729	-0.166180	1.300880
C	0.000000	0.871391	-0.183030
H	2.085805	-0.198229	-0.298662
C	-1.122027	-0.213450	0.206680
H	0.000000	1.365163	-1.146380
H	0.000000	1.573024	0.647499
H	-1.205725	-0.166180	1.300880
H	-2.085807	-0.198229	-0.298659

cyclobutanylidene, triplet

C	0.000000	-1.117792	-0.000071
C	-1.129723	-0.132052	0.000033

H	-1.770855	-0.131380	-0.888165
C	0.000000	0.944564	-0.000030
H	-1.770683	-0.131420	0.888358
C	1.129723	-0.132052	0.000033
H	0.000000	1.574881	0.891444
H	0.000000	1.574714	-0.891619
H	1.770855	-0.131380	-0.888165
H	1.770683	-0.131420	0.888358

cyclobutyl+

H	-0.000058	1.647481	0.465302
C	0.000093	0.864922	-0.287993
C	-1.186112	-0.143013	0.255860
C	1.186069	-0.143080	0.255907
C	-0.000078	-0.782651	-0.205882
H	-0.000095	-1.226419	-1.199799
H	0.000157	1.200453	-1.318256
H	2.085540	-0.252425	-0.341321
H	1.332040	0.052919	1.313806
H	-2.085880	-0.252203	-0.340925
H	-1.331537	0.053121	1.313835

cyclobutane

C	0.000000	1.071275	0.147380
C	1.071275	0.000000	-0.147380
H	1.344096	0.000000	-1.207067
C	0.000000	-1.071275	0.147380
H	1.986456	0.000000	0.451294
C	-1.071275	0.000000	-0.147380
H	0.000000	-1.344096	1.207067
H	0.000000	-1.986456	-0.451294
H	0.000000	1.986456	-0.451294
H	0.000000	1.344096	1.207067
H	-1.344096	0.000000	-1.207067
H	-1.986456	0.000000	0.451294

cyclopentanylidene, singlet

C	0.733029	0.957673	-0.215594
C	1.152803	-0.485595	0.108304
H	2.088932	-0.844905	-0.328642
C	-0.000012	-1.415937	-0.000009
H	1.282702	-0.585699	1.209233
C	-1.152814	-0.485572	-0.108298
C	-0.733007	0.957689	0.215591
H	0.813395	1.132851	-1.294984
H	1.341746	1.712921	0.289066
H	-1.282757	-0.585674	-1.209221
H	-2.088933	-0.844867	0.328682

H	-1.341708	1.712947	-0.289073
H	-0.813368	1.132876	1.294979

cyclopentanylidene, triplet

C	0.729651	-0.911253	0.238668
C	1.250692	0.495625	-0.128901
H	2.060228	0.833713	0.526663
C	0.000000	1.299919	0.000000
H	1.641037	0.509163	-1.156721
C	-1.250691	0.495625	0.128902
C	-0.729651	-0.911253	-0.238668
H	0.758277	-1.033384	1.326787
H	1.324673	-1.715484	-0.204176
H	-1.641037	0.509163	1.156721
H	-2.060228	0.833714	-0.526662
H	-1.324673	-1.715483	0.204176
H	-0.758278	-1.033384	-1.326787

cyclopentyl+

H	-0.000253	2.337538	0.000016
C	-0.000136	1.245856	-0.000010
C	-1.185180	0.436557	-0.101627
C	-0.735865	-0.999155	0.216515
C	0.736104	-0.998993	-0.216509
C	1.185072	0.436825	0.101606
H	-1.329580	0.538277	-1.213217
H	-2.099778	0.847976	0.336349
H	-0.830188	-1.172624	1.293207
H	-1.340237	-1.746323	-0.298795
H	0.830475	-1.172452	-1.293199
H	1.340649	-1.746012	0.298814
H	2.099631	0.848457	-0.336252
H	1.329307	0.538622	1.213230

cyclopentane

C	0.000000	0.000000	1.298624
C	0.000000	1.234235	0.366021
H	-0.998655	1.683573	0.337772
C	0.342408	0.682353	-1.021064
H	0.691885	2.014051	0.697838
C	-0.342408	-0.682353	-1.021064
H	1.426574	0.547662	-1.118543
H	0.016459	1.337508	-1.834980
C	0.000000	-1.234235	0.366021
H	-0.877146	0.004754	1.952302
H	0.877146	-0.004754	1.952302
H	-1.426574	-0.547662	-1.118543
H	-0.016459	-1.337508	-1.834980

H	-0.691885	-2.014051	0.697838
H	0.998655	-1.683573	0.337772

phenylcarbene sets

phenylcarbene, singlet

H	0.837508	-2.164679	0.000000
C	0.285621	-1.228504	-0.000001
C	-1.042291	1.235405	0.000000
C	1.041499	-0.032758	0.000001
C	-1.103321	-1.196885	0.000001
C	-1.762928	0.035609	0.000000
C	0.345744	1.201690	0.000000
C	2.477524	-0.172873	-0.000001
H	-1.678123	-2.119040	0.000000
H	-2.850327	0.063647	0.000000
H	0.919007	2.126999	0.000001
H	-1.571955	2.184413	-0.000001
H	2.892805	0.858554	0.000001

phenylcarbene, triplet, G3

H	2.144621	0.887634	0.000000
C	1.215002	0.326277	0.000000
C	-1.160476	-1.080725	0.000000
C	0.000000	1.028101	0.000000
C	1.229524	-1.039506	0.000000
C	0.045919	-1.756569	0.000000
C	-1.192213	0.285962	0.000000
C	-0.023672	2.436238	0.000000
H	2.179744	-1.566025	0.000000
H	0.064333	-2.841915	0.000000
H	-2.143614	0.810816	0.000000
H	-2.092767	-1.638517	0.000000
H	-0.836828	3.149344	0.000000

benzyl+

C	-2.345471	0.000000	-0.000002
C	-0.973350	0.000000	-0.000001
C	1.798984	0.000000	0.000003
C	-0.258792	-1.245203	-0.000002
C	-0.258791	1.245204	-0.000001
C	1.119284	1.232445	0.000000
C	1.119284	-1.232444	0.000000
H	-0.814708	-2.180063	-0.000012
H	-0.814708	2.180063	-0.000012
H	1.681769	2.160671	0.000002

H	1.681768	-2.160671	0.000002
H	2.886975	0.000000	0.000003
H	-2.913993	0.927303	0.000018
H	-2.913993	-0.927304	0.000017

benzyl+, perp ts

C	-2.371531	-0.000005	0.000007
C	-0.950219	-0.000013	-0.000015
C	1.820751	0.000013	0.000006
C	-0.267627	-1.235424	0.000001
C	-0.267650	1.235412	-0.000004
C	1.125081	1.207681	-0.000002
C	1.125103	-1.207669	0.000001
H	-0.801766	-2.180642	-0.000024
H	-0.801803	2.180623	0.000011
H	1.660961	2.152512	-0.000007
H	1.661000	-2.152490	0.000010
H	2.906291	0.000023	0.000005
H	-2.954050	0.000011	0.926873
H	-2.954082	-0.000006	-0.926839

toluene

C	-0.031126	2.417647	0.000000
C	0.008507	0.912745	0.000000
C	0.006381	-1.900630	0.000000
C	0.007243	0.195996	1.201554
C	0.007243	0.195996	-1.201554
C	0.007243	-1.198309	-1.204938
C	0.007243	-1.198309	1.204938
H	0.011874	0.737000	2.146329
H	0.011874	0.737000	-2.146329
H	0.011111	-1.736688	-2.149649
H	0.011111	-1.736688	2.149649
H	0.009217	-2.987618	0.000000
H	-1.062531	2.786079	0.000000
H	0.465472	2.825044	-0.884895
H	0.465472	2.825044	0.884895

phenylmethylcarbene, singlet

H	0.078315	-2.328066	-0.117863
C	0.443842	-1.306178	-0.060527
C	1.313315	1.343749	-0.045184
C	-0.508403	-0.267462	-0.160798
C	1.791475	-1.025884	0.132581
C	2.229045	0.301033	0.122446
C	-0.045591	1.069226	-0.150679
C	-1.886630	-0.684895	-0.317312

H	2.509565	-1.834254	0.243664
H	3.288100	0.523854	0.229279
H	-0.748555	1.888654	-0.274324
H	1.665125	2.372167	-0.072171
C	-2.882500	0.252629	0.247428
H	-3.106437	-0.236366	1.212563
H	-3.825599	0.232956	-0.305722
H	-2.587825	1.287748	0.476842

phenylmethylcarbene, triplet

H	0.201362	-2.343588	0.000000
C	0.519362	-1.305000	0.000000
C	1.303803	1.339747	0.000000
C	-0.459249	-0.299427	-0.000001
C	1.846336	-0.986280	0.000000
C	2.253911	0.336843	-0.000001
C	-0.030108	1.037214	0.000002
C	-1.831231	-0.624089	0.000002
H	2.588720	-1.779641	0.000000
H	3.310986	0.583922	-0.000002
H	-0.767984	1.834684	0.000003
H	1.616858	2.380389	0.000001
C	-3.062729	0.187470	-0.000001
H	-3.122564	0.830867	0.887562
H	-3.945805	-0.457020	-0.000451
H	-3.122139	0.831519	-0.887120

phenylmethylcarbenium+

H	0.703168	1.931663	-0.000008
C	-0.007076	1.111185	-0.000001
C	-1.855772	-1.033494	0.000001
C	0.446942	-0.243719	-0.000045
C	-1.362711	1.368911	-0.000005
C	-2.280636	0.303189	0.000017
C	-0.503090	-1.312955	-0.000005
C	1.793722	-0.582479	-0.000002
H	-1.725272	2.392111	0.000020
H	-3.345995	0.522150	0.000034
H	-0.147323	-2.341028	-0.000021
H	-2.585328	-1.837142	0.000020
H	2.022523	-1.650476	0.000026
C	2.963712	0.304865	0.000003
H	3.586531	0.060207	-0.871555
H	3.585615	0.061296	0.872523
H	2.735535	1.368201	-0.000824

ethylbenzene

H	-0.269174	2.146733	-0.310393
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C	0.260241	1.202338	-0.191858
C	1.624666	-1.205740	0.095339
C	-0.439661	-0.000004	-0.343638
C	1.624660	1.205744	0.095334
C	2.310799	0.000005	0.241770
C	0.260247	-1.202342	-0.191852
C	-1.924484	-0.000008	-0.592127
H	2.153178	2.149997	0.202737
H	3.375123	0.000008	0.462882
H	-0.269163	-2.146740	-0.310383
H	2.153189	-2.149990	0.202747
H	-2.196239	-0.879240	-1.187555
C	-2.717846	0.000006	0.716318
H	-2.473401	-0.883595	1.312197
H	-3.795605	0.000001	0.527453
H	-2.473405	0.883623	1.312175
H	-2.196241	0.879209	-1.187575

diphenylcarbene, singlet

C	-1.213380	-0.601528	0.055090
C	0.000000	-1.372115	0.000001
C	1.213380	-0.601527	-0.055086
C	-3.681134	0.744872	0.133208
C	-1.339428	0.644919	0.720107
C	-2.369521	-1.165857	-0.536037
C	-3.573552	-0.475149	-0.544272
C	-2.571530	1.287566	0.785959
H	-0.473219	1.064955	1.225122
H	-2.272258	-2.143151	-1.001889
H	-4.445441	-0.901826	-1.033831
H	-2.668226	2.224808	1.328947
H	-4.636873	1.262604	0.168297
C	3.681134	0.744873	-0.133212
C	2.369524	-1.165857	0.536036
C	1.339426	0.644921	-0.720102
C	2.571528	1.287568	-0.785957
C	3.573554	-0.475149	0.544268
H	2.272263	-2.143151	1.001887
H	0.473215	1.064957	-1.225114
H	2.668222	2.224811	-1.328945
H	4.445445	-0.901827	1.033823
H	4.636873	1.262605	-0.168304

diphenylcarbene, triplet

C	1.316974	-0.448226	-0.017727
C	0.000014	-0.974938	0.000162
C	-1.316970	-0.448240	0.017879
C	3.909144	0.546219	-0.089545

C	2.385836	-1.197384	0.480925
C	1.586874	0.808740	-0.570528
C	2.864502	1.294051	-0.594136
C	3.658629	-0.703068	0.443066
H	2.186447	-2.177458	0.904269
H	0.770175	1.389143	-0.989320
H	3.058272	2.272800	-1.024380
H	4.477914	-1.296976	0.838394
H	4.922159	0.935902	-0.115194
C	-3.909152	0.546176	0.089364
C	-1.586958	0.808697	0.570691
C	-2.385748	-1.197388	-0.480952
C	-3.658551	-0.703085	-0.443260
C	-2.864591	1.294002	0.594127
H	-0.770321	1.389094	0.989615
H	-2.186287	-2.177441	-0.904311
H	-4.477774	-1.296986	-0.838727
H	-3.058432	2.272734	1.024380
H	-4.922174	0.935851	0.114878

benzhydryl+

H	2.239570	2.294877	-0.614661
C	2.391327	1.259645	-0.316593
C	2.745745	-1.409099	0.476245
C	1.270431	0.467866	0.055312
C	3.655179	0.695688	-0.352871
C	3.832392	-0.636777	0.041580
C	1.468885	-0.873621	0.483246
C	0.000000	1.079450	0.000000
H	4.509337	1.289063	-0.664655
H	4.829812	-1.069053	0.038582
H	0.640038	-1.438814	0.898054
H	2.910730	-2.423042	0.828420
C	-1.270431	0.467866	-0.055312
H	0.000000	2.172822	0.000000
C	-3.832392	-0.636777	-0.041580
C	-2.391327	1.259645	0.316594
C	-1.468885	-0.873621	-0.483246
C	-2.745745	-1.409099	-0.476245
C	-3.655179	0.695688	0.352871
H	-2.239570	2.294877	0.614661
H	-0.640038	-1.438814	-0.898054
H	-2.910730	-2.423042	-0.828419
H	-4.509337	1.289063	0.664654
H	-4.829812	-1.069053	-0.038582

diphenylmethane

H	2.126971	1.724489	1.490327
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C	2.248130	0.909728	0.778338
C	2.567251	-1.173851	-1.038850
C	1.249714	-0.061869	0.669347
C	3.397200	0.844639	-0.012010
C	3.560205	-0.198543	-0.921507
C	1.421041	-1.103410	-0.251464
H	4.163979	1.609599	0.084297
H	4.453860	-0.251882	-1.538082
H	0.641399	-1.856138	-0.355620
H	2.686762	-1.989440	-1.748045
C	-1.249718	0.059655	0.669503
C	-3.560194	0.201586	-0.920912
C	-2.248265	-0.912141	0.775476
C	-1.420910	1.104082	-0.248058
C	-2.567111	1.177122	-1.035222
C	-3.397325	-0.844445	-0.014667
H	-2.127210	-1.729134	1.484920
H	-0.641167	1.857025	-0.349876
H	-2.686515	1.994929	-1.741875
H	-4.164204	-1.609600	0.079259
H	-4.453841	0.256958	-1.537320
C	-0.000015	-0.002495	1.514664
H	0.049632	0.873911	2.173537
H	-0.049684	-0.881065	2.170647

meta-substituted arylcarbene sets

3-oxyphenylcarbene, singlet

C	-2.384917	-1.273229	0.000013
C	-1.243881	-0.425546	-0.000012
C	1.116297	1.080125	0.000067
C	-1.308041	1.002013	-0.000036
C	0.030368	-1.058344	0.000069
C	1.287993	-0.359303	-0.000018
C	-0.123471	1.725541	-0.000007
H	-2.280066	1.493243	-0.000113
H	0.040309	-2.147556	0.000097
O	2.422591	-0.924394	-0.000061
H	-0.150281	2.817199	0.000018
H	2.033862	1.670285	0.000097
H	-3.270649	-0.585550	-0.000067

3-oxyphenylcarbene-, triplet, G3

C	2.428054	1.167871	0.000000
C	1.197568	0.392322	0.000000
C	-1.150379	-1.077172	0.000000
C	1.274628	-1.006829	0.000000
C	0.000000	1.055341	0.000000

C	-1.276026	0.362742	0.000000
C	0.071484	-1.685612	0.000000
H	2.230658	-1.523081	0.000000
H	-0.036869	2.143180	0.000000
O	-2.368814	0.964666	0.000000
H	0.096178	-2.779775	0.000000
H	-2.075125	-1.651684	0.000000
H	3.463693	0.842042	0.000000

3-oxybenzyl, er ptsons

C	1.200101	0.307367	0.000000
C	-1.226553	-1.009915	0.000000
C	1.186226	-1.147603	0.000000
C	0.000000	1.071938	0.000000
C	-1.309558	0.450499	0.000000
C	-0.036763	-1.766919	0.000000
H	2.125674	-1.693752	0.000000
H	0.056238	2.159294	0.000000
O	-2.390040	1.065109	0.000000
H	-0.102387	-2.852815	0.000000
H	-2.185238	-1.528071	0.000000
C	2.416814	0.930669	0.000000
H	3.344692	0.363285	0.000000
H	2.499743	2.014970	0.000000

3-oxyphenyltoluene-

C	-1.160256	-0.199990	-0.022132
C	1.373577	0.976718	0.012635
C	-1.050339	1.198516	-0.009420
C	-0.015477	-0.991509	-0.010272
C	1.327865	-0.465499	0.000447
C	0.230006	1.764925	0.002604
H	-1.941974	1.825512	-0.025700
H	-0.108247	-2.079590	-0.024089
O	2.367453	-1.201162	0.001296
H	0.332837	2.853315	0.004951
H	2.362181	1.436778	0.017663
C	-2.525421	-0.845686	0.016227
H	-3.264914	-0.244046	-0.525980
H	-2.896316	-0.966225	1.042605
H	-2.502922	-1.841299	-0.440364

3-aminophenylcarbene, singlet

C	2.385868	-1.372424	0.007665
C	1.276844	-0.452296	-0.000192
C	-1.013936	1.154208	-0.007546
C	1.392879	0.959844	0.003509
C	-0.012841	-1.029854	-0.009436

C	-1.166478	-0.243162	-0.001228
C	0.250025	1.748312	0.005715
H	2.382258	1.411526	0.011817
H	-0.068990	-2.116725	-0.012480
N	-2.438035	-0.816211	-0.082655
H	0.325198	2.832764	0.007583
H	-1.903275	1.783117	-0.015246
H	-2.476849	-1.774079	0.248530
H	-3.173682	-0.260960	0.340398
H	3.307436	-0.749932	0.007073

3-aminophenylcarbene, triplet

C	2.406531	-1.263627	0.004561
C	1.250112	-0.448720	0.000121
C	-1.016974	1.141723	-0.005896
C	1.370215	0.945861	0.006418
C	-0.021852	-1.024659	-0.007060
C	-1.152154	-0.243390	-0.008196
C	0.236537	1.710357	0.004121
H	2.353142	1.406376	0.014635
H	-0.111136	-2.108438	-0.014166
N	-2.418779	-0.817989	-0.078443
H	0.321931	2.793991	0.008871
H	-1.905254	1.768275	-0.016284
H	-2.464057	-1.771337	0.261802
H	-3.157626	-0.250385	0.319309
H	3.459958	-1.017826	0.010512

3-aminobenzyl+

C	1.232685	-0.378039	0.001082
C	-1.080592	1.130465	-0.002095
C	1.326584	1.056876	0.001418
C	-0.031584	-1.039679	0.001591
C	-1.211916	-0.287133	0.004383
C	0.157872	1.786877	0.001774
H	2.302874	1.534271	0.002296
H	-0.064727	-2.127347	0.000296
N	-2.438792	-0.854725	-0.031015
H	0.180230	2.872233	0.000348
H	-1.989030	1.731789	-0.008699
H	-2.549594	-1.853531	0.079813
H	-3.271942	-0.298093	0.101540
C	2.392762	-1.111101	-0.000709
H	3.366554	-0.627121	-0.001091
H	2.382309	-2.198716	-0.002064

3-aminotoluene

C	-1.209749	-0.239185	-0.019036
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C	1.266777	1.076643	0.016611
C	-1.152133	1.157914	-0.014755
C	-0.016828	-0.964064	0.000547
C	1.227138	-0.322696	0.002827
C	0.081578	1.806234	-0.003171
H	-2.072606	1.737312	-0.034600
H	-0.051632	-2.053683	-0.001877
N	2.413859	-1.071477	0.089217
H	0.123465	2.892981	-0.004192
H	2.227017	1.589045	0.027350
H	2.329618	-1.998915	-0.314542
H	3.215318	-0.594654	-0.311451
C	-2.534021	-0.955446	0.009762
H	-2.866132	-1.132743	1.038263
H	-2.469788	-1.926723	-0.488877
H	-3.308842	-0.368679	-0.491306

3-hydroxyphenylcarbene, singlet

C	2.411535	1.305261	0.000000
C	1.273300	0.420716	0.000000
C	-1.067913	-1.124338	0.000000
C	1.342994	-0.992898	0.000000
C	0.000000	1.039119	0.000000
C	-1.159798	0.274210	0.000000
C	0.177871	-1.752460	0.000000
H	2.318770	-1.473446	0.000000
H	-0.025272	2.127708	0.000000
H	0.225033	-2.838224	0.000000
H	-1.989040	-1.701432	0.000000
H	3.312607	0.654376	0.000000
O	-2.420317	0.804692	0.000000
H	-2.347506	1.775816	0.000000

3-hydroxyphenylcarbene, triplet

C	2.438631	1.170709	0.000000
C	1.253544	0.403865	0.000000
C	-1.082293	-1.102660	0.000000
C	1.310863	-0.993184	0.000000
C	0.000000	1.031481	0.000000
C	-1.143308	0.284808	0.000000
C	0.146968	-1.717688	0.000000
H	2.274103	-1.493626	0.000000
H	-0.048287	2.118382	0.000000
H	0.193600	-2.803260	0.000000
H	-2.007600	-1.668320	0.000000
H	3.482061	0.886185	0.000000
O	-2.392265	0.836368	0.000000

H	-2.302188	1.805708	0.000000
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3-hydroxybenzyl+

C	1.234838	0.328655	0.000000
C	-1.151188	-1.073789	0.000000
C	1.252262	-1.107153	0.000000
C	0.000000	1.052783	0.000000
C	-1.190899	0.342228	0.000000
C	0.052787	-1.789642	0.000000
H	2.204980	-1.630887	0.000000
H	0.014649	2.141128	0.000000
H	0.029412	-2.874790	0.000000
H	-2.105381	-1.597230	0.000000
O	-2.421519	0.875983	0.000000
H	-2.392731	1.852189	0.000000
C	2.430276	1.003527	0.000000
H	3.378872	0.471767	0.000000
H	2.473909	2.090306	0.000000

3-hydroxytoluene

C	-1.200553	-0.219713	-0.016739
C	1.309735	1.049725	0.008675
C	-1.109075	1.174092	-0.007983
C	-0.021288	-0.972043	-0.009270
C	1.222984	-0.343156	0.000673
C	0.138518	1.799839	0.002126
H	-2.017015	1.772923	-0.017068
H	-0.077383	-2.061301	-0.019538
H	0.199646	2.885364	0.003940
H	2.289877	1.517026	0.013016
O	2.407211	-1.040589	0.002410
H	2.201810	-1.991941	-0.004418
C	-2.538223	-0.909822	0.012387
H	-3.318454	-0.269066	-0.406741
H	-2.831047	-1.163023	1.036905
H	-2.517708	-1.838799	-0.564581

3-sulphyrylphenylcarbene, singlet

C	-2.513589	-1.698375	-0.000149
C	-1.581072	-0.596175	-0.000047
C	0.397533	1.382978	0.000284
C	-1.937056	0.773072	0.000218
C	-0.210462	-0.943364	0.000107
C	0.782372	0.033263	-0.000085
C	-0.949806	1.750082	-0.000341
H	-2.989895	1.047004	-0.000067
H	0.024492	-2.005393	-0.000320
S	2.515111	-0.331286	-0.000068
H	-1.213258	2.804488	-0.000080

H	1.161788	2.158095	0.000242
H	2.377311	-1.664344	0.000824
H	-3.529730	-1.248157	0.000572

3-sulfhydrylphenylcarbene, triplet

C	2.551904	-1.590163	0.009949
C	1.562007	-0.589525	0.003886
C	-0.405672	1.374880	-0.020032
C	1.907005	0.769474	-0.003723
C	0.201009	-0.931938	0.020697
C	-0.763568	0.034422	0.008786
C	0.928451	1.725448	-0.006921
H	2.954761	1.055395	-0.004403
H	-0.076363	-1.981165	0.059015
S	-2.468719	-0.477501	-0.055222
H	1.203551	2.776387	-0.016932
H	-1.171708	2.143507	-0.053175
H	-2.929841	0.433608	0.813269
H	3.632287	-1.543307	0.009920

3-sulfhydrylbenzyl+

C	-1.544362	-0.518836	-0.000074
C	0.452682	1.390192	0.000019
C	-1.900470	0.870159	-0.000113
C	-0.172874	-0.925392	0.000293
C	0.838561	0.027603	0.000097
C	-0.888798	1.806403	0.000105
H	-2.948046	1.160901	-0.000282
H	0.062336	-1.988549	0.000857
S	2.506290	-0.515510	-0.000157
H	-1.114638	2.868366	0.000189
H	1.225933	2.156877	-0.000173
H	3.056359	0.706276	0.000657
C	-2.533858	-1.471210	-0.000080
H	-2.301935	-2.533992	0.000138
H	-3.585945	-1.195244	-0.000353

3-sulfhydryltoluene

C	1.524404	-0.401083	-0.015826
C	-0.617278	1.417328	0.028664
C	1.760802	0.978207	-0.005009
C	0.203115	-0.854923	-0.025509
C	-0.867575	0.043107	0.013365
C	0.698025	1.878523	0.010527
H	2.784434	1.347531	-0.011534
H	0.006074	-1.924975	-0.066626
S	-2.559238	-0.507867	-0.054320
H	0.892470	2.948226	0.019029

H	-1.446526	2.118718	0.069106
H	-2.411740	-1.551460	0.774843
C	2.668304	-1.379282	0.002773
H	2.379210	-2.333079	-0.446513
H	2.997967	-1.580316	1.027559
H	3.527140	-0.990030	-0.550670

3-methylphenylcarbene, singlet

C	-2.400884	1.376453	0.000000
C	-1.295814	0.449749	0.000000
C	0.985701	-1.167203	0.000000
C	-1.416263	-0.962700	0.000000
C	0.000000	1.012966	0.000000
C	1.150240	0.224007	0.000000
C	-0.282418	-1.761011	0.000000
H	-2.409170	-1.408359	0.000000
H	0.062145	2.099840	0.000000
H	-0.367909	-2.844708	0.000000
H	1.869178	-1.804143	0.000000
H	-3.326327	0.759647	0.000000
C	2.518300	0.851408	0.000000
H	3.302651	0.090435	0.000000
H	2.658129	1.482635	0.882303
H	2.658129	1.482635	-0.882303

3-methylphenylcarbene, triplet

C	-2.431834	1.247100	0.000000
C	-1.277641	0.437129	0.000000
C	0.999609	-1.145049	0.000000
C	-1.382529	-0.963775	0.000000
C	0.000000	1.006711	0.000000
C	1.132337	0.232471	0.000000
C	-0.254944	-1.730505	0.000000
H	-2.365434	-1.426499	0.000000
H	0.085182	2.091230	0.000000
H	-0.340885	-2.813771	0.000000
H	1.887697	-1.771517	0.000000
H	-3.486414	1.006622	0.000000
C	2.494433	0.877658	0.000000
H	3.285485	0.124295	0.000000
H	2.628889	1.509600	0.882414
H	2.628889	1.509600	-0.882414

3-methylbenzyl+

C	-1.265926	0.336312	0.000000
C	1.078667	-1.121252	0.000000
C	-1.327500	-1.097733	0.000000
C	0.000000	1.009749	0.000000

C	1.182303	0.287808	0.000000
C	-0.149289	-1.809568	0.000000
H	-2.294430	-1.595271	0.000000
H	0.015863	2.098972	0.000000
H	-0.156764	-2.895119	0.000000
H	1.997718	-1.705567	0.000000
C	2.519116	0.974211	0.000000
H	3.335405	0.250282	0.000000
H	2.624612	1.608101	0.884168
H	2.624612	1.608101	-0.884168
C	-2.426188	1.068366	0.000000
H	-3.401657	0.587173	0.000000
H	-2.412458	2.155976	0.000000

3-methyltoluene

C	-1.222446	0.267502	0.000000
C	1.208235	-1.130730	0.000000
C	-1.208235	-1.130730	0.000000
C	0.000000	0.945892	0.000000
C	1.222446	0.267502	0.000000
C	0.000000	-1.825604	0.000000
H	-2.148865	-1.678160	0.000000
H	0.000000	2.036775	0.000000
H	0.000000	-2.913123	0.000000
H	2.148865	-1.678159	0.000000
C	2.517459	1.036204	0.000000
H	3.376071	0.359667	0.000000
H	2.596312	1.678974	0.882484
H	2.596312	1.678974	-0.882484
C	-2.517459	1.036204	0.000000
H	-3.376071	0.359666	0.000000
H	-2.596311	1.678974	-0.882484
H	-2.596311	1.678974	0.882484

3-fluorophenylcarbene, singlet

C	2.417000	1.297067	0.000000
C	1.264792	0.424361	0.000000
C	-1.091297	-1.108500	0.000000
C	1.319175	-0.991094	0.000000
C	0.000000	1.057330	0.000000
C	-1.145316	0.283047	0.000000
C	0.152328	-1.746455	0.000000
H	2.291029	-1.479444	0.000000
H	-0.047547	2.141796	0.000000
H	0.194395	-2.832055	0.000000
H	-2.019518	-1.672824	0.000000
H	3.308967	0.634301	0.000000
F	-2.358602	0.879299	0.000000

3-fluorophenylcarbene, triplet

C	2.437960	1.165770	0.000000
C	1.247477	0.410169	0.000000
C	-1.104310	-1.086225	0.000000
C	1.287708	-0.992367	0.000000
C	0.000000	1.047549	0.000000
C	-1.129019	0.290710	0.000000
C	0.126263	-1.713322	0.000000
H	2.248069	-1.498676	0.000000
H	-0.072327	2.129540	0.000000
H	0.167956	-2.798582	0.000000
H	-2.035459	-1.641115	0.000000
H	3.479534	0.875227	0.000000
F	-2.331583	0.911100	0.000000

3-fluorobenzyl+

C	1.228193	0.322240	0.000000
C	-1.181305	-1.059697	0.000000
C	1.224521	-1.113103	0.000000
C	0.000000	1.060545	0.000000
C	-1.176268	0.346806	0.000000
C	0.018419	-1.786688	0.000000
H	2.170159	-1.649813	0.000000
H	-0.008361	2.147550	0.000000
H	-0.012311	-2.871650	0.000000
H	-2.142530	-1.569547	0.000000
F	-2.344160	0.981032	0.000000
C	2.427090	0.992645	0.000000
H	3.374454	0.458166	0.000000
H	2.472135	2.079518	0.000000

3-fluorotoluene

C	1.198915	-0.200710	-0.008355
C	-1.350708	1.006417	0.004117
C	1.063998	1.191341	-0.004263
C	0.042254	-0.988360	-0.005435
C	-1.200102	-0.373663	0.000480
C	-0.197398	1.788209	0.001419
H	1.954861	1.815066	-0.008163
H	0.096351	-2.074019	-0.010251
H	-0.284899	2.871490	0.002014
H	-2.344937	1.441370	0.006682
F	-2.312332	-1.152802	0.001053
C	2.554140	-0.855585	0.006276
H	2.749971	-1.332927	0.971707

H	3.345038	-0.123148	-0.172765
H	2.628006	-1.628498	-0.764135

3-chlorophenylcarbene, singlet

C	-1.594082	-2.572448	0.000000
C	-0.535514	-1.587095	0.000000
C	1.364371	0.478593	0.000000
C	0.849029	-1.879451	0.000000
C	-0.946057	-0.234424	0.000000
C	0.000000	0.780533	0.000000
C	1.785949	-0.853792	0.000000
H	1.168738	-2.919305	0.000000
H	-2.011304	-0.022583	0.000000
H	2.849985	-1.074259	0.000000
H	2.090628	1.287078	0.000000
H	-1.095302	-3.565389	0.000000
Cl	-0.502642	2.441351	0.000000

3-chlorophenylcarbene, triplet

C	-1.479643	-2.603282	0.000000
C	-0.525666	-1.567538	0.000000
C	1.353161	0.488658	0.000000
C	0.848995	-1.849584	0.000000
C	-0.933619	-0.226083	0.000000
C	0.000000	0.765959	0.000000
C	1.760223	-0.831282	0.000000
H	1.181071	-2.883494	0.000000
H	-1.991705	0.013873	0.000000
H	2.822232	-1.058878	0.000000
H	2.074965	1.297909	0.000000
H	-1.382187	-3.680182	0.000000
Cl	-0.520299	2.426452	0.000000

3-chlorobenzyl+

C	-0.492528	-1.539049	0.000000
C	1.373639	0.508808	0.000000
C	0.906378	-1.852934	0.000000
C	-0.939094	-0.177451	0.000000
C	0.000000	0.834701	0.000000
C	1.822661	-0.821047	0.000000
H	1.224164	-2.892894	0.000000
H	-2.003075	0.048680	0.000000
H	2.889047	-1.024332	0.000000
H	2.098419	1.320687	0.000000
C	-1.416539	-2.555655	0.000000
H	-1.110758	-3.599541	0.000000
H	-2.485417	-2.353589	0.000000
Cl	-0.478793	2.477456	0.000000

3-chlorotoluene

C	1.512552	-0.390439	-0.016595
C	-0.654840	1.408802	0.008226
C	1.729838	0.991526	-0.007720
C	0.197380	-0.864530	-0.009849
C	-0.867304	0.032638	0.000325
C	0.656602	1.880662	0.002473
H	2.748323	1.374045	-0.016370
H	-0.002090	-1.933353	-0.019523
H	0.838797	2.952314	0.004473
H	-1.499140	2.091395	0.013045
C	2.667488	-1.355166	0.012132
H	2.961584	-1.585007	1.041503
H	3.539922	-0.937478	-0.497165
H	2.406833	-2.297242	-0.477130
Cl	-2.496737	-0.581508	0.001012

3-formylphenylcarbene, singlet

C	-2.739696	-1.421204	0.000000
C	-1.640890	-0.480704	0.000000
C	0.621149	1.190747	0.000000
C	-1.774099	0.928544	0.000000
C	-0.338209	-1.026661	0.000000
C	0.781213	-0.201968	0.000000
C	-0.653687	1.755065	0.000000
H	-2.773583	1.359926	-0.000001
H	-0.247938	-2.111890	0.000001
C	2.144314	-0.786032	0.000000
H	-0.766866	2.835909	0.000001
H	1.512993	1.813383	0.000000
O	3.170107	-0.116896	-0.000001
H	2.185041	-1.893608	0.000002
H	-3.671077	-0.815281	0.000000

3-formylphenylcarbene, triplet

C	2.739610	-1.340512	0.000000
C	1.617956	-0.490695	0.000000
C	-0.610791	1.197597	0.000000
C	1.756461	0.905770	0.000000
C	0.314109	-1.012303	0.000000
C	-0.760452	-0.178936	0.000000
C	0.659640	1.728925	0.000000
H	2.754742	1.334840	0.000000
H	0.175618	-2.091845	0.000000
C	-2.149481	-0.767370	0.000001
H	0.799196	2.805982	0.000000
H	-1.498006	1.822754	0.000001

O	-3.160481	-0.137227	-0.000002
H	-2.153043	-1.883894	0.000004
H	3.803035	-1.144877	-0.000002

3-formylbenzyl+

C	1.602913	-0.404790	0.000001
C	-0.685547	1.166517	-0.000001
C	1.712833	1.026140	-0.000002
C	0.310723	-1.028625	0.000000
C	-0.818291	-0.239012	0.000004
C	0.567007	1.797353	0.000003
H	2.699368	1.484690	0.000000
H	0.239040	-2.116127	0.000003
C	-2.198528	-0.830109	0.000001
H	0.629148	2.881161	-0.000001
H	-1.601583	1.756109	-0.000001
O	-3.189131	-0.120075	-0.000003
H	-2.258534	-1.932975	0.000004
C	2.739708	-1.174936	-0.000002
H	2.690260	-2.261577	0.000000
H	3.730456	-0.725911	-0.000002

3-formyltoluene

C	-1.559498	-0.314760	-0.014864
C	0.815831	1.210490	0.006231
C	-1.597595	1.084487	-0.007671
C	-0.309485	-0.939637	-0.010533
C	0.868130	-0.187748	-0.000782
C	-0.422804	1.841149	0.001822
H	-2.561787	1.590345	-0.014992
H	-0.249191	-2.028584	-0.019626
C	2.174316	-0.877923	-0.002315
H	-0.481205	2.926819	0.002860
H	1.746175	1.772044	0.010843
O	3.259180	-0.305934	0.006341
H	2.122162	-1.987092	-0.011917
C	-2.829626	-1.121274	0.013349
H	-3.180090	-1.265926	1.040621
H	-2.678170	-2.109522	-0.428635
H	-3.626947	-0.619313	-0.541302

3-trifluoromethylphenylcarbene, singlet

C	-3.008655	-1.742959	0.000000
C	-2.105765	-0.611761	0.000000
C	-0.201843	1.450842	-0.000005
C	-2.504715	0.744911	0.000004
C	-0.724040	-0.909614	-0.000006
C	0.212113	0.113460	-0.000009

C	-1.560603	1.766479	0.000001
H	-3.567423	0.979811	0.000008
H	-0.429859	-1.954563	-0.000012
C	1.682302	-0.167117	-0.000001
H	-1.871389	2.807612	0.000002
H	0.543052	2.243441	-0.000011
H	-4.036745	-1.321428	0.000008
F	2.279574	0.374971	1.086074
F	2.279648	0.375344	-1.085849
F	1.955178	-1.485907	-0.000215

3-trifluoromethylphenylcarbene, triplet

C	3.031217	-1.647715	-0.000001
C	2.083254	-0.607570	-0.000003
C	0.200580	1.448707	-0.000074
C	2.477824	0.737382	0.000049
C	0.707834	-0.892726	-0.000074
C	-0.200030	0.120615	-0.000097
C	1.545525	1.741942	0.000010
H	3.537031	0.978708	0.000102
H	0.380446	-1.926385	-0.000132
C	-1.668945	-0.168841	-0.000001
H	1.871958	2.777578	0.000024
H	-0.540731	2.241391	-0.000158
H	4.112497	-1.647433	0.000042
F	-2.275927	0.368078	-1.084415
F	-2.275399	0.366116	1.085672
F	-1.940313	-1.491375	-0.001116

3-trifluoromethylbenzyl+

C	2.068617	-0.539168	0.000000
C	0.149388	1.464503	0.000001
C	2.469992	0.837311	0.000002
C	0.678163	-0.890344	-0.000002
C	-0.259184	0.115743	-0.000006
C	1.505416	1.825327	-0.000004
H	3.529092	1.085601	0.000002
H	0.378878	-1.935548	-0.000004
C	-1.739694	-0.180516	0.000000
H	1.785481	2.874071	0.000001
H	-0.611455	2.243533	-0.000003
F	-2.308495	0.360785	-1.088348
F	-2.308473	0.360717	1.088392
F	-1.969931	-1.501534	-0.000039
C	3.021937	-1.528294	0.000000
H	2.748093	-2.581139	-0.000002
H	4.084198	-1.293611	0.000002

3-trifluoromethyltoluene

C	-2.034598	-0.428253	0.012837
C	-0.027589	1.549494	-0.032273
C	-2.363929	0.932179	0.022311
C	-0.684793	-0.786367	-0.020802
C	0.306120	0.195209	-0.044776
C	-1.372210	1.911556	-0.000063
H	-3.411167	1.227414	0.050660
H	-0.401725	-1.836067	-0.032652
C	1.742706	-0.212652	-0.001647
H	-1.648322	2.962732	0.007925
H	0.751740	2.304915	-0.053302
F	2.182536	-0.356071	1.271523
F	2.547048	0.700236	-0.593222
F	1.952706	-1.396481	-0.622833
C	-3.109156	-1.481334	-0.006772
H	-2.751407	-2.417096	0.430184
H	-3.431162	-1.693642	-1.031502
H	-3.987878	-1.156406	0.556584

3-cyanophenylcarbene, singlet

C	-2.409345	-1.722287	0.000000
C	-1.469155	-0.618847	0.000000
C	0.506513	1.381063	0.000001
C	-1.821360	0.751346	-0.000002
C	-0.101840	-0.966091	0.000002
C	0.878188	0.026877	0.000002
C	-0.842383	1.738656	0.000000
H	-2.875174	1.023233	-0.000004
H	0.158775	-2.021231	0.000003
H	-1.116980	2.789937	-0.000001
H	1.279128	2.146206	0.000003
H	-3.423287	-1.268547	-0.000001
C	2.269597	-0.325282	0.000003
N	3.416607	-0.608887	-0.000004

3-cyanophenylcarbene, triplet

C	2.434043	-1.620832	0.000000
C	1.446890	-0.616953	0.000000
C	-0.511903	1.372295	0.000001
C	1.789651	0.744410	-0.000001
C	0.086122	-0.951775	0.000001
C	-0.856502	0.033255	0.000000
C	0.825742	1.713163	0.000000
H	2.839462	1.023495	-0.000001
H	-0.209410	-1.996059	0.000002
H	1.113751	2.759872	-0.000001
H	-1.284107	2.133927	0.000001

H	3.514388	-1.580255	0.000000
C	-2.268726	-0.336603	0.000001
N	-3.377999	-0.623249	-0.000002

3-cyanobenzyl+

C	1.435527	-0.546042	-0.000001
C	-0.559382	1.386912	-0.000004
C	1.785506	0.843753	0.000004
C	0.061862	-0.951791	-0.000007
C	-0.924133	0.018874	-0.000008
C	0.782644	1.793838	0.000002
H	2.834258	1.132613	0.000009
H	-0.196208	-2.008978	-0.000010
H	1.022226	2.852734	0.000006
H	-1.349258	2.136049	-0.000005
C	-2.310028	-0.346314	-0.000008
N	-3.453135	-0.646284	0.000014
C	2.426210	-1.499540	0.000003
H	2.192904	-2.562245	0.000002
H	3.478775	-1.224321	0.000008

3-cyanotoluene

C	-1.411572	-0.430740	-0.015034
C	0.725489	1.412370	0.007682
C	-1.647642	0.949616	-0.007521
C	-0.090381	-0.881459	-0.009294
C	0.971047	0.033291	0.000828
C	-0.592242	1.860770	0.002328
H	-2.672871	1.314941	-0.015472
H	0.125607	-1.947703	-0.017894
H	-0.797760	2.927967	0.003857
H	1.557023	2.111435	0.012828
C	2.321064	-0.450015	0.000663
N	3.433978	-0.849600	0.001173
C	-2.556316	-1.406900	0.011168
H	-3.399596	-1.038337	-0.578783
H	-2.910727	-1.565634	1.034741
H	-2.256205	-2.377066	-0.392413

3-nitrophenylcarbene, singlet

C	1.800205	-0.586339	-0.000008
C	-0.157058	1.436808	0.000016
C	2.165715	0.780160	0.000011
C	0.429567	-0.923593	-0.000013
C	-0.512796	0.089990	0.000003
C	1.196846	1.777631	0.000019
H	3.221989	1.041666	0.000016
H	0.142419	-1.969598	-0.000028

H	1.481808	2.825983	0.000031
H	-0.933447	2.194507	0.000022
N	-1.944383	-0.258500	0.000000
O	-2.237798	-1.462353	0.000059
O	-2.759715	0.676358	-0.000062
C	2.732322	-1.698575	-0.000031
H	3.749200	-1.251587	-0.000005

3-nitrophenylcarbene, triplet

C	-0.238123	-1.858574	0.000000
C	1.376049	0.426919	0.000000
C	1.163128	-1.951665	0.000000
C	-0.813127	-0.582387	0.000000
C	0.000000	0.508969	0.000000
C	1.945615	-0.829467	0.000000
H	1.625873	-2.934606	0.000000
H	-1.890002	-0.460881	0.000000
H	3.026833	-0.927197	0.000000
H	1.974203	1.329433	0.000000
N	-0.624412	1.847536	0.000000
O	-1.862196	1.907941	0.000000
O	0.129951	2.831221	0.000000
C	-1.049240	-3.011472	0.000000
H	-0.813876	-4.066735	0.000000

3-nitrobenzyl+

C	-1.765038	-0.513270	-0.000001
C	0.209743	1.447771	0.000001
C	-2.129298	0.873341	0.000001
C	-0.386362	-0.904731	-0.000001
C	0.558290	0.089130	-0.000002
C	-1.138759	1.836940	0.000002
H	-3.181154	1.150426	0.000001
H	-0.091877	-1.951418	-0.000001
H	-1.392056	2.892534	0.000004
H	1.005952	2.188583	0.000003
N	1.993069	-0.279816	0.000000
O	2.245738	-1.489094	0.000005
O	2.800294	0.656361	-0.000005
C	-2.743105	-1.479559	-0.000001
H	-2.494148	-2.538619	-0.000003
H	-3.799280	-1.218656	-0.000001

3-nitrotoluene

C	-1.740546	-0.392191	-0.004711
C	0.369713	1.486848	0.001455
C	-1.999025	0.985235	-0.003271

C	-0.413610	-0.826367	-0.002675
C	0.608245	0.117784	0.000128
C	-0.957599	1.911342	-0.000384
H	-3.030009	1.334459	-0.006165
H	-0.164991	-1.882579	-0.004685
H	-1.178397	2.975438	-0.000677
H	1.199223	2.184321	0.002565
C	-2.874428	-1.381030	0.005115
H	-2.505865	-2.403067	-0.108660
H	-3.576665	-1.179427	-0.808911
H	-3.432767	-1.325050	0.944680
N	1.999299	-0.354280	0.000242
O	2.193313	-1.580920	-0.003516
O	2.898920	0.501688	0.004294

para-substituted arylcarbene sets

4-oxyphenylcarbene-, singlet

C	-2.878696	0.143051	0.000001
C	-1.488533	0.026923	-0.000003
C	1.440496	-0.009933	0.000000
C	-0.724837	-1.199658	-0.000002
C	-0.691844	1.230480	-0.000002
C	0.672357	1.228332	0.000002
C	0.639592	-1.229505	0.000002
H	-1.287886	-2.136286	-0.000003
H	-1.254356	2.164441	0.000003
H1	2.47984	2.153128	0.000001
H	1.192926	-2.168096	0.000006
O	2.695667	-0.030507	-0.000001
H	-3.275220	-0.907268	0.000008

4-oxyphenylcarbene-, triplet

C	2.881528	0.090647	-0.000052
C	1.459445	0.057573	0.000000
C	-1.448886	-0.025208	-0.000010
C	0.731291	-1.148794	-0.000012
C	0.663959	1.220158	0.000008
C	-0.687466	1.210811	0.000000
C	-0.619837	-1.216428	-0.000002
H	1.295504	-2.085351	-0.000040
H	1.177893	2.184296	0.000004
H	-1.263967	2.134715	0.000014
H	-1.142442	-2.171856	0.000007
O	-2.694350	-0.059787	0.000013

H 3.607614 -0.716060 0.000322

4-oxyphenylbenzyl (p-quinomethide)

C 0.000000 0.000000 -1.398304
C 0.000000 0.000000 1.481212
C 0.000000 1.246070 -0.644812
C 0.000000 -1.246070 -0.644812
C 0.000000 -1.251517 0.706791
C 0.000000 1.251517 0.706791
H 0.000000 2.180007 -1.204586
H 0.000000 -2.180007 -1.204586
H 0.000000 -2.175540 1.278461
H 0.000000 2.175540 1.278461
O 0.000000 0.000000 2.720516
C 0.000000 0.000000 -2.752254
H 0.000000 0.926014 -3.319775
H 0.000000 -0.926014 -3.319775

4-oxytoluene-

C -1.342716 0.000002 -0.028161
C 1.583584 0.000001 0.008098
C -0.604150 -1.193027 -0.014512
C -0.604149 1.193027 -0.014510
C 0.785308 1.202220 -0.008702
C 0.785305 -1.202219 -0.008700
H -1.141727 -2.146580 -0.027525
H -1.141727 2.146579 -0.027523
H 1.327221 2.148755 -0.010122
H 1.327219 -2.148754 -0.010121
O 2.857022 -0.000003 0.022210
C -2.846322 -0.000002 0.029793
H -3.263177 0.883799 -0.469143
H -3.241908 -0.000362 1.056693
H -3.263229 -0.883426 -0.469772

4-aminophenylcarbene, singlet

C 2.949926 -0.142876 0.012079
C 1.527130 -0.021332 0.001117
C -1.304572 0.006249 0.000317
C 0.797313 1.198120 -0.001576
C 0.771890 -1.222783 -0.000976
C -0.607304 -1.218477 -0.008216
C -0.581677 1.217971 -0.008155
H 1.349740 2.136266 -0.001333
H 1.331164 -2.154746 0.000609
H -1.168551 -2.150761 -0.011726
H -1.125328 2.160850 -0.012543
H 3.354328 0.894094 0.012575

N	-2.678945	0.022787	-0.058982
H	-3.161889	-0.820111	0.225248
H	-3.143087	0.873661	0.232497

4-aminophenylcarbene, triplet

C	-2.920718	0.085303	0.012287
C	-1.511425	0.050426	0.002067
C	1.300381	-0.017384	-0.005410
C	-0.803477	-1.160272	-0.000450
C	-0.746285	1.225086	-0.000058
C	0.614474	1.193268	-0.008073
C	0.559061	-1.193026	-0.008459
H	-1.356697	-2.096007	0.001503
H	-1.259399	2.182719	0.002093
H	1.178020	2.123835	-0.014397
H	1.077185	-2.149688	-0.014905
H	-3.665017	-0.699437	0.013140
N	2.687759	-0.048944	-0.073180
H	3.148759	0.777609	0.288179
H	3.110766	-0.896827	0.285222

4-aminobenzyl+

C	-2.816118	0.000000	0.000003
C	-1.455662	0.000000	-0.000002
C	1.358983	0.000000	0.000004
C	-0.714659	1.240348	0.000003
C	-0.714659	-1.240348	0.000004
C	0.644554	-1.244237	-0.000011
C	0.644554	1.244237	-0.000011
H	-1.263124	2.179382	0.000002
H	-1.263124	-2.179381	0.000002
H	1.201242	-2.177716	-0.000004
H	1.201242	2.177716	-0.000004
N	2.682463	0.000000	0.000005
H	3.216265	0.864208	0.000012
H	3.216265	-0.864208	0.000012
H	-3.383979	0.926341	0.000004
H	-3.383979	-0.926341	0.000005

4-aminotoluene

C	1.397145	-0.000005	-0.017831
C	-1.436308	0.000000	0.005142
C	0.672516	-1.196072	-0.009740
C	0.672518	1.196069	-0.009744
C	-0.719397	1.202536	0.007541
C	-0.719403	-1.202535	0.007540
H	1.205377	-2.145706	-0.017858
H	1.205376	2.145704	-0.017863

H	-1.258053	2.148809	0.012507
H	-1.258063	-2.148805	0.012509
C	2.901982	0.000001	0.006770
N	-2.839615	0.000000	0.093113
H	3.285474	-0.000017	1.032875
H	3.304152	0.884365	-0.495500
H	3.304155	-0.884337	-0.495549
H	-3.262715	-0.829686	-0.310506
H	-3.262710	0.829705	-0.310472

4-hydroxyphenylcarbene, singlet

C	-2.931660	-0.163943	0.000000
C	-1.504888	-0.027834	0.000001
C	1.302995	0.021809	-0.000002
C	-0.789275	1.199969	0.000000
C	-0.748516	-1.225038	-0.000001
C	0.635230	-1.210309	0.000001
C	0.591364	1.231585	0.000002
H	-1.350808	2.132368	0.000003
H	-1.302260	-2.160094	0.000000
H	1.204732	-2.138370	-0.000003
H	1.151395	2.162044	0.000000
O	2.658647	0.119366	-0.000003
H	3.043153	-0.776115	0.000025
H	-3.346884	0.867795	0.000000

4-hydroxyphenylcarbene, triplet

C	0.032814	-2.901773	0.000000
C	0.023682	-1.490991	0.000000
C	0.000000	1.299493	0.000000
C	-1.180730	-0.765920	0.000000
C	1.210687	-0.752734	0.000000
C	1.200305	0.614839	0.000000
C	-1.193699	0.594502	0.000000
H	-2.122963	-1.307324	0.000000
H	2.158955	-1.282162	0.000000
H	2.139913	1.164321	0.000000
H	-2.125793	1.150626	0.000000
O	-0.082787	2.661697	0.000000
H	0.818724	3.028411	0.000000
H	-0.764893	-3.631949	0.000000

4-hydroxybenzyl+

C	-0.006879	-1.432223	0.000000
C	0.000000	1.354761	0.000000
C	-1.247931	-0.697931	0.000000
C	1.237143	-0.704526	0.000000
C	1.241948	0.660947	0.000000

C	-1.243959	0.666533	0.000000
H	-2.187117	-1.246011	0.000000
H	2.173740	-1.257377	0.000000
H	2.176161	1.217467	0.000000
H	-2.157074	1.253461	0.000000
O	-0.080638	2.669483	0.000000
H	0.800275	3.100523	0.000000
C	-0.005440	-2.796628	0.000000
H	0.921619	-3.364210	0.000000
H	-0.931789	-3.365311	0.000000

4-hydroxytoluene

C	1.377992	0.007414	-0.016269
C	-1.435642	-0.015142	0.004033
C	0.663124	-1.197125	-0.009181
C	0.649021	1.199031	-0.009119
C	-0.745754	1.196873	-0.002623
C	-0.727452	-1.217772	-0.002310
H	1.205448	-2.141055	-0.017449
H	1.175723	2.151601	-0.017203
H	-1.292525	2.139055	-0.003402
H	-1.280936	-2.152390	-0.002466
O	-2.807410	-0.096766	0.008981
H	-3.167660	0.807236	0.011619
C	2.882841	0.014013	0.015831
H	3.280916	0.945600	-0.395503
H	3.292849	-0.814445	-0.568626
H	3.260679	-0.085231	1.039008

4-sulfhydrylphenylcarbene, singlet

C	-3.378286	0.136848	0.000000
C	-1.945433	0.018960	0.000000
C	0.876623	0.003153	0.000000
C	-1.218395	-1.198714	0.000000
C	-1.203147	1.223459	0.000000
C	0.181895	1.223121	0.000000
C	0.164733	-1.210154	0.000000
H	-1.767137	-2.138810	0.000000
H	-1.765352	2.153729	0.000000
H	0.729883	2.162467	0.000000
H	0.707680	-2.152686	0.000000
S	2.634161	-0.095648	0.000000
H	2.859866	1.225781	0.000000
H	-3.779455	-0.900143	0.000000

4-sulfhydrylphenylcarbene, triplet

C	-3.335143	0.071648	-0.001699
C	-1.930682	0.044856	-0.001687
C	0.866172	-0.002970	0.010509
C	-1.222494	-1.167578	0.009859
C	-1.180583	1.232292	-0.007888
C	0.181372	1.203884	-0.017853
C	0.142532	-1.183858	0.021914
H	-1.772299	-2.104614	0.021218
H	-1.703642	2.183959	-0.020471
H	0.734651	2.138939	-0.045094
H	0.667441	-2.134712	0.055675
S	2.634717	-0.099877	-0.044589
H	2.869994	1.038353	0.623012
H	-4.078658	-0.713537	0.000167

4-sulfhydrylbenzyl+

C	1.868043	-0.001507	0.000000
C	-0.942937	0.008468	0.000000
C	1.132690	-1.238681	0.000000
C	1.139469	1.239472	0.000000
C	-0.227270	1.241375	0.000000
C	-0.233169	-1.229393	0.000000
H	1.676862	-2.180393	0.000000
H	1.689597	2.177908	0.000000
H	-0.769976	2.182737	0.000000
H	-0.788308	-2.163981	0.000000
S	-2.646867	-0.084351	0.000000
H	-2.887807	1.235992	0.000000
C	3.234091	-0.002503	0.000000
H	3.802839	0.923880	0.000000
H	3.801158	-0.929906	0.000000

4-sulfhydryltoluene

C	-1.822906	0.000676	-0.015029
C	0.998769	-0.001805	-0.010683
C	-1.100453	1.199053	-0.002795
C	-1.103833	-1.198203	-0.020416
C	0.289654	-1.205394	-0.027401
C	0.291797	1.204136	0.019940
H	-1.634832	2.147574	0.004147
H	-1.640082	-2.145396	-0.038076
H	0.829504	-2.148183	-0.066772
H	0.829586	2.148814	0.053551
S	2.776672	-0.059822	0.063373
H	2.998550	0.923933	-0.820687
C	-3.327190	0.004094	0.017709
H	-3.700121	0.029446	1.047169

H	-3.733365	-0.891768	-0.459538
H	-3.731018	0.877392	-0.501722

4-methylphenylcarbene, singlet

C	2.981349	0.139678	0.010516
C	1.546053	0.021119	0.003598
C	-1.283549	-0.004660	-0.015742
C	0.825831	-1.199266	-0.001953
C	0.802709	1.224610	-0.001593
C	-0.584251	1.211151	-0.009574
C	-0.560314	-1.208603	-0.009551
H	1.380232	-2.136251	-0.001281
H	1.364060	2.155373	-0.000097
H	-1.141682	2.145579	-0.017881
H	-1.101296	-2.152938	-0.017952
H	3.381055	-0.898182	0.011904
C	-2.786032	-0.022441	0.014184
H	-3.150537	-0.069278	1.046133
H	-3.181563	-0.892576	-0.516131
H	-3.201051	0.878746	-0.444006

4-methylphenylcarbene, triplet

C	2.938137	0.082118	0.009107
C	1.530823	0.049420	0.004294
C	-1.276914	-0.015899	-0.013444
C	0.830497	-1.166643	-0.001699
C	0.775000	1.231259	-0.001183
C	-0.588436	1.189008	-0.009061
C	-0.535600	-1.186607	-0.009393
H	1.387176	-2.100032	-0.002760
H	1.293505	2.185698	-0.001697
H	-1.149781	2.120898	-0.016710
H	-1.053002	-2.143598	-0.017259
H	3.682907	-0.702145	0.012628
C	-2.780021	-0.048099	0.013642
H	-3.156797	-0.008873	1.041367
H	-3.162775	-0.963687	-0.444292
H	-3.202140	0.804391	-0.524859

4-methylbenzyl+

C	-1.474021	-0.000005	0.002300
C	1.330483	0.000016	-0.017048
C	-0.751177	1.240783	-0.001907
C	-0.751161	-1.240787	-0.001905
C	0.622390	-1.226579	-0.009906
C	0.622380	1.226595	-0.009905
H	-1.302057	2.178739	0.000635
H	-1.302032	-2.178748	0.000635

H	1.178755	-2.159768	-0.016695
H	1.178729	2.159793	-0.016696
C	2.820060	0.000000	0.010784
H	3.158501	-0.000446	1.055581
H	3.230399	0.891574	-0.467852
H	3.230349	-0.891210	-0.468584
C	-2.843752	-0.000008	0.008979
H	-3.411925	-0.927159	0.012313
H	-3.411930	0.927138	0.012311

4-methyltoluene

C	-1.417640	-0.000012	0.019718
C	1.417640	0.000042	-0.019684
C	-0.696692	1.198314	0.007021
C	-0.696640	-1.198323	0.007031
C	0.696680	-1.198298	-0.007070
C	0.696647	1.198341	-0.007058
H	-1.232910	2.146045	0.015521
H	-1.232841	-2.146064	0.015551
H	1.232913	-2.146023	-0.015589
H	1.232828	2.146091	-0.015548
C	2.922485	-0.000016	0.007304
H	3.301052	-0.000298	1.035096
H	3.325365	0.884993	-0.492907
H	3.325348	-0.884787	-0.493358
C	-2.922482	-0.000025	-0.007273
H	-3.325327	-0.884882	0.493257
H	-3.301052	-0.000114	-1.035057
H	-3.325366	0.884897	0.493101

4-fluoromethylphenylcarbene, singlet

C	-3.396074	-0.220745	-0.000416
C	-1.957917	-0.116923	-0.000104
C	0.826122	0.284844	0.000379
C	-1.061170	-1.212128	0.000403
C	-1.410328	1.188538	-0.000386
C	-0.039063	1.388071	-0.000162
C	0.313469	-1.017050	0.000714
H	-1.467467	-2.222146	0.000591
H	-2.108296	2.021561	-0.000865
H	0.369188	2.397671	-0.000521
H	0.999351	-1.857367	0.001040
C	2.310536	0.523510	0.001222
H	-3.630922	-1.307386	-0.000086
F	3.011308	-0.679748	-0.001727
H	2.611344	1.086037	0.891875
H	2.611588	1.090664	-0.886399

4-fluoromethylphenylcarbene, triplet

C	-3.324122	-0.394699	-0.058465
C	-1.935427	-0.168782	-0.013752
C	0.819299	0.276893	0.068566
C	-1.410956	1.133273	-0.050007
C	-1.028325	-1.236115	0.060551
C	0.317179	-1.012374	0.105027
C	-0.062181	1.341120	-0.012401
H	-2.090322	1.978562	-0.117219
H	-1.414415	-2.250942	0.083315
H	1.007221	-1.847937	0.155807
H	0.321257	2.358961	-0.053313
C	2.297129	0.523917	0.164692
H	-4.168952	0.277996	-0.115911
F	3.012829	-0.599979	-0.252498
H	2.598140	0.733902	1.197295
H	2.596031	1.369872	-0.462756

4-fluoromethylbenzyl+

C	-0.481350	-1.822049	0.000000
C	0.000000	0.921817	0.000000
C	0.865077	-1.324732	0.000000
C	-1.582652	-0.899468	0.000000
C	-1.333437	0.451037	0.000000
C	1.093691	0.032070	0.000000
H	1.693216	-2.030271	0.000000
H	-2.600676	-1.282455	0.000000
H	-2.157886	1.160207	0.000000
H	2.100900	0.433073	0.000000
C	0.247095	2.399987	0.000000
F	1.602375	2.662489	0.000000
H	-0.205120	2.854382	0.890218
H	-0.205120	2.854382	-0.890218
C	-0.713230	-3.172918	0.000000
H	0.105113	-3.889225	0.000000
H	-1.722966	-3.576963	0.000000

4-fluoromethyltoluene

C	-1.833828	-0.085592	0.004975
C	0.961859	0.273525	0.075868
C	-0.967790	-1.181715	0.084456
C	-1.273217	1.194911	-0.046058
C	0.107931	1.375019	-0.011184
C	0.413443	-1.009243	0.130277
H	-1.382176	-2.187809	0.122674
H	-1.925869	2.063560	-0.114190
H	0.520842	2.381712	-0.061440
H	1.073019	-1.869967	0.188595

C	2.446291	0.471028	0.180045
F	3.126737	-0.653280	-0.296271
H	2.757172	0.619033	1.220356
H	2.770154	1.337287	-0.406315
C	-3.323503	-0.281795	-0.079995
H	-3.858511	0.573946	0.340683
H	-3.633972	-1.177296	0.465189
H	-3.648408	-0.397779	-1.119411

4-fluorophenylcarbene, singlet

C	2.919686	0.144188	-0.000004
C	1.485773	0.021681	0.000001
C	-1.291157	-0.006658	0.000000
C	0.769760	-1.203083	0.000002
C	0.743307	1.227876	0.000001
C	-0.642983	1.225341	0.000001
C	-0.615688	-1.226050	0.000000
H	1.326608	-2.137828	0.000003
H	1.306039	2.157132	-0.000002
H	-1.230805	2.137666	0.000002
H	-1.185911	-2.149675	-0.000002
F	-2.639152	-0.024004	-0.000001
H	3.324245	-0.891030	0.000001

4-fluorophenylcarbene, triplet

C	0.047159	-2.882421	0.000000
C	0.030024	-1.472139	0.000000
C	0.000000	1.287130	0.000000
C	-1.178866	-0.759742	0.000000
C	1.222423	-0.733960	0.000000
C	1.209846	0.631319	0.000000
C	-1.194839	0.607036	0.000000
H	-2.117673	-1.306070	0.000000
H	2.168983	-1.265591	0.000000
H	2.128417	1.208387	0.000000
H	-2.125627	1.164283	0.000000
F	-0.013750	2.639364	0.000000
H	-0.744826	-3.618621	0.000000

4-fluorobenzyl+

C	0.000000	-1.412152	0.000000
C	0.000000	1.339199	0.000000
C	1.245606	-0.690702	0.000000
C	-1.245606	-0.690702	0.000000
C	-1.244284	0.680471	0.000000
C	1.244284	0.680471	0.000000
H	2.182012	-1.243602	0.000000
H	-2.182012	-1.243602	0.000000

H	-2.156311	1.268890	0.000000
H	2.156311	1.268890	0.000000
F	0.000000	2.654553	0.000000
C	0.000000	-2.780529	0.000000
H	0.927007	-3.348943	0.000000
H	-0.927007	-3.348943	0.000000

4-fluorotoluene

C	-1.360856	0.000027	-0.016387
C	1.423695	-0.000008	0.004168
C	-0.642762	1.201293	-0.009283
C	-0.642790	-1.201257	-0.009293
C	0.751061	-1.213470	-0.002097
C	0.751087	1.213471	-0.002105
H	-1.180260	2.147433	-0.017648
H	-1.180301	-2.147390	-0.017675
H	1.315448	-2.140844	-0.002269
H	1.315501	2.140828	-0.002284
F	2.781003	-0.000022	0.009020
C	-2.865862	-0.000014	0.015489
H	-3.270007	0.884464	-0.484170
H	-3.240851	-0.000188	1.044329
H	-3.269994	-0.884350	-0.484418

4-chlorophenylcarbene, singlet

C	0.137340	-3.360880	0.000000
C	0.019703	-1.923981	0.000000
C	0.000000	0.871900	0.000000
C	-1.200581	-1.203363	0.000000
C	1.226172	-1.185030	0.000000
C	1.226544	0.201906	0.000000
C	-1.217896	0.182722	0.000000
H	-2.138699	-1.755012	0.000000
H	2.155561	-1.748124	0.000000
H	2.151496	0.770597	0.000000
H	-2.150492	0.739081	0.000000
H	-0.899342	-3.761363	0.000000
Cl	-0.015660	2.603246	0.000000

4-chlorophenylcarbene, triplet

C	0.060185	-3.315121	0.000000
C	0.039040	-1.909073	0.000000
C	0.000000	0.865320	0.000000
C	-1.173129	-1.199846	0.000000
C	1.229897	-1.166532	0.000000
C	1.209247	0.197355	0.000000
C	-1.189649	0.165414	0.000000
H	-2.111001	-1.747952	0.000000

H	2.179023	-1.693770	0.000000
H	2.135923	0.762315	0.000000
H	-2.131802	0.704301	0.000000
H	-0.727793	-4.055574	0.000000
Cl	-0.023406	2.600328	0.000000

4-chlorobenzyl+

C	0.000000	-1.847089	0.000000
C	0.000000	0.933095	0.000000
C	1.242137	-1.124230	0.000000
C	-1.242137	-1.124230	0.000000
C	-1.237790	0.247663	0.000000
C	1.237790	0.247663	0.000000
H	2.180602	-1.674147	0.000000
H	-2.180602	-1.674147	0.000000
H	-2.162699	0.816327	0.000000
H	2.162699	0.816327	0.000000
Cl	0.000000	2.622786	0.000000
C	0.000000	-3.216563	0.000000
H	0.927164	-3.784789	0.000000
H	-0.927164	-3.784789	0.000000

4-chlorotoluene

C	-1.802478	0.000003	-0.015865
C	0.998512	0.000001	0.001654
C	-1.082904	-1.199578	-0.009541
C	-1.082904	1.199581	-0.009542
C	0.310312	1.210684	-0.003808
C	0.310309	-1.210683	-0.003810
H	-1.618456	-2.147029	-0.017489
H	-1.618453	2.147033	-0.017490
H	0.859664	2.147616	-0.004112
H	0.859661	-2.147615	-0.004113
Cl	2.738592	-0.000002	0.005976
C	-3.306830	-0.000002	0.017185
H	-3.679455	-0.000150	1.046952
H	-3.711561	-0.884649	-0.481611
H	-3.711566	0.884784	-0.481360

4-formylphenylcarbene, singlet

C	3.322536	-0.142979	0.000000
C	1.876554	-0.088729	0.000000
C	-0.907749	0.223966	0.000000
C	1.018485	-1.218867	0.000000
C	1.293708	1.200292	0.000000
C	-0.086091	1.358099	0.000000
C	-0.358882	-1.067665	0.000000
H	1.461527	-2.213070	0.000000

H	1.968847	2.051801	0.000000
H	-0.534669	2.350130	0.000000
H	-1.033722	-1.919527	0.000000
C	-2.382629	0.388307	0.000000
O	-3.170941	-0.549951	0.000000
H	-2.745872	1.435779	0.000000
H	3.595823	-1.220052	0.000000

4-formylphenylcarbene, triplet

C	-3.257302	-0.195806	-0.000002
C	-1.860356	-0.056391	-0.000001
C	0.892969	0.214415	0.000003
C	-1.024324	-1.192386	0.000002
C	-1.267666	1.216142	-0.000002
C	0.092055	1.338366	0.000000
C	0.327599	-1.050591	0.000003
H	-1.475136	-2.180741	0.000003
H	-1.906080	2.094097	-0.000004
H	0.548350	2.326645	0.000000
H	0.988834	-1.912361	0.000004
C	2.386115	0.351726	0.000003
O	3.160605	-0.554152	-0.000007
H	2.728936	1.414914	0.000014
H	-3.904281	-1.062193	-0.000002

4-formylbenzyl+

C	-1.801476	-0.101193	-0.000001
C	0.950935	0.245760	0.000005
C	-0.935801	-1.247395	0.000002
C	-1.249112	1.224416	-0.000001
C	0.119515	1.383712	0.000002
C	0.428731	-1.063893	0.000006
H	-1.370272	-2.244786	0.000003
H	-1.917683	2.082613	-0.000003
H	0.561022	2.377627	0.000002
H	1.123075	-1.899665	0.000009
C	2.445649	0.407781	0.000004
O	3.182667	-0.566876	-0.000009
H	2.832460	1.441360	-0.000001
C	-3.164058	-0.271919	-0.000005
H	-3.612359	-1.263111	-0.000003
H	-3.843883	0.577364	-0.000006

4-formyltoluene

C	-1.751274	-0.069721	-0.014973
C	1.040927	0.219326	0.002279
C	-0.912100	-1.194225	-0.009916
C	-1.166030	1.201105	-0.008134

C	0.218684	1.348810	-0.002185
C	0.469852	-1.058403	-0.003747
H	-1.355242	-2.188479	-0.018561
H	-1.803170	2.083356	-0.015265
H	0.663701	2.342979	-0.001506
H	1.125899	-1.925078	-0.004079
C	2.508775	0.376221	0.005399
O	3.304467	-0.557281	0.005451
H	2.871385	1.425656	0.008543
C	-3.246507	-0.231953	0.015638
H	-3.604099	-0.380724	1.040086
H	-3.560465	-1.098672	-0.572407
H	-3.747717	0.652245	-0.386592

4-trifluoromethylphenylcarbene, singlet

C	3.957299	0.109060	0.000426
C	2.513420	0.011449	0.000060
C	-0.282306	0.035300	-0.000694
C	1.779232	-1.200526	-0.000141
C	1.797404	1.229567	-0.000139
C	0.407656	1.249092	-0.000485
C	0.392917	-1.192354	-0.000531
H	2.319917	-2.144802	-0.000047
H	2.377404	2.148373	-0.000032
H	-0.140902	2.185077	-0.000710
H	-0.173509	-2.119862	-0.000859
C	-1.781032	0.002447	0.000005
F	-2.249269	-0.644288	1.090824
F	-2.250129	-0.657885	-1.082254
F	-2.326463	1.235525	-0.007449
H	4.342303	-0.933177	0.000545

4-trifluoromethylphenylcarbene, triplet

C	3.903004	0.061772	0.024274
C	2.496184	0.042217	0.005628
C	-0.276161	0.005570	-0.038028
C	1.791609	-1.172596	-0.007493
C	1.760293	1.237190	-0.006177
C	0.397606	1.213752	-0.026070
C	0.427447	-1.184005	-0.027179
H	2.343425	-2.108035	-0.003917
H	2.293065	2.182949	-0.001441
H	-0.162279	2.143241	-0.041539
H	-0.107935	-2.127831	-0.043462
C	-1.769086	-0.012865	0.000559
F	-2.241462	-0.007764	1.270620
F	-2.276685	-1.115080	-0.598193
F	-2.303424	1.066236	-0.616598

H 4.642489 -0.727065 0.034824

4-trifluoromethylbenzyl+

C -2.438655 -0.000010 0.000728
C 0.328746 0.000058 -0.045254
C -1.724168 1.244197 -0.013006
C -1.724115 -1.244185 -0.012994
C -0.346299 -1.234370 -0.036197
C -0.346354 1.234449 -0.036174
H -2.277642 2.180515 -0.005270
H -2.277542 -2.180531 -0.005253
H 0.219734 -2.160311 -0.053040
H 0.219645 2.160410 -0.052998
C 1.844259 0.000018 0.001749
F 2.234413 -0.000475 1.285559
F 2.337692 1.090615 -0.601130
F 2.337571 -1.090223 -0.601899
C -3.811873 -0.000033 0.024958
H -4.380279 0.927451 0.035458
H -4.380250 -0.927534 0.035480

4-trifluoromethyltoluene

C 2.402490 0.000009 0.017985
C -0.400080 0.000005 -0.046752
C 1.685478 -1.201572 -0.000822
C 1.685476 1.201588 -0.000830
C 0.293756 1.210042 -0.027322
C 0.293759 -1.210032 -0.027328
H 2.224651 -2.146702 0.012217
H 2.224649 2.146717 0.012204
H -0.250608 2.149596 -0.043288
H -0.250599 -2.149589 -0.043297
C -1.892422 -0.000001 -0.001091
F -2.353812 -0.000002 1.272591
F -2.417574 -1.090011 -0.606835
F -2.417596 1.089996 -0.606838
C 3.906916 -0.000010 0.007383
H 4.292349 -0.000491 -1.017594
H 4.304080 -0.884955 0.511489
H 4.304081 0.885398 0.510675

4-cyanophenylcarbene, singlet

C -3.265683 0.133050 -0.000015
C -1.822916 0.016785 -0.000004
C 0.978712 0.000918 0.000013
C -1.105066 -1.204625 0.000003
C -1.090202 1.226893 0.000002
C 0.297128 1.229473 0.000010

C	0.281538	-1.220433	0.000010
H	-1.658769	-2.141443	0.000000
H	-1.658364	2.153172	-0.000003
H	0.862606	2.157209	0.000016
H	0.837127	-2.154292	0.000015
C	2.412492	-0.010214	0.000012
N	3.595132	-0.020267	-0.000028
H	-3.664543	-0.903856	-0.000022

4-cyanophenylcarbene, triplet

C	0.058807	-3.207119	0.000000
C	0.037958	-1.802134	0.000000
C	0.000000	0.964400	0.000000
C	-1.179150	-1.099304	0.000000
C	1.234347	-1.066733	0.000000
C	1.211566	0.295459	0.000000
C	-1.192556	0.264096	0.000000
H	-2.113802	-1.652032	0.000000
H	2.179870	-1.599541	0.000000
H	2.138122	0.860974	0.000000
H	-2.134189	0.804265	0.000000
C	-0.019816	2.417556	0.000000
N	-0.035601	3.562568	0.000000
H	-0.727726	-3.948970	0.000000

4-cyanobenzyl+

C	0.000000	-1.750747	0.000000
C	0.000000	1.025545	0.000000
C	1.244394	-1.035456	0.000000
C	-1.244393	-1.035456	0.000000
C	-1.239049	0.340914	0.000000
C	1.239051	0.340914	0.000000
H	2.181058	-1.588693	0.000000
H	-2.181057	-1.588693	0.000000
H	-2.164831	0.909075	0.000000
H	2.164832	0.909075	0.000000
C	0.000000	2.452637	0.000000
N	-0.000003	3.637426	0.000000
C	0.000000	-3.124496	0.000000
H	0.927635	-3.692935	0.000000
H	-0.927634	-3.692935	0.000000

4-cyanotoluene

C	-1.695532	0.000004	-0.015517
C	1.112384	0.000000	0.002044
C	-0.978189	1.202096	-0.009398
C	-0.978191	-1.202092	-0.009398
C	0.412788	-1.213802	-0.003346

C	0.412793	1.213802	-0.003346
H	-1.517603	2.147100	-0.017278
H	-1.517607	-2.147094	-0.017282
H	0.960375	-2.152479	-0.003322
H	0.960382	2.152477	-0.003325
C	2.545786	-0.000002	0.004984
N	3.728125	-0.000003	0.008149
C	-3.199369	-0.000003	0.016955
H	-3.603972	0.885234	-0.480620
H	-3.603982	-0.885135	-0.480798

4-nitrophenylcarbene, singlet

C	3.626243	-0.134068	-0.000002
C	2.183243	-0.017942	0.000000
C	-0.591498	-0.002483	0.000000
C	1.464023	1.202952	0.000008
C	1.449332	-1.227721	-0.000008
C	0.060650	-1.234414	-0.000007
C	0.076205	1.222719	0.000007
H	2.016535	2.140302	0.000014
H	2.016352	-2.154540	-0.000014
H	-0.517327	-2.151451	-0.000012
H	-0.492430	2.145674	0.000012
N	-2.065248	0.008450	0.000000
H	4.025023	0.902648	0.000009
O	-2.629503	1.114090	-0.000019
O	-2.645572	-1.088595	0.000019

4-nitrophenylcarbene, triplet

C	-3.564984	0.066241	0.000000
C	-2.160076	0.043621	0.000000
C	0.586657	0.002646	0.000000
C	-1.459872	-1.176107	0.000004
C	-1.424354	1.240857	-0.000005
C	-0.063512	1.220249	-0.000004
C	-0.098054	-1.194851	0.000004
H	-2.015284	-2.109220	0.000009
H	-1.957667	2.186148	-0.000009
H	0.516446	2.135654	-0.000008
H	0.454863	-2.126920	0.000007
N	2.050952	-0.019316	0.000000
H	-4.308347	-0.718957	0.000003
O	2.612315	-1.126404	-0.000011
O	2.644995	1.070476	0.000012

4-nitrobenzyl+

C	0.000000	-2.110426	0.000000
C	0.000000	0.636853	0.000000

C	1.245638	-1.394420	0.000000
C	-1.245638	-1.394420	0.000000
C	-1.241940	-0.016489	0.000000
C	1.241940	-0.016489	0.000000
H	2.182209	-1.947888	0.000000
H	-2.182209	-1.947888	0.000000
H	-2.155777	0.568457	0.000000
H	2.155777	0.568456	0.000000
N	0.000000	2.118294	0.000000
O	1.110343	2.669128	0.000000
O	-1.110343	2.669128	0.000000
C	0.000000	-3.483146	0.000000
H	-0.927545	-4.052011	0.000000
H	0.927544	-4.052011	0.000000

4-nitrotoluene

C	2.063014	0.000044	-0.015022
C	-0.717628	0.000007	0.000775
C	1.345082	1.201896	-0.009668
C	1.345086	-1.201865	-0.009653
C	-0.046639	-1.217664	-0.004029
C	-0.046685	1.217653	-0.004054
H	1.883864	2.147064	-0.017019
H	1.883894	-2.147017	-0.017006
H	-0.607619	-2.145290	-0.004653
H	-0.607691	2.145264	-0.004702
N	-2.184984	-0.000007	0.003382
O	-2.761919	1.099545	0.005039
O	-2.761888	-1.099572	0.004986
C	3.566720	-0.000020	0.017139
H	3.971136	0.885668	-0.479692
H	3.971222	-0.884639	-0.481503
H	3.936837	-0.001093	1.047773

nonbenzenoid arylcarbene sets

tropylcarbene+, singlet, (cycloheptatrienylcarbene)+

C	-2.676360	-0.000041	-0.117112
C	-1.285377	-0.000026	0.004767
C	-0.651871	-1.276772	-0.018333
C	-0.651912	1.276743	-0.018280
C	0.699943	1.563068	0.000582
H	-1.315812	2.140303	-0.048751
H	-1.315747	-2.140345	-0.048913
C	0.699992	-1.563057	0.000640
H	0.938513	2.624915	0.003232
H	0.938594	-2.624896	0.003289
C	1.808681	-0.692467	0.013775

H	2.783901	-1.173990	0.022562
C	1.808659	0.692514	0.013738
H	2.783864	1.174068	0.022499
H	-3.323842	0.000165	0.767428

tropylcarbene+, singlet, ts

C	-1.301362	0.000000	-0.000025
C	-0.647727	-1.304340	0.000178
C	-0.647727	1.304340	0.000179
C	0.693140	1.560978	0.000103
H	-1.306175	2.169427	0.000373
H	-1.306175	-2.169427	0.000373
C	0.693140	-1.560978	0.000103
H	0.934300	2.622382	0.000250
H	0.934300	-2.622382	0.000251
C	1.818452	-0.684006	-0.000145
H	2.788786	-1.173988	-0.000296
C	1.818452	0.684006	-0.000146
H	2.788786	1.173988	-0.000297
C	-2.616138	0.000000	-0.000272
H	-3.695200	0.000000	-0.000503

tropylcarbene+, triplet

C	2.671630	-0.140342	0.000009
C	1.265007	-0.068748	0.000001
C	0.578489	-1.300067	-0.000005
C	0.689808	1.216459	-0.000006
C	-0.622742	1.568518	-0.000006
H	1.402045	2.039443	-0.000011
H	1.224640	-2.175606	-0.000009
C	-0.759695	-1.535629	-0.000005
H	-0.811863	2.639902	-0.000011
H	-1.044623	-2.585416	-0.000012
C	-1.832718	-0.616320	0.000006
H	-2.825744	-1.059117	0.000016
C	-1.770927	0.752401	0.000005
H	-2.719355	1.284047	0.000017
H	3.461793	0.599120	0.000017

tropylcarbene+, triplet, C2v, ts

C	0.000000	0.000000	1.271561
C	0.000000	1.262120	0.630164
C	0.000000	-1.262120	0.630164
C	0.000000	-1.554385	-0.697152
H	0.000000	-2.111231	1.310037
H	0.000000	2.111231	1.310037
C	0.000000	1.554385	-0.697152
H	0.000000	-2.615946	-0.934596

H	0.000000	2.615946	-0.934596
C	0.000000	0.686045	-1.808030
H	0.000000	1.173029	-2.780207
C	0.000000	-0.686045	-1.808030
H	0.000000	-1.173029	-2.780207
C	0.000000	0.000000	2.658024
H	0.000000	0.000000	3.732225

tropylCH2++

H	2.841584	1.174726	-0.000027
C	1.856364	0.707250	-0.000028
C	1.856364	-0.707250	0.000028
C	0.766986	1.594962	-0.000019
C	-0.598024	1.285693	0.000022
H	1.015711	2.655702	-0.000010
H	2.841584	-1.174726	0.000026
C	0.766986	-1.594962	0.000022
C	-1.217187	0.000000	0.000000
H	-1.274183	2.141770	0.000064
C	-0.598024	-1.285693	-0.000026
H	1.015711	-2.655702	0.000013
C	-2.627471	0.000000	0.000001
H	-1.274183	-2.141770	-0.000067
H	-3.201097	-0.928033	-0.000051
H	-3.201097	0.928032	0.000057

tropylCH2++, perp ts

C	-0.602845	-1.278619	-0.000001
H	-1.264962	-2.147059	-0.000002
C	0.766599	-1.577460	-0.000001
C	-1.186556	0.000000	0.000000
C	-0.602845	1.278619	0.000000
C	-2.652339	0.000000	0.000001
H	1.004577	-2.640605	-0.000002
C	1.862551	-0.701017	0.000001
H	2.842496	-1.177162	0.000002
C	1.862551	0.701017	0.000001
H	-1.264962	2.147059	-0.000001
C	0.766599	1.577460	-0.000001
H	1.004577	2.640605	-0.000002
H	2.842495	1.177162	0.000002
H	-3.223253	-0.000006	0.937320
H	-3.223255	0.000006	-0.937316

tropylCH3+

H	-2.910510	1.176654	0.006295
C	-1.933540	0.697917	0.003097
C	-0.830813	1.557558	0.001521

C	-1.933554	-0.697888	0.003121
C	-0.830844	-1.557553	0.001552
H	-2.910535	-1.176602	0.006360
H	-1.064878	2.620361	0.005667
C	0.531080	1.249195	-0.007272
C	0.531052	-1.249213	-0.007314
H	-1.064929	-2.620352	0.005702
C	1.177763	-0.000012	-0.017018
H	1.194200	2.112998	-0.011329
C	2.681393	-0.000002	0.008206
H	1.194154	-2.113029	-0.011440
H	3.087968	0.886658	-0.481713
H	3.087896	-0.886644	-0.481804
H	3.031409	-0.000070	1.046896

cyclopentadienylcarbene-, singlet

C	-2.215191	-0.178464	0.000006
C	-0.834527	-0.040090	-0.000002
C	0.017055	1.145560	-0.000014
C	0.096521	-1.161067	-0.000008
H	-0.363547	2.165717	0.000018
C	1.335640	0.759595	0.000009
C	1.385312	-0.687693	0.000002
H	-0.229369	-2.198049	0.000009
H	2.299809	-1.278847	0.000008
H	2.207040	1.413357	0.000000
H	-2.622796	0.870771	0.000005

cyclopentadienylcarbene-, triplet

C	2.222947	-0.000037	-0.100658
C	0.802154	-0.000014	-0.025949
C	-0.055694	1.142174	-0.017401
C	-0.055722	-1.142180	-0.017382
H	0.290393	2.173772	-0.029439
C	-1.377277	0.713255	0.020459
C	-1.377296	-0.713228	0.020460
H	0.290332	-2.173790	-0.029390
H	-2.261101	-1.348850	0.049846
H	-2.261066	1.348897	0.049927
H	2.986767	0.000147	0.681886

fulvene

C	-0.753883	0.000000	0.000001
C	0.121629	1.176119	0.000000
C	0.121629	-1.176119	0.000000
H	-0.225329	2.203267	0.000002
C	1.405490	0.733884	-0.000001
C	1.405490	-0.733884	0.000000

H	-0.225329	-2.203267	0.000003
H	2.298471	-1.350102	-0.000001
H	2.298471	1.350102	0.000000
C	-2.101499	0.000000	-0.000001
H	-2.669710	-0.925919	-0.000001
H	-2.669710	0.925919	-0.000001

fulvene, er pts

C	0.000000	0.000000	0.745632
C	0.000000	1.167247	-0.111592
C	0.000000	-1.167247	-0.111592
H	0.000000	2.184737	0.256265
C	0.000000	0.697466	-1.430929
C	0.000000	-0.697466	-1.430929
H	0.000000	-2.184737	0.256265
H	0.000000	-1.352824	-2.295548
H	0.000000	1.352824	-2.295548
C	0.000000	0.000000	2.110658
H	0.914221	0.000000	2.725542
H	-0.914221	0.000000	2.725542

methylcyclopentadienide-

C	0.663567	-0.000003	-0.030782
C	-0.172599	1.138790	-0.011042
C	-0.172604	-1.138793	-0.011042
H	0.171553	2.173927	-0.017737
C	-1.515212	0.705736	0.014268
C	-1.515214	-0.705731	0.014268
H	0.171540	-2.173933	-0.017736
H	-2.396441	-1.346912	0.006069
H	-2.396436	1.346921	0.006069
C	2.163188	-0.000001	0.017606
H	2.580559	-0.882746	-0.487312
H	2.581937	-0.000146	1.038047
H	2.580535	0.882901	-0.487054

cyclopropenylcarbene+, singlet

C	0.000000	0.000000	0.386986
C	0.000000	0.635725	-1.004824
C	0.000000	-0.635725	-1.004824
H	0.000000	1.671886	-1.317564
H	0.000000	-1.671886	-1.317564
C	0.000000	0.000000	1.613545
H	0.000000	0.000000	2.689834

cyclopropenylcarbene+, triplet

H	1.738491	-1.347969	0.000000
C	0.762172	-0.878053	0.000000

C	0.000000	0.279476	0.000000
C	-0.589792	-0.979579	0.000000
C	-0.067474	1.670052	0.000000
H	-1.487304	-1.586519	0.000000
H	-0.880620	2.383115	0.000000

cyclopropenyl+CH2+

C	0.000000	0.000000	0.170281
C	0.000000	0.701836	-1.010125
C	0.000000	-0.701836	-1.010125
H	0.000000	1.640171	-1.572117
H	0.000000	-1.640171	-1.572117
C	0.000000	0.000000	1.643168
H	0.000000	-0.950878	2.192517
H	0.000000	0.950878	2.192517

cyclopropenyl+CH2+, perp

C	0.000000	0.000000	0.209717
C	0.000000	0.671279	-1.021020
C	0.000000	-0.671279	-1.021020
H	0.000000	1.670244	-1.471885
H	0.000000	-1.670244	-1.471885
C	0.000000	0.000000	1.603214
H	0.951588	0.000000	2.159211
H	-0.951588	0.000000	2.159211

cyclopropenylCH3+

C	-0.123044	-0.000001	-0.012810
C	1.073435	-0.681075	0.001589
C	1.073434	0.681076	0.001587
H	1.627260	-1.612003	0.004078
H	1.627260	1.612004	0.004073
C	-1.588362	0.000000	-0.004837
H	-1.976930	0.900321	-0.482252
H	-1.913434	-0.000112	1.043382
H	-1.976930	-0.900211	-0.482458

cyclopropenylidene, singlet

C	0.000000	0.000000	0.938956
C	0.000000	0.664285	-0.324393
C	0.000000	-0.664285	-0.324393
H	0.000000	-1.596901	-0.870506
H	0.000000	1.596901	-0.870506

cyclopropenylidene, triplet

C	0.000000	0.000000	0.966529
C	0.000000	0.668641	-0.327914
C	0.000000	-0.668641	-0.327914

H	0.000000	-1.562516	-0.932103
H	0.000000	1.562516	-0.932103

cyclopropenium+

H	0.000000	0.000000	1.872746
C	0.000000	0.000000	0.789515
C	0.000000	0.683740	-0.394757
C	0.000000	-0.683740	-0.394757
H	0.000000	-1.621845	-0.936374
H	0.000000	1.621845	-0.936374

cyclopropene

C	-0.791702	-0.212659	0.000000
C	0.000000	0.819765	0.000000
H	0.140018	1.889048	0.000000
H	-1.788057	-0.625270	0.000000
C	0.681154	-0.522335	0.000000
H	1.155663	-0.886200	0.912532
H	1.155663	-0.886200	-0.912532

acyclic heteroatomcarbene (XY-C) sets

aminocarbene, singlet

C	0.062292	0.792190	0.000000
N	0.062292	-0.524892	0.000000
H	-0.751328	-1.142768	0.000000
H	0.949455	-1.018070	0.000000
H	-1.007919	1.081943	0.000000

aminocarbene, triplet

H	1.076072	-0.831118	-0.185777
N	0.578175	-0.000004	0.120534
C	-0.772402	0.000010	-0.173924
H	1.076081	0.831119	-0.185735
H	-1.564968	-0.000035	0.571314

aminocarbenium+, ($\text{CH}_2=\text{NH}_2^+$)

N	0.000000	0.000000	0.602556
H	0.000000	0.869951	1.140851
H	0.000000	-0.869951	1.140851
C	0.000000	0.000000	-0.678939
H	0.000000	0.944175	-1.212980
H	0.000000	-0.944175	-1.212980

aminomethane

N	-0.051681	-0.759433	0.000000
H	0.457708	-1.100130	0.812232
H	0.457708	-1.100130	-0.812232

C	-0.051681	0.704304	0.000000
H	0.941900	1.176202	0.000000
H	-0.592732	1.057132	0.880564
H	-0.592732	1.057132	-0.880564

diaminocarbene, singlet

C	0.000000	-0.614141	-0.000022
N	-1.111427	0.141919	0.000067
N	1.111427	0.141919	-0.000060
H	2.009151	-0.314562	0.000032
H	1.131514	1.163552	0.000114
H	-1.131514	1.163552	-0.000063
H	-2.009151	-0.314562	0.000000

diaminocarbene, triplet

C	-0.001047	0.472099	-0.165835
N	-1.271454	-0.024318	0.049577
N	1.210004	-0.191295	0.100678
H	1.573688	-0.708294	-0.701576
H	1.928710	0.453522	0.416237
H	-1.387975	-0.504298	0.938687
H	-1.677989	-0.564235	-0.710131

diaminocarbenium+

H	0.000000	0.000000	1.516239
C	0.000000	0.000000	0.430729
N	0.000000	1.164447	-0.175830
N	0.000000	-1.164447	-0.175830
H	0.000000	-1.263294	-1.187448
H	0.000000	-2.021037	0.367954
H	0.000000	2.021037	0.367954
H	0.000000	1.263294	-1.187448

diaminomethane

H	0.011391	1.095077	1.012849
C	0.000748	0.545857	0.060350
H	-0.040467	1.287494	-0.742172
N	-1.161311	-0.334191	-0.108268
N	1.264683	-0.157381	-0.039646
H	1.367279	-0.791987	0.750611
H	1.231164	-0.745180	-0.871632
H	-1.286551	-0.900726	0.730077
H	-2.010907	0.221188	-0.206434

hydroxycarbene, snglet, anti

H	1.240044	0.755196	0.000001
C	0.713167	-0.225385	0.000000
O	-0.552377	0.156300	0.000000

H -1.100029 -0.653291 0.000001

hydroxycarbene, singlet, syn

H 1.105126 0.906682 0.000000
C 0.740892 -0.153539 0.000000
O -0.573788 -0.098831 0.000000
H -0.960174 0.805195 0.000000

hydroxycarbene, triplet

H 1.465182 -0.242826 0.586948
C 0.725228 0.101234 -0.134650
O -0.596244 -0.129423 -0.011887
H -1.046600 0.670808 0.316046

hydroxycarbene, CH+ (formaldehyde OH+)

O -0.615236 -0.131743 0.000000
H -1.154970 0.702356 0.000003
C 0.629891 0.033819 -0.000002
H 1.219998 -0.878936 0.000006
H 1.077513 1.027607 0.000003

hydroxycarbene, CH2 (methanol)

O 0.750091 0.122712 0.000000
H 1.131645 -0.769070 0.000008
C -0.665708 -0.019527 0.000002
H -1.074676 0.990422 -0.000279
H -1.031748 -0.542708 0.891759
H -1.031706 -0.543182 -0.891501

methoxycarbene, singlet

H -1.621760 -0.165786 -0.893384
C -1.090807 0.161049 0.000002
H -0.944288 1.243834 -0.000428
O 0.205479 -0.500539 -0.000006
H -1.621451 -0.165124 0.893817
C 1.335480 0.146854 0.000008
H 1.075623 1.243972 -0.000018

methoxycarbene, triplet

C -1.254507 0.214740 0.165582
O -0.162879 -0.525395 -0.048967
C 1.083101 0.196839 0.000645
H 1.225380 0.641770 0.987433
H 1.100383 0.978197 -0.763830
H 1.862417 -0.537514 -0.196486
H -1.856709 0.651238 -0.632737

methoxycarbenium+, Z conformation

H	1.677743	-0.232898	0.900347
C	1.203663	0.149333	0.000000
H	1.093232	1.232555	-0.000003
O	-0.151406	-0.479615	0.000000
H	1.677745	-0.232903	-0.900344
C	-1.194861	0.204837	0.000000
H	-1.160406	1.295729	0.000000
H	-2.129883	-0.350579	0.000001

dimethylether

H	1.214027	-0.840599	-0.891754
C	1.165542	-0.199941	0.000000
H	1.214057	-0.840557	0.891783
O	0.000000	0.600159	0.000000
H	2.017696	0.480165	-0.000030
C	-1.165542	-0.199941	0.000000
H	-1.214057	-0.840556	0.891784
H	-1.214027	-0.840600	-0.891753
H	-2.017696	0.480165	-0.000032

methoxymethylcarbene, singlet

H	-2.265409	-0.353090	-0.892632
C	-1.792089	0.056510	0.000014
H	-1.812185	1.145348	-0.000162
O	-0.413662	-0.382779	-0.000021
H	-2.265285	-0.352798	0.892860
C	0.481879	0.580862	-0.000028
C	1.826310	-0.092492	0.000004
H	2.378505	0.270290	0.873843
H	2.378857	0.270746	-0.873415
H	1.798214	-1.187550	-0.000267

methoxymethylcarbene, triplet

H	-1.247369	1.401948	-0.155341
C	-1.610440	0.389754	0.045182
H	-1.917663	0.309927	1.090277
O	-0.593044	-0.582932	-0.256297
H	-2.450058	0.160457	-0.609728
C	0.550816	-0.430715	0.437038
C	1.751978	0.276375	-0.085082
H	2.557820	0.229342	0.649455
H	1.542263	1.334478	-0.291947
H	2.105237	-0.185181	-1.015168

1-methoxyethyl+

H	-2.303649	-0.367908	-0.899171
C	-1.865519	0.057212	0.000000
H	-1.880341	1.146230	-0.000013

O	-0.457689	-0.416808	0.000000
H	-2.303642	-0.367886	0.899185
C	0.508011	0.391101	-0.000001
H	0.290558	1.464026	0.000001
C	1.880954	-0.106905	-0.000001
H	2.399898	0.303350	-0.876092
H	1.918134	-1.195109	-0.000021
H	2.399880	0.303313	0.876120

ethylmethylether

H	-1.983147	0.653601	-0.891709
C	-1.804474	0.036687	0.000000
H	-1.983146	0.653601	0.891709
O	-0.499323	-0.508650	0.000000
H	-2.499484	-0.803576	0.000000
C	0.489902	0.508139	0.000000
H	0.371847	1.150689	0.886881
H	0.371847	1.150688	-0.886881
C	1.843575	-0.165641	0.000000
H	2.644418	0.578783	0.000000
H	1.949115	-0.794848	-0.885856
H	1.949115	-0.794848	0.885856

dimethoxycarbene, singlet, W conformation

C	0.000000	0.360669	-0.000002
O	1.050414	-0.455973	-0.000009
C	2.312079	0.233178	0.000003
H	2.860584	-0.071721	-0.891837
H	2.860417	-0.071408	0.892055
O	-1.050414	-0.455974	0.000009
C	-2.312078	0.233178	-0.000002
H	-2.860438	-0.071449	-0.892026
H	-2.142771	1.309844	0.000147
H	-2.860562	-0.071679	0.891866

dimethoxycarbene, triplet

H	1.630072	1.217069	0.932202
C	1.741426	0.745550	-0.047244
H	1.175193	1.301438	-0.799032
O	1.288707	-0.623681	-0.002890
H	2.792512	0.705130	-0.329058
C	0.009502	-0.770676	0.388037
O	-1.050776	-0.469366	-0.405953
C	-1.924623	0.546935	0.119513
H	-1.378418	1.475850	0.303986
H	-2.395597	0.208506	1.044921
H	-2.685037	0.705529	-0.644114

dimethoxycarbenium+, Z conformation

C	-0.032445	0.720838	0.000000
O	-0.744576	-0.337063	0.000000
C	-2.222916	-0.229684	0.000000
H	-2.515811	0.819417	-0.000003
H	-2.550589	-0.743249	0.899431
H	-2.550589	-0.743255	-0.899427
O	1.235355	0.669629	0.000000
C	1.913981	-0.649937	0.000000
H	1.621150	-1.183213	0.901692
H	2.967570	-0.393881	-0.000001
H	1.621150	-1.183214	-0.901691
H	-0.470831	1.719565	0.000000

dimethoxymethane

H	2.169498	-0.446607	1.192188
C	2.152221	-0.256614	0.110151
H	2.639830	0.708262	-0.083841
O	0.831814	-0.284827	-0.402936
H	2.703767	-1.044490	-0.401732
C	0.025229	0.706161	0.200563
H	0.366583	1.711392	-0.079849
H	0.071571	0.593801	1.301430
O	-1.277013	0.589740	-0.260514
C	-1.882664	-0.638175	0.135107
H	-1.819510	-0.769108	1.223490
H	-1.409903	-1.490180	-0.357796
H	-2.928968	-0.570599	-0.161213

fluorocarbene, singlet

F	0.068512	-0.591459	0.000000
C	0.068512	0.727258	0.000000
H	-1.027686	0.959582	0.000000

fluorocarbene, triplet

F	0.057997	-0.615966	0.000000
C	0.057997	0.711544	0.000000
H	-0.869957	1.274428	0.000000

fluorocarbenium+

F	0.000000	0.000000	0.642803
C	0.000000	0.000000	-0.599629
H	0.000000	0.972255	-1.093724
H	0.000000	-0.972255	-1.093724

fluoromethane

F	0.000000	0.000000	0.754749
C	0.000000	0.000000	-0.635465

H	0.000000	1.031387	-0.993319
H	-0.893207	-0.515693	-0.993319
H	0.893207	-0.515693	-0.993319

difluorocarbene, singlet

F	0.000000	1.036211	-0.201548
C	0.000000	0.000000	0.604644
F	0.000000	-1.036211	-0.201548

difluorocarbene, triplet

F	0.000000	1.148558	-0.166287
C	0.000000	0.000000	0.498861
F	0.000000	-1.148558	-0.166287

difluorocarbenium+

H	0.000000	0.000000	1.508067
C	0.000000	0.000000	0.415503
F	0.000000	1.066609	-0.222283
F	0.000000	-1.066609	-0.222283

difluoromethane

H	0.908454	0.000000	1.106712
C	0.000000	0.000000	0.502939
F	0.000000	1.109672	-0.290615
H	-0.908454	0.000000	1.106712
F	0.000000	-1.109672	-0.290615

silylcarbene, singlet

H	-1.170529	-1.204592	-0.527134
Si	-0.505703	0.011260	-0.007137
C	1.358243	-0.168369	-0.040552
H	-1.191378	1.217986	-0.549536
H	-0.582404	0.032688	1.486983
H	1.874695	0.806500	-0.067083

silylcarbene, triplet

H	-1.077696	1.358443	-0.000439
Si	-0.507823	-0.010146	0.000000
C	1.317672	0.109345	0.000002
H	-0.991966	-0.731680	1.206248
H	-0.991909	-0.732433	-1.205821
H	2.265058	-0.408353	0.000001

methylsilyl+

H	-1.408616	1.251228	0.017026
Si	-0.640393	0.000032	-0.004755
H	1.524051	-0.003132	1.039093
H	-1.407677	-1.251749	0.016987

C	1.180442	0.000137	-0.008004
H	1.587134	-0.897244	-0.481682
H	1.587965	0.899626	-0.476825

silylmethane

H	1.158643	-1.077703	-0.879842
Si	0.635703	0.000000	0.000000
H	1.158639	-0.223115	1.373240
H	1.158640	1.300819	-0.493395
C	-1.244482	0.000000	0.000000
H	-1.636289	0.790097	0.644756
H	-1.636290	-0.953423	0.361867
H	-1.636291	0.163326	-1.006622

disilylcarbene, singlet

Si	1.676741	0.088236	-0.008601
C	0.000004	-0.671104	-0.086663
Si	-1.676743	0.088234	-0.008601
H	2.723404	-0.822281	-0.531884
H	1.915426	1.448690	-0.570076
H	1.744478	0.151565	1.482382
H	-2.723456	-0.822363	-0.531642
H	-1.744413	0.151855	1.482370
H	-1.915437	1.448575	-0.570345

disilylcarbene, triplet

Si	-1.831333	0.000002	0.000001
C	0.000000	-0.000017	-0.000006
Si	1.831333	0.000002	0.000001
H	-2.344197	-0.304883	1.360695
H	-2.344187	1.330847	-0.416300
H	-2.344214	-1.025941	-0.944385
H	2.344195	-0.305370	1.360586
H	2.344215	-1.025604	-0.944751
H	2.344188	1.330996	-0.415823

μ -hydridodisilylmethane+ (C_{2v})

H	-0.000001	1.765568	-0.898291
C	0.000000	1.145421	-0.000001
Si	1.249270	-0.237187	-0.000001
Si	-1.249270	-0.237187	0.000001
H	-1.885770	-0.604579	-1.270348
H	-1.885768	-0.604578	1.270351
H	0.000000	1.765569	0.898289
H	0.000002	-1.344119	0.000001
H	1.885770	-0.604576	-1.270351
H	1.885772	-0.604574	1.270349

silylmethylsilylium+ ($\text{H}_3\text{Si}-\text{CH}_2-\text{SiH}_2^+$)

H	2.159353	-0.663982	1.252939
Si	1.571708	-0.169711	0.000000
C	0.114592	0.859851	0.000001
H	2.159354	-0.663976	-1.252941
Si	-1.534463	-0.220710	0.000000
H	0.048125	1.478732	-0.901156
H	0.048123	1.478732	0.901158
H	-1.505679	-1.051895	1.219959
H	-2.612614	0.781117	-0.000028
H	-1.505656	-1.051934	-1.219932

disilylmethane

H	0.000000	1.485878	0.879004
C	0.000000	0.831113	0.000000
H	0.000000	1.485878	-0.879004
Si	-1.582276	-0.183860	0.000000
Si	1.582276	-0.183860	0.000000
H	1.636312	-1.050568	1.206447
H	1.636313	-1.050566	-1.206448
H	2.780849	0.695955	0.000001
H	-1.636313	-1.050565	1.206448
H	-2.780849	0.695955	-0.000002
H	-1.636311	-1.050569	-1.206446

silylethene

H	1.626487	1.366863	-0.000308
C	1.741285	0.286016	0.000047
H	2.764359	-0.082182	0.000826
Si	-1.079564	0.077455	0.000067
H	-1.057441	1.563029	-0.000048
H	-1.814872	-0.399989	-1.200744
H	-1.813902	-0.400407	1.201281
C	0.681306	-0.539301	-0.000382
H	0.873724	-1.611971	0.000066

(silylmethyl)carbene, triplet

H	-0.815850	1.365001	0.772224
C	-0.732794	0.631237	-0.038202
H	-0.865188	1.191803	-0.975791
Si	1.012027	-0.115068	0.005923
H	1.260885	-0.738779	1.329414
H	1.133675	-1.154099	-1.048742
H	2.036503	0.936039	-0.235884
C	-1.765776	-0.406293	0.118704
H	-1.926976	-1.338678	-0.407158

2-silylethyl+ (symmetrically silyl-bridged cation)

H	1.283884	1.242676	-0.912884
C	1.136081	0.682468	0.006858
H	1.122999	1.247586	0.938204
C	1.136343	-0.682333	0.006764
Si	-1.034247	-0.000030	-0.005401
H	-1.321015	-1.237227	-0.744044
H	-1.327147	-0.000815	1.431003
H	-1.321411	1.237433	-0.743421
H	1.123369	-1.247589	0.938007
H	1.284231	-1.242451	-0.912977

silylethane

H	0.647972	1.329132	-0.875743
C	0.562740	0.675738	-0.000001
H	0.647971	1.329132	0.875742
Si	-1.144369	-0.121714	0.000000
H	-1.309079	-0.978237	-1.205556
H	-1.309171	-0.978021	1.205696
H	-2.219132	0.906721	-0.000132
C	1.700235	-0.350984	0.000000
H	2.678761	0.137508	0.000007
H	1.653002	-0.995378	-0.882395

phosphinocarbene, singlet

H	1.182818	-1.149392	0.000138
P	0.423797	0.017392	-0.000032
H	1.369941	1.077252	0.000174
C	-1.187929	-0.157964	0.000026
H	-1.782135	0.759040	0.000007

phosphinocarbene, triplet

H	0.906967	1.047789	0.730730
P	0.511783	-0.000015	-0.135444
H	0.906998	-1.047632	0.730951
C	-1.234059	0.000030	0.176628
H	-2.086361	-0.000110	-0.489787

phosphinocarbenium+

H	1.233881	-1.188572	0.000023
P	0.510119	0.000000	-0.000015
H	1.233881	1.188572	0.000028
C	-1.127876	0.000000	0.000021
H	-1.676147	0.938527	0.000028
H	-1.676147	-0.938527	0.000024

phosphinomethane

C	-0.069213	1.185321	0.000000
H	-0.607992	1.540751	0.880674

H	-0.607992	1.540751	-0.880674
H	0.929050	1.624306	0.000000
P	-0.069213	-0.672138	0.000000
H	0.870206	-0.867835	-1.041984
H	0.870206	-0.867835	1.041984

thiocarbene, singlet, anti

H	1.620043	-0.774735	0.000010
C	1.151898	0.226239	-0.000002
S	-0.471670	-0.107486	0.000000
H	-0.984707	1.137075	0.000008

thiocarbene, singlet, syn

H	-1.602104	0.876956	0.000000
C	-1.158131	-0.128687	0.000000
S	0.475736	-0.082168	0.000000
H	0.939121	1.209850	0.000000

thiocarbene, triplet

H	-1.952143	-0.016014	0.610808
C	-1.179107	0.041286	-0.146667
S	0.512679	-0.090709	0.013461
H	0.823929	1.219642	0.053827

thiocarbene CH+

S	0.548580	-0.090533	0.000000
H	0.846404	1.223378	0.000001
C	-1.065834	0.025095	0.000000
H	-1.635668	-0.901304	0.000001
H	-1.593011	0.975882	-0.000001

thiomethane (methanethiol)

S	0.047943	-0.664565	0.000000
H	-1.282097	-0.825738	0.000000
C	0.047943	1.149294	0.000000
H	1.092126	1.461722	0.000000
H	-0.432384	1.550650	0.891949
H	-0.432384	1.550650	-0.891949

methylthiocarbene, singlet

S	0.214775	-0.506590	0.000000
C	1.283669	0.737760	-0.000001
H	2.277282	0.252894	0.000005
C	-1.388021	0.325342	0.000000
H	-1.950299	0.037994	-0.889864
H	-1.187073	1.397742	-0.000131
H	-1.950199	0.038197	0.889993

methylthiocarbene, triplet

S	0.179986	-0.572563	0.016874
C	1.371444	0.619747	-0.147563
H	1.953926	1.137012	0.607800
C	-1.346715	0.418351	0.001990
H	-2.180403	-0.283798	0.056666
H	-1.418907	0.990970	-0.922183
H	-1.382763	1.088238	0.861172

methanethiomethyl+

S	0.137806	-0.560202	0.000000
C	-1.402576	0.379019	0.000000
H	-1.963193	0.089760	-0.891098
H	-1.203183	1.450451	-0.000019
H	-1.963177	0.089788	0.891118
C	1.313280	0.543331	0.000000
H	1.120002	1.613855	-0.000001
H	2.340437	0.185285	0.000001

methylthiomethane

S	0.000000	0.663985	0.000000
C	-1.367122	-0.513548	0.000000
H	-2.296668	0.058266	-0.000001
H	-1.346723	-1.144429	0.891644
H	-1.346723	-1.144430	-0.891643
C	1.367122	-0.513548	0.000000
H	2.296668	0.058266	-0.000003
H	1.346721	-1.144432	-0.891642
H	1.346724	-1.144427	0.891645

chlorocarbene, singlet

C	0.045033	1.190167	0.000000
Cl	0.045033	-0.504710	0.000000
H	-1.035769	1.439066	0.000000

chlorocarbene, triplet

C	0.036544	1.157038	0.000000
Cl	0.036544	-0.513669	0.000000
H	-0.840523	1.790143	0.000000

chlorocarbenium+

Cl	0.000000	0.000000	0.550610
C	0.000000	0.000000	-1.036821
H	0.000000	0.949935	-1.569720
H	0.000000	-0.949935	-1.569720

chloromethane

Cl	0.000000	0.000000	0.655761
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C	0.000000	0.000000	-1.121188
H	0.000000	1.029068	-1.473601
H	-0.891199	-0.514534	-1.473601
H	0.891199	-0.514534	-1.473601

dichlorocarbene, singlet

Cl	0.000000	1.405198	-0.147622
C	0.000000	0.000000	0.836523
Cl	0.000000	-1.405198	-0.147622

dichlorocarbene, triplet

Cl	0.000000	1.506798	-0.111246
C	0.000000	0.000000	0.630392
Cl	0.000000	-1.506798	-0.111246

dichlorocarbenium+

H	0.000000	0.000000	1.693371
C	0.000000	0.000000	0.601951
Cl	0.000000	1.432493	-0.156032
Cl	0.000000	-1.432493	-0.156032

dichloromethane

Cl	0.000000	1.473658	-0.215165
C	0.000000	0.000000	0.760303
H	-0.894257	0.000000	1.376898
H	0.894257	0.000000	1.376898
Cl	0.000000	-1.473658	-0.215165

"nitrosocarbene, singlet", (hydrogen cyanide N-oxide)

C	0.000000	0.000000	-1.198167
N	0.000000	0.000000	-0.013964
O	0.000000	0.000000	1.193461
H	0.000000	0.000000	-2.260936

nitrosocarbene, triplet (anti)

C	1.160552	0.036162	0.000000
H	1.627187	-0.949427	0.000000
N	0.000000	0.393593	0.000000
O	-1.073812	-0.252836	0.000000

nitrosomethyl+ ($\text{H}_2\text{C}=\text{N}=\text{O}$)⁺

H	-0.000025	-1.675339	0.973056
C	-0.000026	-1.176265	0.000000
N	0.000000	0.077537	0.000000
H	-0.000025	-1.675339	-0.973056
O	0.000025	1.233189	0.000000

nitrosomethane

H	-1.636134	-0.193909	-0.884678
C	-1.093627	0.150355	-0.000001
H	-0.965252	1.234918	-0.000025
N	0.214909	-0.539560	0.000000
H	-1.636109	-0.193869	0.884708
O	1.161862	0.253456	0.000000

iminocarbene, singlet

H	0.000000	0.000000	1.438998
N	0.000000	0.000000	0.436514
C	0.000000	0.000000	-0.749099

iminocarbene, triplet

C	0.067853	0.731546	0.000000
N	0.067853	-0.496928	0.000000
C	-0.882095	-0.910780	0.000000

iminocarbene, CH+

H	0.000000	0.000000	1.561926
N	0.000000	0.000000	0.541752
C	0.000000	0.000000	-0.610251
H	0.000000	0.000000	-1.692687

formaldimine

C	0.056194	0.589905	0.000000
H	-0.835006	1.225617	0.000000
H	1.014426	1.107643	0.000000
N	0.056194	-0.690739	0.000000
H	-0.909939	-1.037522	0.000000

carbon monoxide, singlet

O	0.000000	0.000000	0.492953
C	0.000000	0.000000	-0.657271

carbon monoxide, triplet

O	0.000000	0.000000	0.504219
C	0.000000	0.000000	-0.672292

formyl+ (carbon monoxide, CH+)

O	0.000000	0.000000	0.600565
C	0.000000	0.000000	-0.529977
H	0.000000	0.000000	-1.624660

formaldehyde

O	0.000000	0.000000	0.683479
C	0.000000	0.000000	-0.536364
H	0.000000	0.934472	-1.124826
H	0.000000	-0.934472	-1.124826

2,2-diaminovinyl+, singlet

N	-1.112067	-0.671847	-0.009730
C	-0.004022	0.063501	0.011955
N	1.206526	-0.484487	0.031598
H	-1.100857	-1.637951	-0.328188
H	-2.023579	-0.261967	0.169050
H	1.359770	-1.441787	0.336484
H	2.018609	0.070095	-0.225326
C	-0.044820	1.496347	-0.136912
H	-0.622103	2.006862	0.644648

2,2-diaminovinyl cation, singlet ts

N	0.000000	1.172082	-0.604429
C	0.000000	0.000000	0.087590
C	0.000000	0.000000	1.415472
N	0.000000	-1.172082	-0.604429
H	0.670693	1.265276	-1.363092
H	-0.316407	2.028815	-0.161952
H	-0.670693	-1.265276	-1.363092
H	0.316407	-2.028815	-0.161952
H	0.000000	0.000000	2.493725

2,2-diaminovinyl+, triplet

N	1.316080	-0.006931	0.000014
C	-0.007673	0.061612	-0.000013
N	-0.764640	-1.029259	-0.000006
H	1.821199	-0.887542	0.000045
H	1.869523	0.843600	-0.000012
H	-0.372132	-1.966240	0.000007
H	-1.776189	-0.959808	0.000012
C	-0.618801	1.358945	-0.000039
H	-1.643637	1.699981	0.000207

diaminomethyl-CH2 dication

N	1.181893	0.633591	0.000004
C	0.000000	0.030597	-0.000001
N	-1.181891	0.633594	-0.000004
H	1.277451	1.657861	0.000015
H	2.068520	0.119013	-0.000023
H	-1.277446	1.657864	-0.000008
H	-2.068520	0.119018	0.000020
C	-0.000002	-1.433211	0.000000
H	0.934982	-2.004188	-0.000003
H	-0.934987	-2.004185	0.000006

1,1-diaminoethyl cation

N	0.705706	-1.149481	0.000003
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C	0.057201	0.000000	-0.015659
N	0.705666	1.149502	0.000005
H	1.719023	-1.213445	0.023439
H	0.195808	-2.025462	-0.012296
H	1.718980	1.213504	0.023445
H	0.195738	2.025465	-0.012306
C	-1.435616	-0.000022	0.003578
H	-1.829573	0.885642	-0.496125
H	-1.779545	0.000063	1.042247
H	-1.829545	-0.885782	-0.495974

cyclic heteroatom carbene sets

NOTE: where cis/trans isomerism exists, only the more stable of the two isomers is listed here.

imidazol-2-ylidene, singlet

H	0.000000	1.388832	-1.751294
C	0.000000	0.681319	-0.935968
C	0.000000	-0.681319	-0.935968
N	0.000000	1.045771	0.398585
H	0.000000	-1.388832	-1.751294
N	0.000000	-1.045771	0.398585
H	0.000000	2.003972	0.720890
H	0.000000	-2.003972	0.720890
C	0.000000	0.000000	1.285373

imidazol-2-ylidene, triplet

H	1.350537	1.749745	-0.061926
C	0.674185	0.907543	-0.000895
C	-0.673803	0.907764	-0.000956
H	-1.349839	1.750225	-0.061932
C	-0.000200	-1.196125	-0.132075
N	1.178448	-0.422322	-0.035947
N	-1.178662	-0.421975	-0.035941
H	1.834407	-0.652806	0.715267
H	-1.834699	-0.652175	0.715356

imidazol-2-ylidene-2-CH⁺ (imidazolium⁺)

H	0.000000	1.393514	-1.788673
C	0.000000	0.684743	-0.974394
C	0.000000	-0.684743	-0.974394
N	0.000000	1.072375	0.344390
H	0.000000	-1.393514	-1.788673
N	0.000000	-1.072375	0.344390
H	0.000000	2.035160	0.676011

H	0.000000	-2.035160	0.676011
C	0.000000	0.000000	1.145212
H	0.000000	0.000000	2.225317

2,2-dihydroimidazole, trans

H	1.420422	1.783037	0.074281
C	0.793727	0.902001	0.018585
C	1.153271	-0.388521	0.093841
H	2.142558	-0.814456	0.188723
C	-1.105911	-0.300383	0.180529
H	-1.325486	-0.294936	1.259659
H	-1.999843	-0.595302	-0.372990
N	-0.004643	-1.240514	-0.047944
H	-0.050474	-1.577463	-1.013929
N	-0.594534	1.016555	-0.256275
H	-1.039454	1.788256	0.236058

4,5-dihydroimidazol-2-ylidene, singlet

H	1.295023	1.579874	-0.566742
C	0.754707	0.922945	0.118831
N	1.056400	-0.495409	-0.122095
C	-0.754708	0.922944	-0.118830
H	0.997271	1.207810	1.150693
N	-1.056399	-0.495410	0.122095
H	-0.997273	1.207809	-1.150692
H	-1.295025	1.579872	0.566742
C	0.000001	-1.334849	0.000000
H	1.995972	-0.852935	-0.024466
H	-1.995971	-0.852938	0.024467

4,5-dihydroimidazol-2-ylidene, triplet

H	-1.388611	1.576188	0.295161
C	-0.767753	0.838703	-0.218503
C	0.718056	0.905346	0.172461
H	-0.880139	0.965216	-1.297879
N	1.186040	-0.460058	-0.155024
H	0.817966	1.124759	1.244774
H	1.275073	1.657977	-0.392256
C	-0.001287	-1.237285	-0.164925
H	1.899092	-0.797121	0.490756
N	-1.185816	-0.537755	0.126559
H	-1.419053	-0.582911	1.124495

4,5-dihydroimidazol-2-CH⁺

H	1.110818	1.037248	-1.332652
C	0.114305	0.764279	-0.977915
N	0.000000	1.092050	0.457619

C	-0.114305	-0.764279	-0.977915
H	-0.639601	1.302442	-1.552476
N	0.000000	-1.092050	0.457619
H	0.639601	-1.302442	-1.552476
H	-1.110818	-1.037248	-1.332652
H	0.071613	2.029066	0.841298
H	-0.071613	-2.029066	0.841298
C	0.000000	0.000000	1.190223
H	0.000000	0.000000	2.274632

2,2,4,5-tetrahydroimidazole cis

H	0.940322	1.493238	1.214162
C	0.081495	0.973160	0.781763
N	0.081495	-0.443505	1.189096
C	0.081495	0.973160	-0.781763
H	-0.824522	1.453598	1.162483
N	0.081495	-0.443505	-1.189096
H	0.940322	1.493238	-1.214162
H	-0.824522	1.453598	-1.162483
H	1.052386	-0.741083	-1.296621
C	-0.450674	-1.116554	0.000000
H	-0.211602	-2.182554	0.000000
H	-1.539598	-0.998478	0.000000
H	1.052386	-0.741083	1.296621

1,3-dioxol-2-ylidene, singlet

H	0.000000	1.430911	-1.665035
C	0.000000	0.668454	-0.904683
C	0.000000	-0.668454	-0.904683
O	0.000000	1.070612	0.420190
H	0.000000	-1.430911	-1.665035
C	0.000000	0.000000	1.243871
O	0.000000	-1.070612	0.420190

1,3-dioxol-2-ylidene, triplet

O	1.082269	-0.429043	0.002998
C	0.007142	-1.230064	0.044440
O	-1.077129	-0.441144	0.006017
C	-0.765327	0.930091	-0.119408
C	0.754856	0.939217	-0.116348
H	-1.368035	1.557031	0.532734
H	1.346884	1.568999	0.543046

1,3-dioxole-2-CH+

H	0.000000	1.449351	-1.701384
C	0.000000	0.673562	-0.950820
C	0.000000	-0.673562	-0.950820
O	0.000000	1.077635	0.378419

H	0.000000	-1.449351	-1.701384
O	0.000000	-1.077635	0.378419
C	0.000000	0.000000	1.096359
H	0.000000	0.000000	2.179746

1,3-dioxole-2-CH₂

H	-1.767510	1.394782	0.099947
C	-0.973276	0.667673	0.043622
C	-0.973279	-0.667670	0.043610
O	0.319185	1.149243	-0.139875
H	-1.767511	-1.394779	0.099981
O	0.319181	-1.149245	-0.139873
C	1.119650	-0.000002	0.136406
H	1.391490	0.000007	1.204109
H	1.998035	-0.000008	-0.507878

4,5-dihydro-1,3-dioxole-2-ylidene, singlet

H	-0.893673	1.206100	-1.340295
C	0.000000	0.757126	-0.906942
H	0.893022	1.206166	-1.341539
C	0.000000	-0.757126	-0.906942
O	-0.000980	-1.080943	0.528840
H	0.893673	-1.206100	-1.340295
C	0.000000	0.000000	1.297589
O	0.000980	1.080943	0.528840
H	-0.893022	-1.206166	-1.341539

4,5-dihydro-1,3-dioxol-2-ylidene, triplet

H	-0.842856	0.980189	-1.286563
C	-0.732949	0.843819	-0.205459
H	-1.360556	1.551234	0.336736
C	0.733016	0.843410	0.206585
O	1.149253	-0.488895	-0.168533
H	0.843161	0.976666	1.288060
C	0.000657	-1.226093	0.002453
O	-1.149836	-0.489485	0.165308
H	1.360572	1.552129	-0.333909

4,5-dihydro-1,3-dioxole-2-CH⁺

H	1.369399	-1.224582	0.899166
C	0.960203	-0.767453	0.000058
H	1.369697	-1.224581	-0.898914
C	0.960202	0.767453	0.000065
O	-0.493698	1.097354	0.000098
H	1.369524	1.224593	-0.898980
O	-0.493698	-1.097354	-0.000170
H	1.369571	1.224571	0.899100
C	-1.144971	0.000000	-0.000069

H -2.231624 0.000000 -0.000124

2,2,4,5-tetrahydro-1,3-dioxole

H -0.106698 1.391528 -1.659209
C 0.319000 0.686838 -0.942815
H 1.405324 0.617430 -1.086649
C -0.319000 -0.686838 -0.942815
O 0.000000 1.150418 0.370166
H 0.106698 -1.391528 -1.659209
H -1.405324 -0.617430 -1.086649
O 0.000000 -1.150418 0.370166
C 0.000000 0.000000 1.203980
H -0.899646 0.044858 1.829485
H 0.899646 -0.044858 1.829485

oxazole-2-ylidene, singlet

H -1.957559 1.026743 -0.000005
C -0.970264 0.593597 0.000007
C 0.276198 1.110141 0.000008
O -0.872662 -0.776034 0.000006
H 0.634033 2.127483 -0.000010
N 1.103264 -0.007713 0.000004
C 0.438590 -1.189622 -0.000028
H 2.114827 0.023343 0.000019

oxazole-2-ylidene, triplet

H 1.247547 1.473720 0.791324
C 0.761948 0.946373 -0.033055
C -0.752526 0.942550 -0.179258
O 1.124929 -0.418235 -0.075139
H -1.399016 1.697094 0.256199
C 0.041835 -1.244384 0.053404
N -1.027721 -0.413212 0.056654
H -1.961458 -0.799680 0.110465

oxazole-2-CH+

H 2.150798 -0.646950 0.000050
C 1.148823 -0.246234 0.000012
C 0.618023 1.003643 0.000008
O 0.118802 -1.154157 -0.000037
H 1.077585 1.980810 0.000004
N -0.753508 0.813238 0.000007
H -1.460913 1.549589 0.000021
C -1.012829 -0.482787 0.000001
H -1.967430 -0.990595 0.000045

oxazole-2-CH2

H -2.000543 -1.043605 0.056673

C	-1.082295	-0.475090	0.009408
C	-0.853920	0.842998	0.088090
H	-1.560633	1.651563	0.205594
N	0.562384	1.091750	-0.057661
H	0.754459	1.383350	-1.019912
O	0.075403	-1.204260	-0.174563
C	1.099859	-0.235289	0.184477
H	2.000225	-0.443206	-0.393339
H	1.284720	-0.351984	1.259268

4,5-dihydrooxazol-2-ylidene, singlet

H	0.611696	1.586488	-1.042163
C	0.416068	1.124669	-0.068952
N	1.137564	-0.146402	0.064207
C	-1.010933	0.607210	0.068938
H	0.691806	1.827969	0.720213
H	-1.689086	0.955198	-0.710136
H	-1.441392	0.812735	1.051695
O	-0.886412	-0.849087	-0.061746
C	0.396307	-1.258773	-0.004108
H	2.146673	-0.203514	0.049647

4,5-dihydrooxazol-2-ylidene, triplet

H	-1.193722	1.709357	0.298128
C	-0.656635	0.915734	-0.225742
N	-1.212152	-0.413244	0.109652
C	0.819758	0.795956	0.176191
H	-0.752204	1.064959	-1.303502
H	0.970260	1.017390	1.239165
H	1.501528	1.400868	-0.424537
O	1.132075	-0.601504	-0.053720
C	-0.099920	-1.219166	-0.158189
H	-1.476622	-0.442987	1.099381

4,5-dihydrooxazole-2-CH⁺

H	1.209213	1.426660	0.893415
C	0.828678	0.929252	0.000072
N	-0.646797	0.963190	0.000065
C	1.080016	-0.592685	0.000015
H	1.209217	1.426731	-0.893230
H	1.573916	-0.963685	0.896207
H	1.574051	-0.963598	-0.896138
O	-0.277112	-1.198138	-0.000113
H	-1.210233	1.811594	0.000118
C	-1.143793	-0.238484	-0.000055
H	-2.201095	-0.483423	-0.000109

2,2,4,5-tetrahydrooxazole

C	-1.095823	-0.577179	-0.045108
H	-1.636823	-0.764760	-0.978157
H	-1.670373	-1.003492	0.785251
O	0.186482	-1.212249	-0.141137
C	1.154047	-0.214923	0.218910
H	2.095099	-0.458493	-0.276943
H	1.297278	-0.203893	1.307830
C	-0.785404	0.921891	0.171010
H	-1.413818	1.590021	-0.421565
H	-0.897522	1.192126	1.225056
N	0.629664	1.066110	-0.195295
H	0.689735	1.104975	-1.214183

1,3-diphosphole-2-ylidene, singlet, trans

C	-0.683384	1.318575	-0.059436
P	-1.288554	-0.346746	0.099323
H	-2.453930	-0.595241	-0.639949
C	-0.000151	-1.441932	-0.000510
P	1.288537	-0.346846	-0.099041
C	0.683569	1.318548	0.059198
H	-1.299409	2.211953	-0.079244
H	1.299692	2.211857	0.079011
H	2.453693	-0.595838	0.640447

1,3-diphosphole-2-ylidene, triplet, trans

C	-0.674133	1.243303	-0.008597
P	-1.557116	-0.362206	0.108259
H	-2.013790	-0.475453	-1.236499
C	0.674138	1.243305	0.008589
H	-1.243524	2.170884	-0.002870
H	1.243525	2.170888	0.002822
C	-0.000004	-1.240713	-0.000048
P	1.557124	-0.362207	-0.108237
H	2.013662	-0.475489	1.236560

1,3-diphosphole-2-CH+, trans

H	1.289874	2.210957	-0.083841
C	0.683662	1.310601	-0.061385
C	-0.683498	1.310632	0.061387
H	-1.289610	2.211058	0.083799
C	-0.000021	-1.300595	-0.000007
H	-0.000009	-2.385922	-0.000065
P	1.380191	-0.292028	0.102592
H	2.478481	-0.600214	-0.711677
P	-1.380279	-0.291951	-0.102612
H	-2.478281	-0.600020	0.712109

1,3-diphosphole-2-CH2, trans

H	1.258905	2.233226	0.168859
C	0.673954	1.317781	0.095978
C	-0.671483	1.329565	0.098195
P	1.492876	-0.276294	-0.228245
H	-1.238736	2.251930	0.199912
P	-1.544318	-0.275773	-0.029184
H	2.270153	-0.363598	0.957108
C	0.003238	-1.269275	0.288404
H	0.039186	-1.508903	1.354134
H	-0.051077	-2.209908	-0.265264
H	-1.541067	-0.390176	-1.448771

4,5-dihydro-1,3-diphospholane-2-ylidene, trans, singlet

H	0.678536	1.406083	-1.377938
C	0.710196	1.293683	-0.288034
P	1.340278	-0.408444	0.180487
C	-0.710152	1.293688	0.288042
H	1.326560	2.087590	0.138509
P	-1.340305	-0.408419	-0.180504
H	-1.326496	2.087618	-0.138486
H	-0.678484	1.406070	1.377946
C	-0.000007	-1.454352	0.000010
H	2.388987	-0.766298	-0.690689
H	-2.388909	-0.766231	0.690820

4,5-dihydro-1,3-diphospholane, triplet, cis

H	0.636207	1.282396	-1.414834
C	0.710842	1.187434	-0.326115
P	1.574151	-0.438288	0.022874
C	-0.684289	1.213221	0.312936
H	1.325844	2.020493	0.030434
P	-1.558718	-0.385611	-0.159602
H	-1.258859	2.075716	-0.038702
H	-0.592236	1.284029	1.400587
C	-0.006424	-1.284862	-0.065214
H	-2.116834	-0.724263	1.104492
H	1.653612	-0.274638	1.439307

4,5-dihydro-1,3-diphospholane-2-C+, trans

H	0.658078	1.359962	-1.400984
C	0.703664	1.284022	-0.308269
P	1.420606	-0.350583	0.178866
C	-0.703539	1.283911	0.308217
H	1.307513	2.103920	0.084051
P	-1.420860	-0.350583	-0.178876
H	-1.307385	2.103882	-0.083972
H	-0.657828	1.359824	1.400932
H	2.420502	-0.806994	-0.701114

H	-2.419349	-0.806875	0.702826
C	0.000207	-1.302128	-0.000172
H	0.000282	-2.391067	-0.000253

4,5-dihydro-1,3-diphospholane-2-CH₂, cis

H	0.833882	1.313195	-1.422404
C	0.766782	1.257268	-0.329757
P	1.526462	-0.363167	0.157532
C	-0.696725	1.349342	0.122038
H	1.357147	2.091703	0.063396
P	-1.547237	-0.323107	-0.009535
H	-1.240371	2.079704	-0.484284
H	-0.745003	1.690622	1.159670
H	-1.606057	-0.600090	1.380873
C	0.004812	-1.307585	-0.333233
H	0.077259	-1.531435	-1.401900
H	-0.047165	-2.270764	0.183668
H	1.232719	-0.272972	1.546736

1,3-dithiol-2-ylidene, singlet

C	0.000000	1.238794	0.679556
S	0.000000	-0.351613	1.373340
C	0.000003	-1.310027	0.000000
S	0.000000	-0.351613	-1.373340
C	0.000000	1.238794	-0.679556
H	-0.000001	2.123122	1.306521
H	-0.000001	2.123122	-1.306521

1,3-dithiol-2-ylidene, triplet

C	-0.674427	1.196036	0.042718
S	-1.487665	-0.357309	-0.068012
C	0.000000	-1.183672	0.247853
S	1.487665	-0.357309	-0.068012
C	0.674427	1.196036	0.042718
H	-1.283103	2.091742	0.088326
H	1.283103	2.091742	0.088326

1,3-dithiole-2-CH⁺

C	-0.685036	1.230244	0.000000
S	-1.427759	-0.302023	-0.000001
S	1.427759	-0.302023	-0.000001
C	0.685036	1.230244	0.000000
H	-1.307974	2.119163	0.000006
H	1.307974	2.119163	0.000006
C	0.000000	-1.178573	0.000005
H	0.000000	-2.265076	-0.000002

1,3-dithiole-2-CH₂

C	0.670913	1.270451	0.100786
S	1.484133	-0.268918	-0.140196
S	-1.484133	-0.268919	-0.140196
C	-0.670914	1.270450	0.100787
H	1.279725	2.162275	0.195489
H	-1.279726	2.162275	0.195486
C	0.000000	-1.226760	0.297860
H	0.000000	-1.445410	1.368048
H	0.000001	-2.158584	-0.269357

4,5-dihydro-1,3-dithiol-2-ylidene, singlet

S	0.000000	1.399752	0.445732
S	0.000000	-1.399752	0.445732
C	0.000000	0.000000	1.335324
C	-0.224761	0.722066	-1.275218
C	0.224761	-0.722066	-1.275218
H	0.358796	1.329273	-1.969651
H	-1.286905	0.814909	-1.516722
H	-0.358796	-1.329273	-1.969651
H	1.286905	-0.814909	-1.516722

4,5-dihydro-1,3-dithiol-2-ylidene, triplet

S	-1.509720	-0.404704	0.038875
S	1.487599	-0.417349	-0.139022
C	0.004828	-1.241324	0.167364
C	-0.671198	1.191509	-0.291553
C	0.708686	1.158081	0.358212
H	-1.286921	1.992590	0.125047
H	-0.578929	1.327431	-1.371359
H	1.332809	1.979902	-0.002314
H	0.633065	1.203332	1.446828

4,5-dihydro-1,3-dithiole, 2-CH⁺

S	-1.454399	0.386712	-0.078678
S	1.454399	0.386712	0.078678
C	0.000000	1.194410	0.000000
H	0.000000	2.284464	0.000000
C	-0.712216	-1.249929	0.261870
C	0.712216	-1.249929	-0.261870
H	-1.314630	-2.013552	-0.235558
H	-0.759544	-1.399724	1.344887
H	1.314629	-2.013552	0.235558
H	0.759544	-1.399724	-1.344887

1,3-dithiolane, (4,5-dihydro-1,3-dithiole, 2-CH₂)

S	1.499419	0.305014	0.091478
S	-1.499419	0.305014	-0.091479
C	0.000000	1.340778	0.000000

H	0.019258	1.973687	-0.888495
H	-0.019258	1.973687	0.888496
C	0.674824	-1.246179	-0.346406
C	-0.674824	-1.246179	0.346406
H	1.306661	-2.064320	0.011929
H	0.553408	-1.334855	-1.428484
H	-1.306661	-2.064320	-0.011929
H	-0.553407	-1.334854	1.428484

N,N'-dimethylimidazol-2-ylidene, singlet

H	-1.389418	2.030594	-0.000003
C	-0.682355	1.213012	0.000007
C	0.682355	1.213012	0.000001
N	-1.057934	-0.115809	-0.000002
H	1.389418	2.030594	-0.000016
N	1.057934	-0.115808	-0.000015
C	-2.435371	-0.571998	0.000010
C	2.435371	-0.571998	0.000015
C	0.000000	-0.990528	-0.000026
H	-2.406934	-1.660190	-0.000260
H	-2.959119	-0.216894	-0.891189
H	-2.958956	-0.217351	0.891487
H	2.958918	-0.217439	0.891549
H	2.959157	-0.216805	-0.891127
H	2.406934	-1.660190	-0.000359

N,N'-dimethylimidazol-2-ylidene, triplet, cis

H	1.355384	2.012971	0.313101
C	0.675512	1.202140	0.082424
C	-0.675442	1.202142	0.082481
H	-1.355270	2.013015	0.313135
C	-0.000004	-0.722402	-0.751046
N	-1.177436	-0.029230	-0.400639
C	-2.194680	-0.704991	0.407679
H	-2.543857	-1.586817	-0.131901
H	-3.039197	-0.025883	0.545687
H	-1.809785	-1.011112	1.389842
N	1.177429	-0.029257	-0.400647
C	2.194632	-0.705028	0.407697
H	1.809789	-1.010840	1.389976
H	3.039295	-0.026046	0.545452
H	2.543583	-1.587050	-0.131708

N,N'-dimethylimidazole-2-CH⁺

H	1.391350	-2.049774	0.000009
C	0.685079	-1.232164	0.000016
C	-0.685079	-1.232164	-0.000015
N	1.086971	0.081626	0.000017

H	-1.391350	-2.049774	0.000005
N	-1.086971	0.081626	-0.000038
C	2.478923	0.549246	-0.000001
C	-2.478923	0.549246	0.000022
H	2.479756	1.638202	0.000344
H	2.978641	0.180898	-0.895564
H	2.978833	0.180342	0.895224
H	-2.978621	0.180874	0.895586
H	-2.978853	0.180365	-0.895201
H	-2.479756	1.638202	-0.000295
C	0.000000	0.867462	-0.000014
H	0.000000	1.948149	0.000001

N,N'-dimethylimidazole-2-CH₂, cis

H	-1.353031	2.069093	0.155739
C	-0.671849	1.235703	0.040505
C	0.671848	1.235703	0.040504
H	1.353032	2.069092	0.155742
C	-2.362050	-0.513802	0.259719
C	2.362050	-0.513802	0.259719
H	-2.680773	-1.441573	-0.222927
H	-3.155618	0.225752	0.131907
H	-2.222663	-0.706720	1.336511
H	2.222664	-0.706720	1.336511
H	3.155618	0.225753	0.131906
H	2.680773	-1.441572	-0.222928
N	-1.151063	-0.030785	-0.380168
N	1.151063	-0.030785	-0.380167
C	0.000000	-0.910550	-0.178539
H	0.000000	-1.309910	0.868008
H	0.000000	-1.751716	-0.879579

4,5-dimethylimidazol-2-ylidene, singlet

C	1.679858	-1.371958	-0.000049
C	0.684422	-0.264968	0.000055
C	-0.684421	-0.264971	-0.000123
N	1.042775	1.076681	0.000055
C	-1.679852	-1.371966	0.000076
N	-1.042780	1.076676	-0.000056
C	-0.000004	1.965403	0.000021
H	2.002912	1.396455	0.000158
H	-2.002918	1.396446	-0.000138
H	1.172329	-2.339309	-0.000140
H	2.323749	-1.334334	0.885072
H	2.323783	-1.334165	-0.885136
H	-2.324125	-1.334032	-0.884753
H	-2.323396	-1.334486	0.885455
H	-1.172318	-2.339314	-0.000395

4,5-dimethylimidazol-2-ylidene, triplet, cis

C	-1.650678	1.366693	0.017607
C	-0.677441	0.241937	-0.030399
C	0.677446	0.241928	-0.030405
C	1.650697	1.366670	0.017606
C	-0.000013	-1.866872	0.159708
N	1.176136	-1.097848	0.035621
N	-1.176154	-1.097834	0.035619
H	1.813295	-1.340552	-0.730368
H	-1.813307	-1.340523	-0.730381
H	2.383081	1.280580	-0.793469
H	2.204715	1.365209	0.961137
H	1.144930	2.328530	-0.088982
H	-1.144899	2.328546	-0.088980
H	-2.204701	1.365240	0.961134
H	-2.383059	1.280611	-0.793472

4,5-dimethylimidazole-2-CH+, G3

C	-1.413665	-1.684814	-0.000028
C	-0.306327	-0.690295	0.000028
C	-0.306327	0.690295	-0.000037
N	1.022088	-1.068746	0.000023
C	-1.413665	1.684814	0.000032
N	1.022088	1.068745	-0.000024
H	1.353108	-2.031533	0.000070
H	1.353108	2.031533	-0.000095
H	-2.375169	-1.170387	0.000433
H	-1.372179	-2.321007	0.888266
H	-1.372669	-2.320390	-0.888787
H	-1.372148	2.321053	-0.888227
H	-1.372699	2.320344	0.888826
H	-2.375169	1.170388	-0.000490
C	1.826377	0.000000	0.000004
H	2.906229	0.000000	0.000015

4,5-dimethylimidazole-2-CH2, cis

C	1.463216	-1.645842	0.039876
C	0.337353	-0.674813	-0.024414
C	0.337352	0.674814	-0.024413
C	1.463214	1.645844	0.039877
H	2.430443	-1.138589	0.044379
H	1.438820	-2.319552	-0.825015
H	1.387177	-2.269281	0.935753
H	1.387172	2.269285	0.935751
H	1.438818	2.319552	-0.825016
H	2.430441	1.138592	0.044382
C	-1.811051	-0.000001	0.237382

H	-2.767203	-0.000002	-0.291694
H	-1.996601	-0.000001	1.316126
N	-1.005686	1.194263	-0.067061
N	-1.005684	-1.194265	-0.067060
H	-1.204989	1.562296	-1.002837
H	-1.204987	-1.562298	-1.002835

4,5-difluoroimidazol-2-ylidene, singlet

F	0.000000	1.556111	-1.331894
C	0.000000	0.678485	-0.324793
C	0.000000	-0.678485	-0.324793
F	0.000000	-1.556111	-1.331894
N	0.000000	1.053010	0.997627
N	0.000000	-1.053010	0.997627
C	0.000000	0.000000	1.882765
H	0.000000	2.017662	1.304117
H	0.000000	-2.017662	1.304117

4,5-difluoroimidazol-2-ylidene, triplet

C	0.000002	1.774357	0.000000
N	-0.963208	0.915908	0.467418
H	-1.821275	1.261547	0.875188
N	0.963209	0.915907	-0.467418
H	1.821279	1.261544	-0.875184
C	0.691286	-0.442238	-0.279537
C	-0.691287	-0.442237	0.279537
F	1.628202	-1.149173	0.402963
F	-1.628204	-1.149170	-0.402962

4,5-difluoroimidazol-2-CH⁺

F	0.000000	1.550875	-1.357285
C	0.000000	0.685114	-0.374505
C	0.000000	-0.685114	-0.374505
F	0.000000	-1.550875	-1.357285
N	0.000000	1.075778	0.939572
N	0.000000	-1.075778	0.939572
H	0.000000	2.047644	1.252244
H	0.000000	-2.047644	1.252244
C	0.000000	0.000000	1.740978
H	0.000000	0.000000	2.820832

4,5-difluoroimidazole-2-CH₂, cis

F	-1.426490	-1.497122	0.050627
C	-0.377677	-0.669933	-0.032878
C	-0.377673	0.669935	-0.032873
F	-1.426481	1.497129	0.050627
C	1.718950	-0.000004	0.263459
H	2.692559	-0.000008	-0.227856

H	1.846718	-0.000004	1.348229
N	0.932800	1.205099	-0.083747
N	0.932793	-1.205105	-0.083745
H	1.148352	-1.554708	-1.022737
H	1.148361	1.554714	-1.022733

1,3,4,5-tetramethylimidazol-2-ylidene, singlet

C	-1.668857	1.754568	-0.000084
C	-0.685941	0.636139	-0.000054
C	0.685941	0.636140	0.000020
N	-1.055487	-0.701370	-0.000107
C	1.668856	1.754569	0.000100
N	1.055487	-0.701370	0.000052
C	0.000000	-1.577088	-0.000015
C	-2.429057	-1.164788	0.000119
C	2.429058	-1.164788	-0.000067
H	-2.960670	-0.815786	-0.889749
H	-2.959838	-0.817543	0.891185
H	-2.389470	-2.252912	-0.000994
H	2.960488	-0.816154	0.890057
H	2.960020	-0.817174	-0.890878
H	2.389470	-2.252913	0.000579
H	2.315520	1.728725	-0.883745
H	2.315316	1.728788	0.884095
H	1.146132	2.714060	0.000007
H	-1.146133	2.714059	0.000055
H	-2.315529	1.728686	0.883754
H	-2.315309	1.728824	-0.884086

1,3,4,5-tetramethylimidazol-2-ylidene, triplet, trans

C	1.638629	1.760922	0.083189
C	0.679232	0.635542	-0.100047
C	-0.679252	0.635532	-0.100071
N	1.176849	-0.657536	-0.436831
C	-1.638674	1.760891	0.083150
N	-1.176852	-0.657568	-0.436846
C	0.000013	-1.377175	-0.715974
C	2.155962	-1.259812	0.473570
C	-2.155912	-1.259851	0.473617
H	1.760720	-1.377906	1.492732
H	3.053821	-0.639213	0.501412
H	2.431116	-2.240631	0.082402
H	-2.431050	-2.240690	0.082489
H	-3.053789	-0.639278	0.501475
H	-1.760624	-1.377900	1.492766
H	-2.254254	1.630010	0.979593
H	-2.312815	1.833541	-0.776158

H	-1.106570	2.708921	0.185429
H	1.106500	2.708934	0.185503
H	2.312756	1.833614	-0.776127
H	2.254224	1.630031	0.979621

1,3,4,5-tetramethylimidazole-2-CH⁺

C	1.673154	-1.779256	-0.000011
C	0.690756	-0.661678	-0.000008
C	-0.690756	-0.661678	0.000002
N	1.083671	0.663031	-0.000006
C	-1.673154	-1.779256	0.000014
N	-1.083671	0.663031	0.000004
C	2.468523	1.139157	0.000012
C	-2.468524	1.139157	-0.000010
H	2.977100	0.777345	-0.893791
H	2.977032	0.777473	0.893907
H	2.460257	2.228341	-0.000072
H	-2.977087	0.777376	0.893814
H	-2.977046	0.777442	-0.893885
H	-2.460257	2.228341	0.000034
H	-2.312384	-1.749868	-0.887127
H	-2.312379	-1.749852	0.887157
H	-1.146962	-2.734534	0.000021
H	1.146962	-2.734533	-0.000052
H	2.312359	-1.749884	0.887149
H	2.312405	-1.749835	-0.887135
C	0.000000	1.451499	0.000000
H	0.000000	2.532081	0.000005

1,3,4,5-tetramethylimidazol-2-CH₂, cis

C	1.879697	1.580861	-0.435028
C	0.806404	0.565846	-0.256566
C	-0.486702	0.706740	0.111339
N	1.132168	-0.836760	-0.396306
C	-1.256984	1.939672	0.432987
N	-1.092275	-0.574120	0.266870
C	1.846578	-1.316994	0.797106
C	-2.479709	-0.704634	-0.141555
H	1.290387	-1.135438	1.728242
H	2.813201	-0.812486	0.858777
H	2.035268	-2.388487	0.691196
H	-2.629056	-0.492534	-1.214589
H	-3.111415	-0.033637	0.443417
H	-2.807605	-1.729014	0.054856
H	-1.674012	1.869976	1.443481
H	-2.091634	2.099276	-0.258157
H	-0.612287	2.819492	0.391634
H	1.474213	2.594830	-0.401318

H	2.374300	1.437840	-1.400722
H	2.651301	1.505869	0.340444
C	-0.192287	-1.434655	-0.514343
H	-0.202785	-2.468389	-0.155208
H	-0.491118	-1.412163	-1.579640

1,3,4,5-tetrasilylimidazol-2-ylidene singlet

Si	1.927033	1.983223	0.000081
C	0.692367	0.576637	-0.000018
C	-0.692366	0.576637	0.000000
N	1.071641	-0.778322	-0.000054
Si	-1.927036	1.983220	-0.000072
N	-1.071639	-0.778324	-0.000018
C	0.000002	-1.632465	-0.000047
Si	2.651469	-1.610424	-0.000034
Si	-2.651468	-1.610425	0.000072
H	2.782279	-2.433457	1.219227
H	2.781791	-2.434313	-1.218759
H	3.684488	-0.547028	-0.000600
H	2.790470	1.905864	-1.205324
H	1.198245	3.270390	0.000567
H	2.790899	1.905230	1.205138
H	-1.198253	3.270390	-0.000464
H	-2.790859	1.905285	-1.205164
H	-2.790515	1.905796	1.205299
H	-2.782215	-2.433692	-1.219034
H	-2.781850	-2.434082	1.218951
H	-3.684487	-0.547029	0.000397

1,3,4,5-tetrasilylimidazol-2-ylidene, triplet, trans

Si	-1.948650	1.781125	-0.888533
C	-0.770194	0.601543	-0.075814
C	0.738543	0.667477	-0.084685
N	-1.019226	-0.755611	0.252220
Si	1.741062	1.864957	0.936532
N	1.103300	-0.695600	-0.303029
C	0.078888	-1.559789	0.017863
Si	-2.548447	-1.592919	0.609360
Si	2.710208	-1.402659	-0.596510
H	-2.311135	-2.601285	1.660583
H	-3.482384	-0.547061	1.089814
H	-3.100904	-2.231958	-0.607494
H	-3.123442	1.031186	-1.403558
H	-2.438247	2.821616	0.054725
H	-1.229995	2.465279	-1.995136
H	1.496898	3.243805	0.446063
H	1.357036	1.811631	2.376408
H	3.179302	1.529307	0.792981

H	2.530481	-2.666312	-1.334849
H	3.468913	-0.417439	-1.401539
H	3.423118	-1.642735	0.681583

1,3,4,5-tetrasilylimidazole-2-CH+

Si	1.874100	1.998527	0.006952
C	0.694458	0.511114	0.000979
C	-0.694460	0.511113	-0.000980
N	1.100064	-0.825543	0.003260
Si	-1.874100	1.998525	-0.006951
N	-1.100063	-0.825545	-0.003263
Si	2.809563	-1.511209	-0.005087
Si	-2.809563	-1.511208	0.005089
H	2.568617	-2.947742	0.213589
H	3.387456	-1.208058	-1.323884
H	3.507168	-0.849346	1.108641
H	3.127827	1.542515	-0.630449
H	1.220587	3.059555	-0.784088
H	2.113374	2.422115	1.403124
H	-1.220533	3.059588	0.783998
H	-2.113456	2.422048	-1.403130
H	-3.127791	1.542550	0.630545
H	-3.507174	-0.849329	-1.108627
H	-2.568624	-2.947739	-0.213605
H	-3.387447	-1.208068	1.323892
C	0.000000	-1.596631	-0.000001
H	0.000001	-2.678947	-0.000002

1,3,4,5-tetrasilylimidazol-2-CH₂, cis

Si	-2.147461	1.800921	0.087514
C	-0.798889	0.513269	0.206740
C	0.564505	0.635404	0.117187
Si	1.622864	2.136599	-0.236433
Si	2.660074	-1.280048	-0.234224
H	-3.033998	1.700500	1.274267
H	-1.543862	3.152019	0.030047
H	-2.978090	1.594589	-1.127747
H	0.807168	3.220040	-0.827184
H	2.296962	2.627326	0.993772
H	2.674022	1.731987	-1.205142
H	3.838150	-0.524797	0.261312
H	2.704241	-2.670707	0.278509
H	2.726734	-1.293812	-1.720638
C	0.115277	-1.395540	1.064033
H	0.148807	-1.190034	2.147299
H	0.215397	-2.470769	0.895906
N	1.168328	-0.619760	0.395457
N	-1.129706	-0.851501	0.524242

Si	-2.140909	-1.792304	-0.561263
H	-1.639220	-1.882962	-1.963386
H	-2.212587	-3.158286	0.011879
H	-3.483382	-1.167411	-0.592864

1,2-diaziridin-3-ylidene, singlet, trans

C	0.000000	0.000000	0.875609
N	0.000000	0.754099	-0.289204
H	0.912290	1.091597	-0.602401
N	0.000000	-0.754099	-0.289204
H	-0.912290	-1.091597	-0.602401

1,2-diazet-3-ylidene, triplet, trans

C	0.000000	0.000000	0.848529
N	0.000000	0.814545	-0.282537
H	0.966948	1.024187	-0.567827
N	0.000000	-0.814545	-0.282537
H	-0.966948	-1.024187	-0.567827

1,2-diazet-3-ylidene, CH+, trans

C	0.000000	0.000000	0.700628
H	0.000000	0.000000	1.789298
N	0.000000	0.822381	-0.318777
H	-0.841513	1.214790	-0.765093
N	0.000000	-0.822381	-0.318777
H	0.841513	-1.214790	-0.765093

1,2-diazet-3-ylidene, CH2, trans

N	0.000000	0.752677	-0.441328
H	-0.967593	0.986644	-0.677472
N	0.000000	-0.752677	-0.441328
H	0.967593	-0.986644	-0.677472
C	0.000000	0.000000	0.795832
H	-0.912791	-0.083946	1.379272
H	0.912791	0.083946	1.379272

1,3-diazet-2-ylidene, singlet, trans

H	0.060939	1.578732	0.898470
C	0.000028	0.955589	0.000005
H	-0.060851	1.578790	-0.898421
C	-0.000037	-1.118840	0.000010
N	0.969266	-0.131077	-0.082256
H	1.919800	-0.171700	0.262208
N	-0.969260	-0.131026	0.082210
H	-1.919875	-0.171596	-0.262030

1,3-diazet-2-ylidene, triplet, trans

H	-0.899719	0.023231	-1.514553
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C	0.000000	0.000000	-0.893989
H	0.899719	-0.023231	-1.514553
N	0.000000	-1.087934	0.127885
N	0.000000	1.087934	0.127885
C	0.000000	0.000000	1.057982
H	0.865981	1.630652	0.127383
H	-0.865981	-1.630652	0.127383

1,3-diazet-2-ylidene-2-CH⁺, trans

H	-0.042402	1.607280	-0.912536
C	-0.000011	1.011860	0.000000
H	0.042368	1.607278	0.912540
C	0.000011	-0.965884	0.000001
H	0.000023	-2.050840	0.000001
N	-0.991529	-0.082715	0.052256
H	-1.982742	-0.140880	-0.163424
N	0.991530	-0.082693	-0.052255
H	1.982747	-0.140839	0.163409

1,3-diazet-2-ylidene-CH₂, cis-diequatorial

H	1.076326	-0.285092	1.388763
C	0.070814	-0.018757	1.017336
N	0.070814	1.052866	0.000000
H	-0.593137	0.157107	1.869805
N	-0.459663	-0.949871	0.000000
H	-0.008893	-1.863408	0.000000
H	0.914690	1.623495	0.000000
C	0.070814	-0.018757	-1.017336
H	1.076326	-0.285092	-1.388763
H	-0.593137	0.157107	-1.869805

azet-2-ylidene, singlet

H	0.139954	1.615457	0.754038
C	0.016277	0.811901	0.022354
C	-1.088577	-0.027400	-0.168332
H	-2.158506	0.059578	-0.086090
C	-0.110262	-0.918604	0.277861
N	1.039998	-0.113869	-0.263964
H	1.833936	-0.073339	0.388501

azet-2-ylidene, triplet

H	0.487873	1.969812	0.000335
C	0.164899	0.936145	-0.000058
C	-1.010071	0.130259	0.000030
H	-2.068561	0.358516	-0.000097
C	-0.254491	-1.137823	0.000052
N	0.896889	-0.215932	-0.000098
H	1.900446	-0.388286	0.000302

azet-2-ylidene-2-CH+

H	1.324320	-1.578279	0.000002
C	0.612354	-0.756075	0.000000
C	-0.898828	-0.577315	0.000000
H	-1.747960	-1.244493	0.000000
N	0.844157	0.509571	-0.000002
H	1.701696	1.065836	0.000005
C	-0.710138	0.747002	0.000001
H	-1.207481	1.708264	-0.000001

azet-2-ylidene-2-CH2

H	1.768147	-1.099497	0.002840
C	0.886182	-0.465444	0.012008
C	0.621071	0.856629	0.039066
H	1.203129	1.764038	-0.046895
N	-0.464380	-0.910134	-0.140574
H	-0.812047	-1.516080	0.606246
C	-0.853697	0.538921	0.006291
H	-1.404077	0.741338	0.930693
H	-1.425824	0.900505	-0.853055

azetidine-2-ylidene, singlet

H	0.023397	1.622731	0.894740
C	0.040999	0.992312	-0.000005
N	-0.960118	-0.070598	0.000007
C	1.035221	-0.195795	0.000004
H	0.023391	1.622705	-0.894769
H	1.665443	-0.280562	0.889312
H	1.665496	-0.280552	-0.889268
C	-0.189313	-1.158112	-0.000012
H	-1.978345	-0.020568	0.000010

azetidine-2-ylidene, triplet

H	-0.132611	1.449722	0.971071
C	-0.056220	0.920289	0.017372
N	-1.083925	-0.156732	-0.146713
C	1.108005	-0.107908	-0.000290
H	-0.071710	1.630584	-0.812451
H	1.775258	-0.072364	0.865769
H	1.707587	-0.110289	-0.916009
C	-0.027889	-1.086783	0.045154
H	-1.834424	-0.154122	0.545195

azetidine-2-ylidene-2-CH+

H	0.616504	1.534135	0.902418
C	0.432320	0.950697	-0.000013
N	-0.928267	0.338869	0.000012

C	0.946111	-0.518988	0.000010
H	0.616468	1.534078	-0.902489
H	1.493622	-0.831477	0.893048
H	1.493724	-0.831510	-0.892952
H	-1.878115	0.723483	0.000040
C	-0.502663	-0.883088	-0.000015
H	-1.098945	-1.792517	-0.000044

azetidine-2-ylidene-2-CH2

H	1.932507	-0.049373	-0.522144
C	1.042258	-0.038288	0.114178
N	0.000000	-1.022700	-0.261761
C	0.000000	1.072675	-0.097669
H	1.354305	-0.095081	1.167625
H	0.000000	1.436478	-1.126523
H	0.000000	1.916237	0.594738
H	0.000000	-1.881497	0.289031
C	-1.042258	-0.038288	0.114178
H	-1.932507	-0.049373	-0.522144
H	-1.354305	-0.095081	1.167625

miscellaneous carbenes

diethynylcarbene, singlet

H	0.000000	3.305911	-0.818063
C	0.000000	2.357864	-0.327570
C	0.000000	1.195025	0.082412
C	0.000000	0.000000	0.763005
C	0.000000	-1.195025	0.082412
C	0.000000	-2.357864	-0.327570
H	0.000000	-3.305911	-0.818063

diethynylcarbene, triplet

H	0.000000	3.598364	-0.000593
C	0.000000	2.532986	-0.000235
C	0.000000	1.314889	-0.000031
C	0.000000	0.000000	0.000731
C	0.000000	-1.314889	-0.000031
C	0.000000	-2.532986	-0.000235
H	0.000000	-3.598364	-0.000593

diethynylmethyl+

H	0.000000	3.267429	-0.950295
C	0.000000	2.311702	-0.457416
C	0.000000	1.210040	0.087295
C	0.000000	0.000000	0.749594
C	0.000000	-1.210040	0.087295
H	0.000000	0.000000	1.844477

C	0.000000	-2.311702	-0.457416
H	0.000000	-3.267429	-0.950295

diethynylmethane

H	0.000000	3.148171	-1.159204
C	0.000000	2.261239	-0.567661
C	0.000000	1.220376	0.065414
C	0.000000	-1.220376	0.065414
C	0.000000	-2.261239	-0.567661
H	0.000000	-3.148171	-1.159204
C	0.000000	0.000000	0.878667
H	0.877665	0.000000	1.536681
H	-0.877665	0.000000	1.536681

cyanocarbene, singlet

C	0.119376	-1.300055	0.000000
C	0.000000	0.098492	0.000000
N	-0.271702	1.254590	0.000000
H	1.185657	-1.572754	0.000000

cyanocarbene, triplet

C	0.275735	-1.227963	0.000000
C	0.000000	0.119244	0.000000
N	-0.191487	1.254368	0.000000
H	-0.314002	-2.128267	0.000000

cyanomethyl+

C	0.000000	0.000000	-1.201225
C	0.000000	0.000000	0.185363
N	0.000000	0.000000	1.370454
H	0.000000	0.945880	-1.749006
H	0.000000	-0.945880	-1.749006

acetonitrile

C	0.000000	0.273873	0.000000
N	-0.000438	1.452206	0.000000
C	0.000314	-1.186931	0.000000
H	-1.024593	-1.562585	0.000000
H	0.512888	-1.562255	0.887664
H	0.512888	-1.562255	-0.887664

dicyanocarbene, singlet

C	0.000000	0.000000	0.800428
C	0.000000	1.188122	0.062996
N	0.000000	2.282781	-0.397037
C	0.000000	-1.188122	0.062996
N	0.000000	-2.282781	-0.397037

dicyanocarbene, triplet

C	0.000000	0.000000	0.004063
C	0.000000	1.333755	0.000337
N	0.000000	2.492776	-0.002030
C	0.000000	-1.333755	0.000337
N	0.000000	-2.492776	-0.002030

dicyanomethyl+

C	0.000000	0.750767	0.000000
C	-1.214507	0.060121	0.000000
N	-2.260117	-0.505293	0.000000
H	0.000000	1.848056	0.000000
C	1.214506	0.060120	0.000000
N	2.260117	-0.505293	0.000000

dicyanomethane (malonitrile)

C	0.000000	0.000000	0.852540
C	0.000000	1.214795	0.031043
N	0.000000	2.206438	-0.606387
H	-0.882933	0.000000	1.500834
H	0.882933	0.000000	1.500834
C	0.000000	-1.214795	0.031043
N	0.000000	-2.206438	-0.606387

nitrocarbene, singlet (nitrosocarbaldehyde)

C	-0.716990	0.482377	0.073970
N	0.784166	0.588145	-0.135179
O	-1.321405	-0.555290	-0.053097
O	1.318438	-0.504262	0.079461
H	-1.163484	1.465140	0.291526

nitrocarbene, triplet

C	-1.017202	-0.913504	-0.000002
N	0.065039	0.010368	0.000000
O	1.208735	-0.459308	0.000001
O	-0.245875	1.211004	0.000000
H	-2.054940	-0.605116	0.000011

nitromethyl+

C	-1.039185	-0.592861	0.000002
N	0.279148	-0.073068	-0.000012
O	-0.567249	0.912669	0.000004
O	1.463022	-0.175329	0.000004
H	-1.442546	-0.915045	0.957286
H	-1.442575	-0.915030	-0.957275

nitromethane

N	0.165852	0.000001	-0.014189
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O	0.731199	1.103802	0.004135
O	0.731330	-1.103731	0.004136
C	-1.319467	-0.000060	-0.001274
H	-1.631786	-0.000035	1.043198
H	-1.656256	-0.904822	-0.501175
H	-1.656352	0.904642	-0.501221

dinitrocarbene, singlet

N	1.163768	-0.106021	0.078099
C	0.073744	0.060150	0.932104
N	-1.125448	-0.037340	0.048315
O	1.901797	-0.886865	-0.480921
O	1.152957	1.180101	0.121507
O	-1.599382	-1.180294	0.078008
O	-1.544210	0.967386	-0.528286

dinitrocarbene, triplet

N	1.265398	-0.071175	-0.083288
C	-0.000004	-0.760969	-0.000021
N	-1.265394	-0.071169	0.083288
O	2.222649	-0.665797	0.424044
O	1.261784	1.013436	-0.673857
O	-1.261784	1.013443	0.673852
O	-2.222649	-0.665804	-0.424023

dinitromethyl+

C	-0.020072	-0.705958	0.324133
N	-1.254230	-0.169621	-0.116114
O	-1.052840	0.118080	1.142222
O	-2.092949	0.059843	-0.924105
N	1.195234	0.077971	-0.054236
H	0.079192	-1.760493	0.589380
O	1.060172	1.300788	-0.021637
O	2.142394	-0.648987	-0.364196

dinitromethane

H	-0.160502	-1.491638	-0.909216
C	-0.081809	-0.898019	-0.000581
H	-0.160800	-1.492823	0.907248
N	-1.205482	0.095745	-0.000111
N	1.205815	-0.169103	0.000101
O	1.679043	0.116196	-1.110394
O	1.677933	0.115955	1.111125
O	-2.328358	-0.420799	0.000212
O	-0.927389	1.299407	-0.000252

aminocyanocarbene, singlet

H	1.314464	1.282667	0.000009
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N	1.491487	0.275392	-0.000002
C	0.581514	-0.670274	-0.000002
H	2.470734	0.006761	-0.000010
C	-0.747017	-0.104743	0.000012
N	-1.890370	0.204704	-0.000007

aminocyanocarbene, triplet

H	-2.174715	-0.237041	-0.841504
N	-1.606185	-0.268852	0.000004
C	-0.506172	0.540483	-0.000022
H	-2.174694	-0.236981	0.841521
C	0.842377	0.105156	0.000027
N	1.939353	-0.216836	-0.000011

aminocyanomethyl+

C	0.000000	0.756867	0.000000
C	-0.628415	-0.518874	0.000000
N	-1.180597	-1.566476	0.000000
H	-0.602269	1.664559	0.000000
N	1.285801	0.864052	0.000000
H	1.737978	1.783453	0.000000
H	1.898358	0.041005	0.000000

aminocyanomethane

C	-0.535877	0.608284	0.047280
C	0.843394	0.105906	-0.008849
N	1.952701	-0.292313	-0.021251
H	-0.675779	1.306003	-0.783619
H	-0.643583	1.187221	0.977292
N	-1.476613	-0.499192	-0.116282
H	-1.434482	-1.109811	0.697364
H	-2.423878	-0.128019	-0.158887

aminonitrocarbene, singlet

N	1.681316	-0.035037	0.155349
C	0.723825	-0.787152	-0.314477
N	-0.539694	-0.000482	-0.056732
H	1.519894	0.910643	0.518135
H	2.637292	-0.366750	0.087210
O	-0.517157	1.247389	-0.095098
O	-1.544279	-0.693933	0.168999

aminonitrocarbene, triplet

N	1.844266	-0.048576	-0.102910
C	0.663376	-0.651386	0.177794
N	-0.598260	0.000969	0.005017
H	2.178329	0.646110	0.560842
H	2.573463	-0.656530	-0.457085

O	-0.570933	1.244738	-0.022263
O	-1.610828	-0.713240	-0.038396

aminonitrocarbenium ion

H	-1.650495	1.034885	-0.000177
N	-1.738957	0.005119	-0.000059
C	-0.668802	-0.688295	0.000080
H	-2.670494	-0.424581	-0.000043
N	0.602444	0.052563	0.000018
H	-0.627303	-1.775380	0.000225
O	1.607588	-0.674705	-0.000073
O	0.506999	1.286088	0.000048

aminonitromethane

C	-0.675032	-0.752918	0.000038
N	0.627080	0.058631	0.000004
O	0.541500	1.295487	0.000016
O	1.674814	-0.600868	-0.000029
N	-1.863178	0.013082	-0.000029
H	-0.595791	-1.381693	0.888158
H	-0.595782	-1.381827	-0.887984
H	-1.917997	0.611004	-0.819861
H	-1.918051	0.611083	0.819741

imidazol-5-ylidene, singlet

H	-1.176374	-1.774127	0.000000
N	-0.578247	-0.955728	0.000000
C	-1.081510	0.295339	0.000000
C	0.822384	-1.052456	0.000000
H	-2.113068	0.613036	0.000000
C	1.138380	0.306356	0.000000
N	0.000000	1.094727	0.000000
H	2.108069	0.784827	0.000000
H	-0.046420	2.107838	0.000000

imidazol-5-ylidene, triplet

C	-0.635633	0.948603	-0.144906
C	-0.043421	-1.205355	-0.001496
H	-1.197470	1.700987	0.406854
C	1.078972	-0.546694	0.013916
H	2.101421	-0.887758	-0.023929
N	-1.151011	-0.391146	-0.090241
H	-1.940951	-0.577286	0.520616
N	0.761000	0.833951	0.126602
H	1.367572	1.485089	-0.363149

imidazol-2-ylidene-5-CH⁺ (imidazolium⁺)

H	0.000000	1.393514	-1.788673
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C	0.000000	0.684743	-0.974394
C	0.000000	-0.684743	-0.974394
N	0.000000	1.072375	0.344390
H	0.000000	-1.393514	-1.788673
N	0.000000	-1.072375	0.344390
H	0.000000	2.035160	0.676011
H	0.000000	-2.035160	0.676011
C	0.000000	0.000000	1.145212
H	0.000000	0.000000	2.225317

imidazol-5-ylidene, 5-CH2

C	-0.750721	-0.935822	0.166223
N	-1.085526	0.372294	0.042285
H	-2.052206	0.679061	0.024974
H	-1.445017	-1.693009	-0.190623
N	0.616426	-0.975950	-0.238086
H	1.130958	-1.736576	0.200024
C	-0.032904	1.204753	-0.200945
H	-0.125294	2.247975	0.081788
C	1.163526	0.354351	0.121834
H	2.053999	0.582515	-0.470693
H	1.441854	0.405927	1.202471

Table S6. G3MP2 enthalpies of hydrogenation and singlet-triplet enthalpy gaps for a large range of singlet carbene types. HIA and ΔH_{ACID} for the corresponding carbenium ions, 298 K, kcal/mol.^a

Carbene	$\Delta H_{\text{HYDROG(singlet)}}$	ΔH_{ST}	HIA	ΔH_{ACID}
<u>Type 1. alkyl, alkenyl and alkynyl carbenes^b</u>				
CH ₂	-118.1	9.4	-314.5	205.2
CH ₃ CH	-106.0	2.9	-269.3	235.6
(CH ₃) ₂ CH-CH	-104.9	0.6	NA	NA
(CH ₃) ₂ C	-97.1	-1.9	-250.2	245.9
CH ₂ =CH-CH	-100.1	8.2	-256.3	242.8
CH≡C-CH	-96.1	11.4	-272.7	222.3
diethynylcarbene	-78.6	12.6	-252.5	225.1
cyclopropylidene	-97.1	-16.7	-245.3	250.7
cyclobutylidene	-91.6	-10.4	-239.3	251.3
cyclopentylidene	-90.5	-9.9	-243.6	245.8
cyclopropenylidene	-49.0	-71.7	-222.5	225.4
cyclopropylcarbinylidene	-95.1	-6.5	-241.2	252.9
cyclobut-1-en-3-ylidene	-72.5	-24.2	-239.6	231.8
cyclopent-1-en-1-ylidene	-86.6	-7.6	-226.3	259.2
2,4-cyclohexadienylidene	-83.4	3.2	-215.0	267.3
2,5-cyclohexadienylidene	-85.7	3.2	-215.1	269.5
6,6-dimethylcyclohexa-2,4-dienylidene	-87.4	5.3	-214.6	271.9
spiro[2.5]octa-4,6-dien-8-ylidene	-71.5	-7.4	-195.6	274.8
spiro[2.5]octa-4,6-dien-6-ylidene	-81.1	0.8	-196.5	283.6
<u>Type 2. aryl carbenes^c</u>				
PhCH	-99.4	2.13	-240.5	259.9
3-oxyphenyl [†]	-87.2	-8.2	-127.1	359.0
3-aminophenyl	-98.9	1.53	-231.5	266.4
3-hydroxyphenyl	-99.1	1.70	-237.8	260.3
3-sulphydrylphenyl	-99.7	1.63	-239.4	259.2
3-methylphenyl	-99.6	1.63	-236.0	262.6
3-fluorophenyl	-100.7	2.72	-244.6	255.1
3-chlorophenyl	-100.8	2.47	-243.9	255.8
3-formylphenyl	-100.6	2.24	-245.6	254.0
3-trifluoromethylphenyl	-101.4	3.02	-247.9	252.5
3-cyanophenyl	-102.1	3.05	-252.1	249.0
3-nitrophenyl	-102.4	3.38	-252.7	248.6
4-oxyphenyl [†]	-64.5	-24.3	-87.5	376.0
4-aminophenyl	-92.5	-4.05	-210.6	280.9
4-hydroxyphenyl	-95.5	-1.70	-224.8	269.6
4-sulphydrylphenyl	-97.8	-0.04	-227.1	269.7
4-methylphenyl	-98.0	0.78	0231.3	265.6
4-fluoromethylphenyl	-99.1	1.49	-236.6	261.5

Table S6. G3MP2 enthalpies of hydrogenation and singlet-triplet enthalpy gaps for a large range of singlet carbene types. HIA and ΔH_{ACID} for the corresponding carbenium ions, 298 K, kcal/mol.^a

Carbene	$\Delta H_{\text{HYDROG(singlet)}}$	ΔH_{ST}	HIA	ΔH_{ACID}
4-fluorophenyl	-98.2	0.22	-237.5	259.6
4-chlorophenyl	-99.3	1.40	-237.4	260.5
4-formylphenyl	-101.9	4.52	-246.6	254.3
4-trifluoromethylphenyl	-192.6	3.79	-249.0	252.5
4-cyanophenyl	-102.4	4.39	-251.2	250.2
4-nitrophenyl	-103.0	4.98	-253.6	248.4
PhCCH ₃	-93.2	0.8	-229.3	264.9
Ph ₂ C	-86.4	-2.6	-217.4	268.0
cycloheptatrienylcarbene ⁺	-108.2	9.2	-369.9	137.2
cyclopentadienylcarbene ⁻	-59.8	-26.4	-70.0	388.7
cyclopropenylcarbene ⁺	-83.2	-20.7	-428.7	53.4

Type 3, acyclic heteroatom and cyano carbenes^c

NH ₂ CH	-60.0	-34.5	-217.1	241.9
(NH ₂) ₂ C	-35.2	-57.4	-184.5	249.6
HOCH (anti)	-71.8	-25.6	-249.9	220.9
HOCH (syn)	-76.4	-21.0	-249.9	225.5
CH ₃ OCH	-70.2	-28.1	-238.9	232.2
CH ₃ OCCH ₃	-64.6	-32.7	-221.1	242.5
(CH ₃ O) ₂ C	-40.8	-59.8	-206.2	235.6
FCH	-89.6	-14.6	-289.5	199.1
F ₂ C	-59.5	-56.3	-282.7	175.7
SiH ₃ CH	-117.4	18.1	-241.4 ^d	274.9 ^d
(SiH ₃) ₂ C	-113.7	22.0	-226.4 ^e	281.7 ^e
PH ₂ CH	-83.9	-13.4	-249.3	233.5
HSCH (anti)	-75.4	-20.6	-247.7	226.7
HSCH (syn)	-76.6	-19.4	-247.7	227.9
CH ₃ SCH	-69.7	-24.9	-233.9	234.7
ClCH	-93.7	-6.9	-279.7	212.9
Cl ₂ C	-74.4	-21.8	-266.2	207.1
(NH ₂) ₂ CCH ⁺	-120.1	12.1	-428.3	90.7
cyanocarbene	-106.6	9.9	-313.5	192.0
dicyanocarbene	-94.5	11.8	-315.3	178.2
nitrocarbene	NA ^f	NA ^f	-293.6	NA ^f
dinitrocarbene	-93.1	-19.7	-309.0	183.0
aminocyanocarbene	-52.8	-32.4	-234.2	217.6
aminonitrocarbene	-58.0	-41.5	-245.8	211.2
O=NCH	-21.7	-60.4	-255.9	164.8
HN=C	-22.9	-106.8	-238.8	183.0
O=C	2.2	-138.1	-256.5	140.3

Table S6. G3MP2 enthalpies of hydrogenation and singlet-triplet enthalpy gaps for a large range of singlet carbene types. HIA and ΔH_{ACID} for the corresponding carbenium ions, 298 K, kcal/mol.^a

Carbene	$\Delta H_{\text{HYDROG(singlet)}}$	ΔH_{ST}	HIA	ΔH_{ACID}
<u>Type 4. Five-membered cyclic 1,3-diheteroatom carbenes^g</u>				
imidazol-2-ylidene	-15.0	-85.7	-163.9	250.1
4,5-dihydroimidazol-2-ylidene	-30.7	-72.3	-176.9	252.8
<i>N,N'</i> -dimethylimidazol-2-ylidene	-14.9	-87.6	-155.5	258.4
4,5-dimethylimidazol-2-ylidene	-16.7	-83.6	-158.9	257.6
4,5, <i>N,N'</i> -tetramethylimidazol-2-ylidene	-14.5	-86.3	-148.4	265.0
imidazol-5-ylidene	-3.8	65.3	-133.3	269.5
1,3-dioxol-2-ylidene	-33.7	-86.6	-212.0	220.6
1,3-dioxolane-2-ylidene	-38.1	-72.7	-208.5	228.5
oxazol-2-ylidene	-26.3	-86.8	-188.0	237.3
4,5-dihydrooxazol-2-ylidene	-36.2	-70.2	-192.5	242.7
4,5-difluoroimidazol-2-ylidene	-24.5	-65.8	-184.7	238.7
4,5, <i>N,N'</i> -tetrasilylimidazol-2-ylidene	-16.9	-83.0	-157.6	258.2
1,3-diphosphole-2-ylidene	-70.0	-26.1	-226.0	243.0
1,3-diphospholan-2-ylidene	-74.9	-22.0	-228.9	245.0
1,3-dithiol-2-ylidene	-35.6	-56.9	-200.3	234.3
1,3-dithiolan-2-ylidene	-46.9	-47.2	-210.6	235.3
<u>Type 5. small-ring aza- and diazacarbenes^g</u>				
diazirene-3-ylidene	=61.6	-30.5	-288.2	172.4
diazirane-3-ylidene	-64.5	-55.0	-260.5	203.0
1,3-diazetid-2-ylidene	-38.7	-62.8	-191.3	246.4
azet-2-ylidene	-71.3	-39.3	-241.9	228.4
azetid-2-ylidene	-53.8	-46.9	-203.2	249.6

^aHydrogenation of the carbene occurs with the addition of two hydrogen atoms to the carbenic carbon. A negative value for ΔH_{ST} indicates the singlet is more stable. HIA = the reaction enthalpy for addition of hydride⁻ to the carbenium ion. ΔH_{ACID} is the reaction enthalpy for loss of a proton from the α -carbon of the carbenium ion. ^bSee also Keeffe, J. R.; More O'Ferrall, R. A. *ARKIVOC* **2008**, 183. ^c ΔH_{ST} and ΔH_{HYDROG} values for a number of examples of Types 1, 2 and 3 carbenes are given in Gronert, S.; Keeffe, J. R.; More O'Ferrall, R. A. *J. Org. Chem.* **2009**, 74, 5250. ^dProtonation of singlet silylcarbene leads to rearrangement resulting in the methylsilylium ion. The listed values are obtained using the latter species. ^eProtonation of singlet disilylcarbene leads to rearrangement resulting first in silylmethylsilylium ion, $\text{H}_3\text{Si-CH}_2\text{-SiH}_2^+$, then the symmetrical (C_{2v}) 1,3-bridged μ -hydrido-disilylmethane cation, 10.6 kcal/mol more stable. The listed values are obtained using the latter structure. ^fSinglet nitrocarbene shows a partially oxygen-bridged structure at HF/3-21G, and a C_s structure at HF/6-31G* with the nitro group perpendicular to the CH moiety. However it rearranges at MP2/6-31G* by a 1,2-oxygen migration from nitrogen to carbon yielding "nitrosocarbaldehyde". See also Tao, Y.; Ding, Y.; Li, Z.; Huang, X.; Sun, C.-C. *J. Phys. Chem. A* **2001**, 105, 3388. ^gWhere cis and trans isomers exist, the more stable of the two is used for the ΔH calculations.