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ENERGIES FOR THE SURFACE DESCRIBING H-ABSTRACTION BY 2,5-DEHYDROPYRIDYNE

Pyridyne	Methanol	CAS(4,4)/3-21G	delta E's	CAS(4,4)/6-31G**	delta E's	CAS(4,4)MP2/6-31G**	delta E's
1.1	1.2	-358.369 644	38.74				
1.1	1.3	-358.388 216	27.08				
1.1	2	-358.445 452	-8.83				
1.2	1.1	-358.347 122	52.87				
1.2	1.2	-358.384 091	29.67				
1.2	1.3	-358.397 111	21.50				
1.2	1.4	-358.407 385	15.05				
1.2	1.5	-358.415 943	9.68				
1.2	1.7	-358.428 997	1.49				
1.2	2	-358.440 256	-5.57				
1.3	1.1	-358.360 638	44.39				
1.3	1.2	-358.392 472	24.41				
1.3	1.3	-358.400 286	19.51	-360.429 545	20.79	-361.550 029	13.19
1.3	1.4	-358.406 228	15.78	-360.435 727	16.91	-361.554 370	10.47
1.3	1.5	-358.411 429	12.52	-360.440 917	13.65	-361.557 673	8.39
1.3	1.7	-358.420 265	6.97				
1.3	2	-358.428 844	1.59				
1.35	1.25	-358.398 550	20.60	-360.427 840	21.86	-361.548 140	14.38
1.35	1.35	-358.402 898	17.87	-360.432 454	18.96	-361.551 277	12.41
1.35	1.45	-358.406 463	15.63	-360.435 913	16.79	-361.552 986	11.34
1.4	1.1	-358.371 601	37.51	-360.418 679	27.61	-361.540 175	19.37
1.4	1.2	-358.398 162	20.84	-360.427 311	22.19	-361.547 216	14.96
1.4	1.25	-358.400 051	19.66	-360.429 404	20.88	-361.548 691	14.03
1.4	1.275	-358.400 727	19.23	-360.430 119	20.43	-361.549 123	13.76
1.4	1.3	-358.401 287	18.88	-360.430 761	20.02	-361.549 428	13.57
1.4	1.325	-358.401 768	18.58	-360.431 022	19.86	-361.549 959	13.24
1.4	1.35	-358.402 200	18.31				
1.4	1.4	-358.403 007	17.80	-360.432 565	18.89	-361.549 905	13.27
1.4	1.5	-358.404 723	16.72	-360.434 184	17.88	-361.550 058	13.17
1.4	1.7	-358.408 942	14.08				
1.4	2	-358.414 562	10.55				
1.425	1.25	-358.400 745	19.22	-360.430 358	20.28	-361.549 066	13.80
1.425	1.275	-358.401 154	18.96	-360.431 045	19.85	-361.549 391	13.59
1.425	1.3	-358.401 449	18.78	-360.430 785	20.01	-361.549 038	13.81
1.425	1.325	-358.401 668	18.64	-360.431 146	19.78	-361.549 163	13.73
1.425	1.35	-358.401 843	18.53	-360.431 385	19.63	-361.549 064	13.80
1.425	1.375	-358.401 998	18.43				
1.45	1.15	-358.398 578	20.58	-360.427 477	22.09	-361.546 776	15.23
1.45	1.25	-358.401 425	18.79	-360.430 811	19.99	-361.549 052	13.80
1.45	1.275	-358.401 578	18.70	-360.431 070	19.83	-361.549 064	13.80
1.45	1.3	-358.401 618	18.67	-360.431 093	19.82	-361.548 847	13.93
1.45	1.325	-358.401 583	18.69	-360.431 062	19.84	-361.548 579	14.10
1.45	1.35	-358.401 506	18.74	-360.430 764	20.02	-361.548 074	14.42
1.45	1.45	-358.401 226	18.92	-360.430 614	20.12	-361.546 768	15.24
1.475	1.25	-358.402 100	18.37	-360.431 613	19.49	-361.549 314	13.64
1.475	1.275	-358.402 012	18.43	-360.431 497	19.56	-361.548 992	13.84
1.475	1.3	-358.401 807	18.55	-360.431 254	19.71	-361.548 561	14.11
1.475	1.325	-358.401 528	18.73	-360.430 988	19.88	-361.548 089	14.41
1.475	1.35	-358.401 208	18.93	-360.430 668	20.08	-361.547 519	14.77
1.475	1.375	-358.400 875	19.14				
1.5	1.2	-358.402 856	17.90	-360.432 074	19.20	-361.549 746	13.37

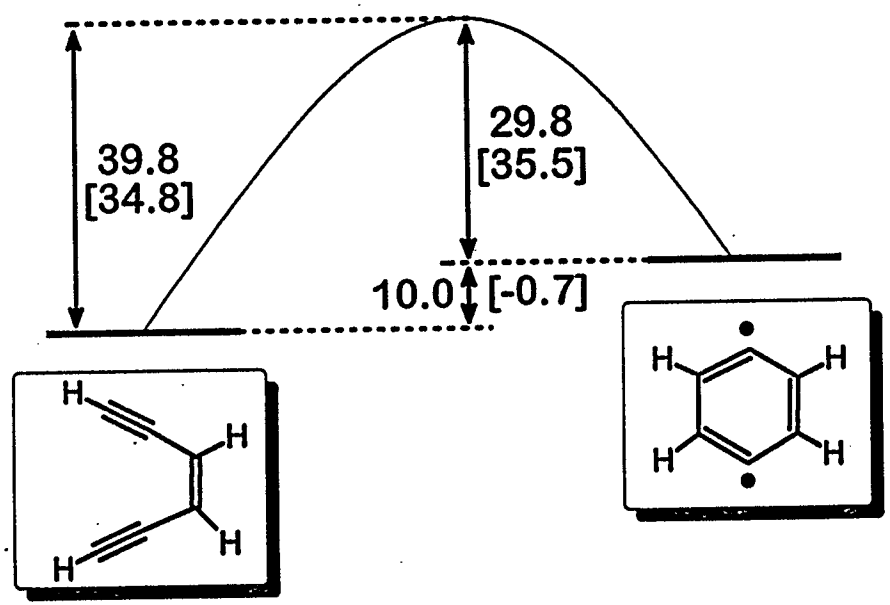
1.5	1.25	-358.402 781	17.94	-360.432 196	19.12	-361.549 422	13.57
1.5	1.275	-358.402 463	18.14	-360.431 928	19.29	-361.548 926	13.88
1.5	1.3	-358.402 026	18.42	-360.431 459	19.59	-361.548 238	14.31
1.5	1.325	-358.401 513	18.74	-360.430 709	20.06	-361.547 413	14.83
1.5	1.35	-358.400 959	19.09	-360.430 233	20.36	-361.546 682	15.29
1.5	1.4	-358.399 838	19.79	-360.429 230	20.99	-361.545 165	16.24
1.5	1.5	-358.398 027	20.93	-360.427 248	22.23	-361.542 173	18.12
1.5	1.7	-358.397 146	21.48				
1.5	2	-358.399 361	20.09				
1.55	1.25	-358.404 176	17.07	-360.433 404	18.37	-361.549 710	13.39
1.55	1.35	-358.400 644	19.28	-360.429 863	20.59	-361.545 500	16.03
1.55	1.45	-358.396 762	21.72	-360.425 867	23.10	-361.540 749	19.01
1.6	1.1	-358.405 880	16.00				
1.6	1.2	-358.407 191	15.18	-360.436 384	16.50	-361.552 114	11.88
1.6	1.3	-358.403 300	17.62	-360.432 619	18.86	-361.547 576	14.73
1.6	1.4	-358.397 794	21.07	-360.426 939	22.42	-361.541 261	18.69
1.6	1.5	-358.392 645	24.30	-360.421 535	25.81	-361.535 274	22.45
1.6	1.7	-358.386 258	28.31				
1.6	2	-358.384 408	29.47				
1.7	1.1	-358.411 814	12.27				
1.7	1.2	-358.411 241	12.63				
1.7	1.3	-358.405 171	16.44				
1.7	1.5	-358.389 167	26.49				
1.7	1.7	-358.377 245	33.97				
1.7	2	-358.370 509	38.19				
1.8	1.1	-358.416 702	9.21				
1.8	1.2	-358.414 882	10.35				
1.8	1.3	-358.407 361	15.07				
1.8	1.4	-358.397 584	21.20				
1.8	1.5	-358.387 521	27.52				
1.8	1.7	-358.370 692	38.08				
1.8	2	-358.358 303	45.85				
2	1.1	-358.423 700	4.82				
2	1.2	-358.420 566	6.78				
2	1.3	-358.411 538	12.45				
2	1.4	-358.399 952	19.72				
2	1.5	-358.387 641	27.44				
2	1.7	-358.364 608	41.90				
2	2	-358.341 013	56.70				
10	1.1	-358.431 402	-0.02	-360.462 672	0.00	-361.571 051	0.00
30	1.1	-358.431 375	0.00				

		3-21g		6-31g*	
		Vertical Excitation	Triplet Relaxed	Vertical Excitation	Triplet Relaxed
p-Benzyne		**CAS(6,6)**		**CAS(6,6)**	
	singlet	-228.1440195		-229.4235532	
	triplet	-228.1402493	-228.140926	-229.4209942	-229.4217876
	ΔEST (kcal/mol)	**2.37**	**1.94**	**1.61**	**1.11**
		CAS(6,6)MP2		**CAS(6,6)MP2**	
	singlet	-228.5642106		-230.0963386	
	triplet	-228.5598879	-228.5615452	-230.0929887	-230.095204
	ΔEST (kcal/mol)	**2.71**	**1.67**	**2.1**	**0.71**

		3-21g		6-31g*	
		Vertical Excitation	Triplet Relaxed	Vertical Excitation	Triplet Relaxed
Pyridyne		**CAS(6,6)**		**CAS(6,6)**	
	singlet	-244.0449993		-245.4234846	
	triplet	-244.0328382	-244.0354053	-245.4134308	-245.4170952
	ΔEST (kcal/mol)	**7.63**	**6.02**	**6.31**	**4.01**
		CAS(6,6)MP2		**CAS(6,6)MP2**	
	singlet	-244.4831999		-246.1206479	
	triplet	-244.4688041	-244.4726243	-246.1075771	-246.1135411
	ΔEST (kcal/mol)	**9.03**	**6.64**	**8.2**	**4.46**
Protonated Pyridyne		**CAS(6,6)**		**CAS(6,6)**	
	singlet	-244.4026047		-245.7745936	
	triplet	-244.3976452	-244.398418	-245.7710849	-245.7720467
	ΔEST (kcal/mol)	**3.11**	**2.63**	**2.2**	**1.6**
		CAS(6,6)MP2		**CAS(6,6)MP2**	
	singlet	-244.8330325		-246.4582237	
	triplet	-244.8275941	-244.8295511	-246.4540073	-246.4568635
	ΔEST (kcal/mol)	**3.41**	**2.18**	**2.65**	**0.85**

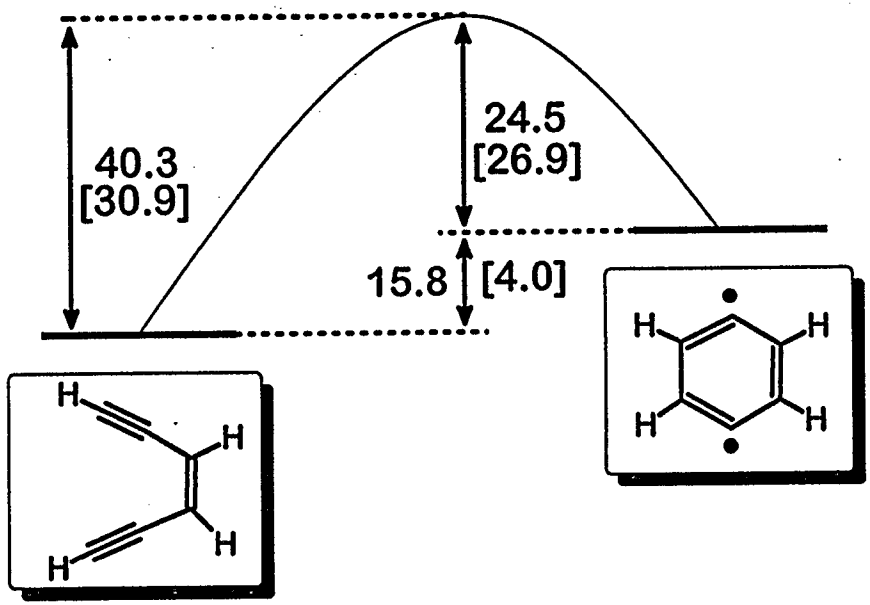
A_E_DY02.CW1

CAS(6,6)/6-31g*
[CAS-MP2/6-31g*]
all numbers in kcal/mol



A_E_DY01.CW1

CAS(6,6)/3-21g
[CAS-MP2/3-21g]
all numbers in kcal/mol



Singlet
p-Benzyne, CAS(6,6)/3-21g optimized
(benzyne1.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.684936	0.000000			
3	C	1.366441	2.383255	0.000000		
4	C	2.383255	1.366441	2.808069	0.000000	
5	C	1.366441	2.383255	2.422542	1.420051	0.000000
6	C	2.383255	1.366441	1.420051	2.422542	2.808069
7	H	2.141751	3.355935	1.070353	3.878392	3.392851
8	H	3.355935	2.141751	3.878392	1.070353	2.162439
9	H	2.141751	3.355935	3.392851	2.162439	1.070353
10	H	3.355935	2.141751	2.162439	3.392851	3.878392

		6	7	8	9	10
6	C	0.000000				
7	H	2.162439	0.000000			
8	H	3.392851	4.948728	0.000000		
9	H	3.878392	4.278887	2.486169	0.000000	
10	H	1.070353	2.486169	4.278887	4.948728	0.000000

Interatomic angles:

C1-C3-C2= 87.0237	C1-C4-C2= 87.0237	C3-C1-C4= 92.9763
C3-C2-C4= 92.9763	C1-C5-C2= 87.0237	C3-C1-C5=124.859
C3-C2-C5= 61.0936	C1-C5-C4=117.5705	C2-C4-C5=117.5705
C3-C5-C4= 90.	C1-C6-C2= 87.0237	C1-C3-C6=117.5705
C2-C6-C3=117.5705	C4-C1-C6= 61.0936	C4-C2-C6=124.859
C3-C6-C4= 90.	C5-C1-C6= 92.9763	C5-C2-C6= 92.9763
C5-C3-C6= 90.	C5-C4-C6= 90.	C2-C1-H7= 87.3404
C1-C3-H7=122.5603	C2-C3-H7=150.416	C4-C1-H7=117.8872
C4-C3-H7=179.4911	C5-C1-H7=149.7699	C5-C3-H7=150.1308
C1-H7-C6= 67.2413	C2-C6-H7=142.9889	C6-C3-H7=119.8692
C4-C6-H7=115.4184	C5-C6-H7= 85.0403	C1-C2-H8= 87.3404
C3-C2-H8=117.8872	C1-C4-H8=150.416	C2-C4-H8=122.5603
C3-C4-H8=179.4911	C1-C5-H8=142.9889	C2-H8-C5= 67.2413
C3-C5-H8=115.4184	C5-C4-H8=119.8692	C6-C2-H8=149.7699
C6-C4-H8=150.1308	C6-C5-H8= 85.0403	C2-C1-H9= 87.3404
C3-C1-H9=149.7699	C1-H9-C4= 67.2413	C2-C4-H9=142.9889
C3-C4-H9= 85.0403	C1-C5-H9=122.5603	C2-C5-H9=150.416
C3-C5-H9=150.1308	C4-C5-H9=119.8692	C6-C1-H9=117.8872
C6-C4-H9=115.4184	C6-C5-H9=179.4911	H7-C1-H9=174.6807
C1-H9-H8= 92.6596	C2-H8-H9= 92.6596	H8-C4-H9= 94.4508
H8-C5-H9= 94.4508	C1-C2-H10= 87.3404	C1-C3-H10=142.9889
C2-H10-C3= 67.2413	C4-C2-H10=149.7699	C4-C3-H10= 85.0403
C5-C2-H10=117.8872	C5-C3-H10=115.4184	C1-C6-H10=150.416
C2-C6-H10=122.5603	C3-C6-H10=119.8692	C4-C6-H10=150.1308
C5-C6-H10=179.4911	C1-H7-H10= 92.6596	C2-H10-H7= 92.6596
H7-C3-H10= 94.4508	H7-C6-H10= 94.4508	H8-C2-H10=174.6807

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Population analysis using the SCF density.

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Orbital Symmetries:

Occupied (B3G) (B2U) (B1U) (AG) (B1U) (AG) (AG) (B1U) (B2U)
(B3G) (AG) (B1U) (B2U) (B3G) (B2G) (B3U) (B1G)
(AG) (B2U) (B1U)

Virtual (AG) (B1U) (B3G) (B3U) (AG) (B2U) (B1U) (B2G)
(B3G) (AU) (AG) (B2U) (B1U) (B3G) (AG) (B2U) (B3U)
(B3G) (B2G) (B1G) (B1U) (AG) (AU) (B3U) (AG) (B1U)
(B2G) (B2U) (B1U) (B3G) (AG) (B2U) (B3G) (B2U)
(AG) (B1U) (B3G) (B1U) (B2U) (B3G) (AG) (B1U)

The electronic state is 1-AG.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.198926D+01				
2	0.000000D+00	0.198860D+01			
3	0.000000D+00	0.000000D+00	0.122359D+01		
4	-0.113037D-04	0.000000D+00	0.000000D+00	0.776321D+00	
5	0.000000D+00	0.000000D+00	0.338475D-05	0.000000D+00	0.109688D-01
6	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00

	6
6	0.112686D-01

Zero-point correction= 0.080405 (Hartree/Particle)
Thermal correction to Energy= 0.084342
Thermal correction to Enthalpy= 0.085286
Thermal correction to Gibbs Free Energy= 0.054604
Sum of electronic and zero-point Energies= -228.063614
Sum of electronic and thermal Energies= -228.059678
Sum of electronic and thermal Enthalpies= -228.058733
Sum of electronic and thermal Free Energies= -228.089415

Test job not archived.
1\1\GINC-C4-32\Freq\CASSCF\3-21G\C6H4\MSCHOTT\23-May-1997\0\\#P CAS(6,
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MP2=-228.5642106

Singlet
p-Benzyne, CAS(6,6)/6-31g* (3-21g geometry)
(benzyne1.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.684936	0.000000			
3	C	1.366441	2.383255	0.000000		
4	C	2.383255	1.366441	2.808069	0.000000	
5	C	1.366441	2.383255	2.422542	1.420051	0.000000
6	C	2.383255	1.366441	1.420051	2.422542	2.808069
7	H	2.141751	3.355935	1.070353	3.878392	3.392851
8	H	3.355935	2.141751	3.878392	1.070353	2.162439
9	H	2.141751	3.355935	3.392851	2.162439	1.070353
10	H	3.355935	2.141751	2.162439	3.392851	3.878392

		6	7	8	9	10
6	C	0.000000				
7	H	2.162439	0.000000			
8	H	3.392851	4.948728	0.000000		
9	H	3.878392	4.278887	2.486169	0.000000	
10	H	1.070353	2.486169	4.278887	4.948728	0.000000

Interatomic angles:

C1-C3-C2= 87.0237	C1-C4-C2= 87.0237	C3-C1-C4= 92.9763
C3-C2-C4= 92.9763	C1-C5-C2= 87.0237	C3-C1-C5=124.859
C3-C2-C5= 61.0936	C1-C5-C4=117.5705	C2-C4-C5=117.5705
C3-C5-C4= 90.	C1-C6-C2= 87.0237	C1-C3-C6=117.5705
C2-C6-C3=117.5705	C4-C1-C6= 61.0936	C4-C2-C6=124.859
C3-C6-C4= 90.	C5-C1-C6= 92.9763	C5-C2-C6= 92.9763
C5-C3-C6= 90.	C5-C4-C6= 90.	C2-C1-H7= 87.3404
C1-C3-H7=122.5603	C2-C3-H7=150.416	C4-C1-H7=117.8872
C4-C3-H7=179.4911	C5-C1-H7=142.7699	C5-C3-H7=150.1308
C1-H7-C6= 67.2413	C2-C6-H7=142.9889	C6-C3-H7=119.8692
C4-C6-H7=115.4184	C5-C6-H7= 85.0403	C1-C2-H8= 87.3404
C3-C2-H8=117.8872	C1-C4-H8=150.416	C2-C4-H8=122.5603
C3-C4-H8=179.4911	C1-C5-H8=142.9889	C2-H8-C5= 67.2413
C3-C5-H8=115.4184	C5-C4-H8=119.8692	C6-C2-H8=149.7699
C6-C4-H8=150.1308	C6-C5-H8= 85.0403	C2-C1-H9= 87.3404
C3-C1-H9=149.7699	C1-H9-C4= 67.2413	C2-C4-H9=142.9889
C3-C4-H9= 85.0403	C1-C5-H9=122.5603	C2-C5-H9=150.416
C3-C5-H9=150.1308	C4-C5-H9=119.8692	C6-C1-H9=117.8872
C6-C4-H9=115.4184	C6-C5-H9=179.4911	H7-C1-H9=174.6807
C1-H9-H8= 92.6596	C2-H8-H9= 92.6596	H8-C4-H9= 94.4508
H8-C5-H9= 94.4508	C1-C2-H10= 87.3404	C1-C3-H10=142.9889
C2-H10-C3= 67.2413	C4-C2-H10=149.7699	C4-C3-H10= 85.0403
C5-C2-H10=117.8872	C5-C3-H10=115.4184	C1-C6-H10=150.416
C2-C6-H10=122.5603	C3-C6-H10=119.8692	C4-C6-H10=150.1308
C5-C6-H10=179.4911	C1-H7-H10= 92.6596	C2-H10-H7= 92.6596
H7-C3-H10= 94.4508	H7-C6-H10= 94.4508	H8-C2-H10=174.6807

****

Population analysis using the SCF density.

****

Orbital Symmetries:

Occupied (B3G) (B2U) (B1U) (AG) (B1U) (AG) (AG) (B1U) (B2U)
(B3G) (AG) (B1U) (B2U) (B3G) (B2G) (B3U) (B1G)
(AG) (B3G) (AG)

Virtual (B1U) (B1U) (B2U) (B3U) (AG) (B2U) (B1U) (B2G)
(B3G) (AU) (AG) (B2U) (B1U) (B3G) (AG) (B2U) (B3U)
(B3G) (B2G) (B1G) (B1U) (AG) (AU) (B3U) (AG) (B1U)
(B2G) (B2U) (B1U) (B3G) (AG) (B2U) (B3G) (B2U)
(AG) (B1U) (B3G) (B1U) (B2U) (B3G) (AG) (B1U)
(AG) (B3G) (AG) (AG) (B2G) (B3G) (AG) (AG) (AG)
(AG) (B1G) (B2G) (B3G) (B1U) (B2U) (B1U) (B1U)
(B3U) (B2U) (B1U) (B1U) (B1U) (AU) (B3U) (B2U)
(B3G) (B3G) (B1G) (B2U) (B2U) (B1U) (B1G) (B2G)
(AU) (AU) (B3U)

The electronic state is 1-AG.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.198961D+01				
2	0.000000D+00	0.108839D-01			
3	0.192732D-04	0.000000D+00	0.800262D+00		
4	0.000000D+00	0.000000D+00	0.000000D+00	0.119967D+01	
5	0.000000D+00	0.000000D+00	0.000000D+00	0.262450D-04	0.106083D-01
6	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00

	6
6	0.198897D+01

Test job not archived.
1\1\GINC-C4-32\SP\CASSCF\6-31G(d)\C6H4\MSCHOTT\24-May-1997\0\\#P CAS(6
,6)/6-31G* GEOM=CHECK GUESS=READ SCF=(CONVER=6) # GFINPUT IOP(6/7=3)\\
p-benzyne, ring opening\\0,1\C,0.,0.,1.3424680767\C,0.,0.,-1.342468076
7\C,0.,1.211270894,0.7100253893\C,0.,-1.211270894,-0.7100253893\C,0.,-
1.211270894,0.7100253893\C,0.,1.211270894,-0.7100253893\H,0.,2.1394434
172,1.2430844704\H,0.,-2.1394434172,-1.2430844704\H,0.,-2.1394434172,1
.2430844704\H,0.,2.1394434172,-1.2430844704\\Version=DEC-AXP-OSF/1-G94
RevC.3\State=1-AG\HF=-229.4235532\RMSD=0.000e+00\Dipole=0.,0.,0.\PG=D0
2H [C2*(C1.C1),SG(C4H4)]\\@

MP2=-230.0963386

Triplet
p-Benzyne, CAS(6,6)/3-21g (singlet geometry)
(benzyne1.t.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.684936	0.000000			
3	C	1.366441	2.383255	0.000000		
4	C	2.383255	1.366441	2.808069	0.000000	
5	C	1.366441	2.383255	2.422542	1.420051	0.000000
6	C	2.383255	1.366441	1.420051	2.422542	2.808069
7	H	2.141751	3.355935	1.070353	3.878392	3.392851
8	H	3.355935	2.141751	3.878392	1.070353	2.162439
9	H	2.141751	3.355935	3.392851	2.162439	1.070353
10	H	3.355935	2.141751	2.162439	3.392851	3.878392

		6	7	8	9	10
6	C	0.000000				
7	H	2.162439	0.000000			
8	H	3.392851	4.948728	0.000000		
9	H	3.878392	4.278887	2.486169	0.000000	
10	H	1.070353	2.486169	4.278887	4.948728	0.000000

Interatomic angles:

C1-C3-C2= 87.0237	C1-C4-C2= 87.0237	C3-C1-C4= 92.9763
C3-C2-C4= 92.9763	C1-C5-C2= 87.0237	C3-C1-C5=124.859
C3-C2-C5= 61.0936	C1-C5-C4=117.5705	C2-C4-C5=117.5705
C3-C5-C4= 90.	C1-C6-C2= 87.0237	C1-C3-C6=117.5705
C2-C6-C3=117.5705	C4-C1-C6= 61.0936	C4-C2-C6=124.859
C3-C6-C4= 90.	C5-C1-C6= 92.9763	C5-C2-C6= 92.9763
C5-C3-C6= 90.	C5-C4-C6= 90.	C2-C1-H7= 87.3404
C1-C3-H7=122.5603	C2-C3-H7=150.416	C4-C1-H7=117.8872
C4-C3-H7=179.4911	C5-C1-H7=149.7699	C5-C3-H7=150.1308
C1-H7-C6= 67.2413	C2-C6-H7=142.9889	C6-C3-H7=119.8692
C4-C6-H7=115.4184	C5-C6-H7= 85.0403	C1-C2-H8= 87.3404
C3-C2-H8=117.8872	C1-C4-H8=150.416	C2-C4-H8=122.5603
C3-C4-H8=179.4911	C1-C5-H8=142.9889	C2-H8-C5= 67.2413
C3-C5-H8=115.4184	C5-C4-H8=119.8692	C6-C2-H8=149.7699
C6-C4-H8=150.1308	C6-C5-H8= 85.0403	C2-C1-H9= 87.3404
C3-C1-H9=149.7699	C1-H9-C4= 67.2413	C2-C4-H9=142.9889
C3-C4-H9= 85.0403	C1-C5-H9=122.5603	C2-C5-H9=150.416
C3-C5-H9=150.1308	C4-C5-H9=119.8692	C6-C1-H9=117.8872
C6-C4-H9=115.4184	C6-C5-H9=179.4911	H7-C1-H9=174.6807
C1-H9-H8= 92.6596	C2-H8-H9= 92.6596	H8-C4-H9= 94.4508
H8-C5-H9= 94.4508	C1-C2-H10= 87.3404	C1-C3-H10=142.9889
C2-H10-C3= 67.2413	C4-C2-H10=149.7699	C4-C3-H10= 85.0403
C5-C2-H10=117.8872	C5-C3-H10=115.4184	C1-C6-H10=150.416
C2-C6-H10=122.5603	C3-C6-H10=119.8692	C4-C6-H10=150.1308
C5-C6-H10=179.4911	C1-H7-H10= 92.6596	C2-H10-H7= 92.6596
H7-C3-H10= 94.4508	H7-C6-H10= 94.4508	H8-C2-H10=174.6807

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Population analysis using the SCF density.

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Orbital Symmetries:

Occupied (B3G) (B2U) (B1U) (AG) (B1U) (AG) (AG) (B1U) (B2U)
(B3G) (AG) (B1U) (B2U) (B3G) (B2G) (B3U) (B1G)
(AG) (B2U) (B1U) (AG)

Virtual (B1U) (B3G) (B3U) (AG) (B2U) (B1U) (B2G) (B3G)
(AU) (AG) (B2U) (B1U) (B3G) (AG) (B2U) (B3U) (B3G)
(B2G) (B1G) (B1U) (AG) (AU) (B3U) (AG) (B1U) (B2G)
(B2U) (B1U) (B3G) (AG) (B2U) (B3G) (B2U) (AG)
(B1U) (B3G) (B1U) (B2U) (B3G) (AG) (B1U)

The electronic state is 3-B1U.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.198962D+01				
2	0.000000D+00	0.198883D+01			
3	0.000000D+00	0.000000D+00	0.100049D+01		
4	-0.451986D-04	0.000000D+00	0.000000D+00	0.999300D+00	
5	0.000000D+00	0.000000D+00	0.281844D-04	0.000000D+00	0.106157D-01
6	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00

	6
6	0.111480D-01

Test job not archived.

1\1\GINC-C4-32\SP\CASSCF\3-21G\C6H4(3)\MSCHOTT\24-May-1997\0\\#P CAS(6
,6)/3-21G GEOM=CHECK GUESS=READ SCF=(CONVER=6) # GFINPUT IOP(6/7=3)\\p
-benzyne, ring opening\\0,3\C,0.,0.,1.3424680767\C,0.,0.,-1.3424680767
\C,0.,1.211270894,0.7100253893\C,0.,-1.211270894,-0.7100253893\C,0.,-1
.211270894,0.7100253893\C,0.,1.211270894,-0.7100253893\H,0.,2.13944341
72,1.2430844704\H,0.,-2.1394434172,-1.2430844704\H,0.,-2.1394434172,1.
2430844704\H,0.,2.1394434172,-1.2430844704\\Version=DEC-AXP-OSF/1-G94R
evC.3\State=3-B1U\HF=-228.1402493\RMSD=0.000e+00\Dipole=0.,0.,0.\PG=D0
2H [C2"(C1.C1),SG(C4H4)]\\@

MP2=-228.5598879

Triplet
p-Benzyne, CAS(6,6)/3-21g (triplet geometry)
(benzyne1.t.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.659358	0.000000			
3	C	1.373250	2.372454	0.000000		
4	C	2.372454	1.373250	2.820730	0.000000	
5	C	1.373250	2.372454	2.444546	1.407379	0.000000
6	C	2.372454	1.373250	1.407379	2.444546	2.820730
7	H	2.141090	3.355621	1.070505	3.891098	3.406997
8	H	3.355621	2.141090	3.891098	1.070505	2.163099
9	H	2.141090	3.355621	3.406997	2.163099	1.070505
10	H	3.355621	2.141090	2.163099	3.406997	3.891098

		6	7	8	9	10
6	C	0.000000				
7	H	2.163099	0.000000			
8	H	3.406997	4.961525	0.000000		
9	H	3.891098	4.279588	2.510351	0.000000	
10	H	1.070505	2.510351	4.279588	4.961525	0.000000

Interatomic angles:

C1-C3-C2= 86.109	C1-C4-C2= 86.109	C3-C1-C4= 93.891
C3-C2-C4= 93.891	C1-C5-C2= 86.109	C3-C1-C5=125.7613
C3-C2-C5= 62.0208	C1-C5-C4=117.1194	C2-C4-C5=117.1194
C3-C5-C4= 90.	C1-C6-C2= 86.109	C1-C3-C6=117.1194
C2-C6-C3=117.1194	C4-C1-C6= 62.0208	C4-C2-C6=125.7613
C3-C6-C4= 90.	C5-C1-C6= 93.891	C5-C2-C6= 93.891
C5-C3-C6= 90.	C5-C4-C6= 90.	C2-C1-H7= 88.0059
C1-C3-H7=121.8722	C2-C3-H7=152.0188	C4-C1-H7=119.0163
C4-C3-H7=178.9215	C5-C1-H7=150.8865	C5-C3-H7=148.9916
C1-H7-C6= 66.896	C2-C6-H7=142.2175	C6-C3-H7=121.0084
C4-C6-H7=115.0981	C5-C6-H7= 85.1681	C1-C2-H8= 88.0059
C3-C2-H8=119.0163	C1-C4-H8=152.0188	C2-C4-H8=121.8722
C3-C4-H8=178.9215	C1-C5-H8=142.2175	C2-H8-C5= 66.896
C3-C5-H8=115.0981	C5-C4-H8=121.0084	C6-C2-H8=150.8865
C6-C4-H8=148.9916	C6-C5-H8= 85.1681	C2-C1-H9= 88.0059
C3-C1-H9=150.8865	C1-H9-C4= 66.896	C2-C4-H9=142.2175
C3-C4-H9= 85.1681	C1-C5-H9=121.8722	C2-C5-H9=152.0188
C3-C5-H9=148.9916	C4-C5-H9=121.0084	C6-C1-H9=119.0163
C6-C4-H9=115.0981	C6-C5-H9=178.9215	H7-C1-H9=176.0117
C1-H9-H8= 91.9941	C2-H8-H9= 91.9941	H8-C4-H9= 95.9103
H8-C5-H9= 95.9103	C1-C2-H10= 88.0059	C1-C3-H10=142.2175
C2-H10-C3= 66.896	C4-C2-H10=150.8865	C4-C3-H10= 85.1681
C5-C2-H10=119.0163	C5-C3-H10=115.0981	C1-C6-H10=152.0188
C2-C6-H10=121.8722	C3-C6-H10=121.0084	C4-C6-H10=148.9916
C5-C6-H10=178.9215	C1-H7-H10= 91.9941	C2-H10-H7= 91.9941
H7-C3-H10= 95.9103	H7-C6-H10= 95.9103	H8-C2-H10=176.0117

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Population analysis using the SCF density.

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Orbital Symmetries:

Occupied (B3G) (B2U) (B1U) (AG) (B1U) (AG) (AG) (B1U) (B2U)
(B3G) (AG) (B1U) (B2U) (B3G) (B2G) (B3U) (B1G)
(AG) (B3G) (AG) (B1U)

Virtual (B1U) (B2U) (B3U) (AG) (B2U) (B1U) (B2G) (B3G)
(AU) (AG) (B2U) (B1U) (B3G) (AG) (B2U) (B3U) (B3G)
(B2G) (B1G) (B1U) (AG) (AU) (B3U) (AG) (B1U) (B2G)
(B2U) (B1U) (B3G) (AG) (B2U) (B3G) (B2U) (AG)
(B1U) (B3G) (B1U) (B2U) (B3G) (AG) (B1U)

The electronic state is 3-B1U.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.199005D+01				
2	0.000000D+00	0.106359D-01			
3	0.140414D-04	0.000000D+00	0.999353D+00		
4	0.000000D+00	0.000000D+00	0.000000D+00	0.100044D+01	
5	0.000000D+00	0.000000D+00	0.000000D+00	0.824192D-05	0.101595D-01
6	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00

	6
6	0.198936D+01

Zero-point correction= 0.080758 (Hartree/Particle)
Thermal correction to Energy= 0.084710
Thermal correction to Enthalpy= 0.085654
Thermal correction to Gibbs Free Energy= 0.053902
Sum of electronic and zero-point Energies= -228.060168
Sum of electronic and thermal Energies= -228.056216
Sum of electronic and thermal Enthalpies= -228.055272
Sum of electronic and thermal Free Energies= -228.087024

Test job not archived.
1\1\GINC-C4-32\Freq\CASSCF\3-21G\C6H4(3)\MSCHOTT\24-May-1997\0\\#P CAS
(6,6)/3-21G FREQ GEOM=CHECK GUESS=READ SCF=(CONVER=6) # GFINPUT IOP(6/
7=3)\\p-benzyne, ring opening\\0,3\C,0.,0.,1.3296790566\C,0.,0.,-1.329
6790566\C,0.,1.2222729866,0.703689368\C,0.,-1.2222729866,-0.703689368\
C,0.,-1.2222729866,0.703689368\C,0.,1.2222729866,-0.703689368\H,0.,2.1
397938416,1.2551753335\H,0.,-2.1397938416,-1.2551753335\H,0.,-2.139793
8416,1.2551753335\H,0.,2.1397938416,-1.2551753335\\Version=DEC-AXP-OSF
/1-G94RevC.3\State=3-B1U\HF=-228.140926\RMSD=0.000e+00\RMSF=1.125e-04\
PG=D02H [C2"(C1.C1),SG(C4H4)]\NImag=0

MP2=-228.5615452

Triplet
p-Benzyne, CAS(6,6)/6-31g* (singlet geometry)
(benzyne1.t.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.684936	0.000000			
3	C	1.366441	2.383255	0.000000		
4	C	2.383255	1.366441	2.808069	0.000000	
5	C	1.366441	2.383255	2.422542	1.420051	0.000000
6	C	2.383255	1.366441	1.420051	2.422542	2.808069
7	H	2.141751	3.355935	1.070353	3.878392	3.392851
8	H	3.355935	2.141751	3.878392	1.070353	2.162439
9	H	2.141751	3.355935	3.392851	2.162439	1.070353
10	H	3.355935	2.141751	2.162439	3.392851	3.878392

		6	7	8	9	10
6	C	0.000000				
7	H	2.162439	0.000000			
8	H	3.392851	4.948728	0.000000		
9	H	3.878392	4.278887	2.486169	0.000000	
10	H	1.070353	2.486169	4.278887	4.948728	0.000000

Interatomic angles:

C1-C3-C2= 87.0237	C1-C4-C2= 87.0237	C3-C1-C4= 92.9763
C3-C2-C4= 92.9763	C1-C5-C2= 87.0237	C3-C1-C5=124.859
C3-C2-C5= 61.0936	C1-C5-C4=117.5705	C2-C4-C5=117.5705
C3-C5-C4= 90.	C1-C6-C2= 87.0237	C1-C3-C6=117.5705
C2-C6-C3=117.5705	C4-C1-C6= 61.0936	C4-C2-C6=124.859
C3-C6-C4= 90.	C5-C1-C6= 92.9763	C5-C2-C6= 92.9763
C5-C3-C6= 90.	C5-C4-C6= 90.	C2-C1-H7= 87.3404
C1-C3-H7=122.5603	C2-C3-H7=150.416	C4-C1-H7=117.8872
C4-C3-H7=179.4911	C5-C1-H7=149.7699	C5-C3-H7=150.1308
C1-H7-C6= 67.2413	C2-C6-H7=142.9889	C6-C3-H7=119.8692
C4-C6-H7=115.4184	C5-C6-H7= 85.0403	C1-C2-H8= 87.3404
C3-C2-H8=117.8872	C1-C4-H8=150.416	C2-C4-H8=122.5603
C3-C4-H8=179.4911	C1-C5-H8=142.9889	C2-H8-C5= 67.2413
C3-C5-H8=115.4184	C5-C4-H8=119.8692	C6-C2-H8=149.7699
C6-C4-H8=150.1308	C6-C5-H8= 85.0403	C2-C1-H9= 87.3404
C3-C1-H9=149.7699	C1-H9-C4= 67.2413	C2-C4-H9=142.9889
C3-C4-H9= 85.0403	C1-C5-H9=122.5603	C2-C5-H9=150.416
C3-C5-H9=150.1308	C4-C5-H9=119.8692	C6-C1-H9=117.8872
C6-C4-H9=115.4184	C6-C5-H9=179.4911	H7-C1-H9=174.6807
C1-H9-H8= 92.6596	C2-H8-H9= 92.6596	H8-C4-H9= 94.4508
H8-C5-H9= 94.4508	C1-C2-H10= 87.3404	C1-C3-H10=142.9889
C2-H10-C3= 67.2413	C4-C2-H10=149.7699	C4-C3-H10= 85.0403
C5-C2-H10=117.8872	C5-C3-H10=115.4184	C1-C6-H10=150.416
C2-C6-H10=122.5603	C3-C6-H10=119.8692	C4-C6-H10=150.1308
C5-C6-H10=179.4911	C1-H7-H10= 92.6596	C2-H10-H7= 92.6596
H7-C3-H10= 94.4508	H7-C6-H10= 94.4508	H8-C2-H10=174.6807

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Population analysis using the SCF density.

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Orbital Symmetries:

Occupied (B3G) (B2U) (B1U) (AG) (B1U) (AG) (AG) (B1U) (B2U)
(B3G) (AG) (B1U) (B2U) (B3G) (B2G) (B3U) (B1G)
(AG) (B3G) (AG) (B1U)

Virtual (B1U) (B2U) (B3U) (AG) (B2U) (B1U) (B2G) (B3G)
(AU) (AG) (B2U) (B1U) (B3G) (AG) (B2U) (B3U) (B3G)
(B2G) (B1G) (B1U) (AG) (AU) (B3U) (AG) (B1U) (B2G)
(B2U) (B1U) (B3G) (AG) (B2U) (B3G) (B2U) (AG)
(B1U) (B3G) (B1U) (B2U) (B3G) (AG) (B1U) (AG)
(B3G) (AG) (AG) (B2G) (B3G) (AG) (AG) (AG) (AG)
(B1G) (B2G) (B3G) (B1U) (B2U) (B1U) (B1U) (B3U)
(B2U) (B1U) (B1U) (B1U) (AU) (B3U) (B2U) (B3G)
(B3G) (B1G) (B2U) (B2U) (B1U) (B1G) (B2G) (AU)
(AU) (B3U)

The electronic state is 3-B1U.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.198995D+01				
2	0.000000D+00	0.107682D-01			
3	-0.177200D-04	0.000000D+00	0.999383D+00		
4	0.000000D+00	0.000000D+00	0.000000D+00	0.100041D+01	
5	0.000000D+00	0.000000D+00	0.000000D+00	0.494940D-05	0.102822D-01
6	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00

	6
6	0.198920D+01

Test job not archived.
1\1\GINC-C4-31\SP\CASSCF\6-31G(d)\C6H4(3)\MSCHOTT\24-May-1997\0\\#P CA
S(6,6)/6-31G* GEOM=CHECK GUESS=READ SCF=(CONVER=6) # GFINPUT IOP(6/7=3
)\\p-benzyne, ring opening\\0,3\C,0.,0.,1.3424680767\C,0.,0.,-1.342468
0767\C,0.,1.211270894,0.7100253893\C,0.,-1.211270894,-0.7100253893\C,0
.,-1.211270894,0.7100253893\C,0.,1.211270894,-0.7100253893\H,0.,2.1394
434172,1.2430844704\H,0.,-2.1394434172,-1.2430844704\H,0.,-2.139443417
2,1.2430844704\H,0.,2.1394434172,-1.2430844704\\Version=DEC-AXP-OSF/1-
G94RevC.3\State=3-B1U\HF=-229.4209942\RMSD=0.000e+00\Dipole=0.,0.,0.\P
G=D02H [C2*(C1.C1),SG(C4H4)]\\@

MP2=-230.0929887

Triplet
p-Benzyne, CAS(6,6)/6-31g* (triplet geometry)
(benzyne1.t.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.659358	0.000000			
3	C	1.373250	2.372454	0.000000		
4	C	2.372454	1.373250	2.820730	0.000000	
5	C	1.373250	2.372454	2.444546	1.407379	0.000000
6	C	2.372454	1.373250	1.407379	2.444546	2.820730
7	H	2.141090	3.355621	1.070505	3.891098	3.406997
8	H	3.355621	2.141090	3.891098	1.070505	2.163099
9	H	2.141090	3.355621	3.406997	2.163099	1.070505
10	H	3.355621	2.141090	2.163099	3.406997	3.891098

		6	7	8	9	10
6	C	0.000000				
7	H	2.163099	0.000000			
8	H	3.406997	4.961525	0.000000		
9	H	3.891098	4.279588	2.510351	0.000000	
10	H	1.070505	2.510351	4.279588	4.961525	0.000000

Interatomic angles:

C1-C3-C2= 86.109	C1-C4-C2= 86.109	C3-C1-C4= 93.891
C3-C2-C4= 93.891	C1-C5-C2= 86.109	C3-C1-C5=125.7613
C3-C2-C5= 62.0208	C1-C5-C4=117.1194	C2-C4-C5=117.1194
C3-C5-C4= 90.	C1-C6-C2= 86.109	C1-C3-C6=117.1194
C2-C6-C3=117.1194	C4-C1-C6= 62.0208	C4-C2-C6=125.7613
C3-C6-C4= 90.	C5-C1-C6= 93.891	C5-C2-C6= 93.891
C5-C3-C6= 90.	C5-C4-C6= 90.	C2-C1-H7= 88.0059
C1-C3-H7=121.8722	C2-C3-H7=152.0188	C4-C1-H7=119.0163
C4-C3-H7=178.9215	C5-C1-H7=150.8865	C5-C3-H7=148.9916
C1-H7-C6= 66.896	C2-C6-H7=142.2175	C6-C3-H7=121.0084
C4-C6-H7=115.0981	C5-C6-H7= 85.1681	C1-C2-H8= 88.0059
C3-C2-H8=119.0163	C1-C4-H8=152.0188	C2-C4-H8=121.8722
C3-C4-H8=178.9215	C1-C5-H8=142.2175	C2-H8-C5= 66.896
C3-C5-H8=115.0981	C5-C4-H8=121.0084	C6-C2-H8=150.8865
C6-C4-H8=148.9916	C6-C5-H8= 85.1681	C2-C1-H9= 88.0059
C3-C1-H9=150.8865	C1-H9-C4= 66.896	C2-C4-H9=142.2175
C3-C4-H9= 85.1681	C1-C5-H9=121.8722	C2-C5-H9=152.0188
C3-C5-H9=148.9916	C4-C5-H9=121.0084	C6-C1-H9=119.0163
C6-C4-H9=115.0981	C6-C5-H9=178.9215	H7-C1-H9=176.0117
C1-H9-H8= 91.9941	C2-H8-H9= 91.9941	H8-C4-H9= 95.9103
H8-C5-H9= 95.9103	C1-C2-H10= 88.0059	C1-C3-H10=142.2175
C2-H10-C3= 66.896	C4-C2-H10=150.8865	C4-C3-H10= 85.1681
C5-C2-H10=119.0163	C5-C3-H10=115.0981	C1-C6-H10=152.0188
C2-C6-H10=121.8722	C3-C6-H10=121.0084	C4-C6-H10=148.9916
C5-C6-H10=178.9215	C1-H7-H10= 91.9941	C2-H10-H7= 91.9941
H7-C3-H10= 95.9103	H7-C6-H10= 95.9103	H8-C2-H10=176.0117

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Population analysis using the SCF density.

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Orbital Symmetries:

Occupied (B3G) (B2U) (B1U) (AG) (B1U) (AG) (AG) (B1U) (B2U)
(B3G) (AG) (B1U) (B2U) (B3G) (B2G) (B3U) (B1G)
(AG) (B3G) (AG) (B1U)

Virtual (B1U) (B2U) (B3U) (AG) (B2U) (B1U) (B2G) (B3G)
(AU) (AG) (B2U) (B1U) (B3G) (AG) (B2U) (B3U) (B3G)
(B2G) (B1G) (B1U) (AG) (AU) (B3U) (AG) (B1U) (B2G)
(B2U) (B1U) (B3G) (AG) (B2U) (B3G) (B2U) (AG)
(B1U) (B3G) (B1U) (B2U) (B3G) (AG) (B1U) (AG)
(B3G) (AG) (AG) (B2G) (B3G) (AG) (AG) (AG) (AG)
(B1G) (B2G) (B3G) (B1U) (B2U) (B1U) (B1U) (B3U)
(B2U) (B1U) (B1U) (B1U) (AU) (B3U) (B2U) (B3G)
(B3G) (B1G) (B2U) (B2U) (B1U) (B1G) (B2G) (AU)
(AU) (B3U)

The electronic state is 3-B1U.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.199038D+01				
2	0.000000D+00	0.102664D-01			
3	-0.222114D-04	0.000000D+00	0.999428D+00		
4	0.000000D+00	0.000000D+00	0.000000D+00	0.100036D+01	
5	0.000000D+00	0.000000D+00	0.000000D+00	0.516041D-05	0.983261D-02
6	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00

	6
6	0.198972D+01

Test job not archived.
1\1\GINC-C4-32\SP\CASSCF\6-31G(d)\C6H4(3)\MSCHOTT\24-May-1997\0\\#P CA
S(6,6)/6-31G* GEOM=CHECK GUESS=READ SCF=(CONVER=6) # GFINPUT IOP(6/7=3
)\\p-benzyne, ring opening\\0,3\C,0.,0.,1.3296790566\C,0.,0.,-1.329679
0566\C,0.,1.2222729866,0.703689368\C,0.,-1.2222729866,-0.703689368\C,0
.,-1.2222729866,0.703689368\C,0.,1.2222729866,-0.703689368\H,0.,2.1397
938416,1.2551753335\H,0.,-2.1397938416,-1.2551753335\H,0.,-2.139793841
6,1.2551753335\H,0.,2.1397938416,-1.2551753335\\Version=DEC-AXP-OSF/1-
G94RevC.3\State=3-B1U\HF=-229.4217876\RMSD=0.000e+00\Dipole=0.,0.,0.\P
G=D02H [C2*(C1.C1),SG(C4H4)]\\@

MP2=-230.095204

Ene-diyne, CAS(6,6)/3-21g optimized
(benzyne3.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.945227	0.000000			
3	C	1.199651	3.770882	0.000000		
4	C	2.443672	1.425816	3.563038	0.000000	
5	C	1.425816	2.443672	2.625324	1.337276	0.000000
6	C	3.770882	1.199651	4.339357	2.625324	3.563038
7	H	2.250364	4.626509	1.050728	4.575222	3.676045
8	H	3.400127	2.133723	4.565242	1.072468	2.081393
9	H	2.133723	3.400127	3.242847	2.081393	1.072468
10	H	4.626509	2.250364	5.017895	3.676045	4.575222

		6	7	8	9	10
6	C	0.000000				
7	H	5.017895	0.000000			
8	H	3.242847	5.596434	0.000000		
9	H	4.565242	4.256582	2.379472	0.000000	
10	H	1.050728	5.548112	4.256582	5.596434	0.000000

Interatomic angles:

C2-C1-C3=125.5249	C1-C4-C2= 95.5164	C3-C1-C4=154.3324
C1-C5-C2= 95.5164	C3-C1-C5=178.799	C2-C5-C3= 96.0651
C1-C5-C4=124.3239	C2-C4-C5=124.3239	C3-C5-C4=124.8727
C1-C2-C6=125.5249	C1-C4-C6= 96.0651	C4-C2-C6=178.799
C5-C2-C6=154.3324	C5-C4-C6=124.8727	C2-C1-H7=125.3328
C1-C3-H7=179.5886	C4-C1-H7=154.1404	C5-C1-H7=178.991
C5-C3-H7=179.7591	C1-C2-H8= 82.3816	C1-C4-H8=147.8781
C2-C4-H8=116.6055	C1-C5-H8=151.0902	C2-H8-C5= 70.8521
C3-C5-H8=151.6389	C5-C4-H8=119.0706	C6-C2-H8=152.0935
C6-C4-H8=116.0567	C2-C1-H9= 82.3816	C3-C1-H9=152.0935
C1-H9-C4= 70.8521	C2-C4-H9=151.0902	C1-C5-H9=116.6055
C2-C5-H9=147.8781	C3-C5-H9=116.0567	C4-C5-H9=119.0706
C6-C4-H9=151.6389	H7-C1-H9=152.2855	C1-H9-H8= 97.6184
C2-H8-H9= 97.6184	H8-C4-H9= 92.3043	H8-C5-H9= 92.3043
C1-C2-H10=125.3328	C4-C2-H10=178.991	C5-C2-H10=154.1404
C2-C6-H10=179.5886	C4-C6-H10=179.7591	H8-C2-H10=152.2855

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Population analysis using the SCF density.

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Orbital Symmetries:

Occupied	(B2)	(A1)	(B2)	(A1)	(B2)	(A1)	(A1)	(B2)	(A1)	(B2)
	(A1)	(B2)	(A1)	(B2)	(B1)	(B1)	(A2)	(A1)	(A1)	(B2)
Virtual	(A1)	(B2)	(B2)	(B1)	(B2)	(A1)	(B2)	(A2)	(A1)	(A2)
	(A1)	(B2)	(A1)	(B2)	(A1)	(B1)	(B2)	(A1)	(A2)	(B1)
	(B2)	(A1)	(A2)	(A1)	(B1)	(A2)	(B2)	(B2)	(A1)	(B2)
	(B2)	(A1)	(A1)	(B2)	(A1)	(B2)	(A1)	(B2)	(A1)	(B2)
	(A1)	(B2)								

The electronic state is 1-A1.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.199178D+01				
2	0.244003D-05	0.194072D+01			
3	0.000000D+00	0.000000D+00	0.193722D+01		
4	-0.162264D-04	0.229757D-06	0.000000D+00	0.614825D-01	
5	0.000000D+00	0.000000D+00	0.432709D-06	0.000000D+00	0.606855D-01
6	0.000000D+00	0.000000D+00	0.545803D-05	0.000000D+00	0.218523D-05

	6
6	0.811600D-02

Zero-point correction= 0.076027 (Hartree/Particle)
Thermal correction to Energy= 0.081965
Thermal correction to Enthalpy= 0.082909
Thermal correction to Gibbs Free Energy= 0.047184
Sum of electronic and zero-point Energies= -228.093172
Sum of electronic and thermal Energies= -228.087234
Sum of electronic and thermal Enthalpies= -228.086290
Sum of electronic and thermal Free Energies= -228.122016

Test job not archived.
1\1\GINC-C4-32\Freq\CASSCF\3-21G\C6H4\MSCHOTT\22-May-1997\0\\#P CAS(6,
6)/3-21G FREQ GEOM=CHECK GUESS=READ SCF=(CONVER=6) # GFINPUT IOP(6/7=3
)\\p-benzyne, ring opening\\0,1\C,0.,1.4726133372,-0.074304751\C,0.,-1
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79996,1.1032243776\C,0.,0.6686379996,1.1032243776\C,0.,-2.1696786672,-
1.0506560846\H,0.,2.7740558398,-1.9101656044\H,0.,-1.1897361799,2.0405
84353\H,0.,1.1897361799,2.040584353\H,0.,-2.7740558398,-1.9101656044\\
Version=DEC-AXP-OSF/1-G94RevC.3\State=1-A1\HF=-228.1691992\RMSD=0.000e
+00\RMSP=7.385e-05\PG=C02V [SGV(C6H4)]\NImag=0

MP2=-228.5707064

Ene-diyne, CAS(6,6)/6-31g* (3-21g geometry)
(benzyne3.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.945227	0.000000			
3	C	1.199651	3.770882	0.000000		
4	C	2.443672	1.425816	3.563038	0.000000	
5	C	1.425816	2.443672	2.625324	1.337276	0.000000
6	C	3.770882	1.199651	4.339357	2.625324	3.563038
7	H	2.250364	4.626509	1.050728	4.575222	3.676045
8	H	3.400127	2.133723	4.565242	1.072468	2.081393
9	H	2.133723	3.400127	3.242847	2.081393	1.072468
10	H	4.626509	2.250364	5.017895	3.676045	4.575222

		6	7	8	9	10
6	C	0.000000				
7	H	5.017895	0.000000			
8	H	3.242847	5.596434	0.000000		
9	H	4.565242	4.256582	2.379472	0.000000	
10	H	1.050728	5.548112	4.256582	5.596434	0.000000

Interatomic angles:

C2-C1-C3=125.5249	C1-C4-C2= 95.5164	C3-C1-C4=154.3324
C1-C5-C2= 95.5164	C3-C1-C5=178.799	C2-C5-C3= 96.0651
C1-C5-C4=124.3239	C2-C4-C5=124.3239	C3-C5-C4=124.8727
C1-C2-C6=125.5249	C1-C4-C6= 96.0651	C4-C2-C6=178.799
C5-C2-C6=154.3324	C5-C4-C6=124.8727	C2-C1-H7=125.3328
C1-C3-H7=179.5886	C4-C1-H7=154.1404	C5-C1-H7=178.991
C5-C3-H7=179.7591	C1-C2-H8= 82.3816	C1-C4-H8=147.8781
C2-C4-H8=116.6055	C1-C5-H8=151.0902	C2-H8-C5= 70.8521
C3-C5-H8=151.6389	C5-C4-H8=119.0706	C6-C2-H8=152.0935
C6-C4-H8=116.0567	C2-C1-H9= 82.3816	C3-C1-H9=152.0935
C1-H9-C4= 70.8521	C2-C4-H9=151.0902	C1-C5-H9=116.6055
C2-C5-H9=147.8781	C3-C5-H9=116.0567	C4-C5-H9=119.0706
C6-C4-H9=151.6389	H7-C1-H9=152.2855	C1-H9-H8= 97.6184
C2-H8-H9= 97.6184	H8-C4-H9= 92.3043	H8-C5-H9= 92.3043
C1-C2-H10=125.3328	C4-C2-H10=178.991	C5-C2-H10=154.1404
C2-C6-H10=179.5886	C4-C6-H10=179.7591	H8-C2-H10=152.2855

****

Population analysis using the SCF density.

****

Orbital Symmetries:

Occupied	(B2)	(A1)	(B2)	(A1)	(B2)	(A1)	(A1)	(B2)	(A1)	(B2)
	(A1)	(B2)	(A1)	(B2)	(B1)	(B1)	(A2)	(A1)	(A1)	(B2)
Virtual	(A1)	(B2)	(B2)	(B1)	(B2)	(A1)	(B2)	(A2)	(A1)	(A2)
	(A1)	(B2)	(A1)	(B2)	(A1)	(B1)	(B2)	(A1)	(A2)	(B1)
	(B2)	(A1)	(A2)	(A1)	(B1)	(A2)	(B2)	(B2)	(A1)	(B2)
	(B2)	(A1)	(A1)	(B2)	(A1)	(B2)	(A1)	(B2)	(A1)	(B2)
	(A1)	(B2)	(A1)	(A2)	(A1)	(A1)	(A1)	(A1)	(A1)	(A1)
	(A1)	(A2)	(A2)	(A1)	(B2)	(B1)	(B2)	(B2)	(B2)	(B2)
	(B2)	(B2)	(B2)	(B1)	(B1)	(B2)	(A1)	(A1)	(A1)	(A2)
	(A2)	(B2)	(B2)	(A2)	(B1)	(B1)	(B2)	(B1)		

The electronic state is 1-A1.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.199204D+01				
2	-0.322960D-04	0.591453D-01			
3	0.000000D+00	0.000000D+00	0.193957D+01		
4	0.145923D-05	0.879450D-04	0.000000D+00	0.194320D+01	
5	0.000000D+00	0.000000D+00	0.489858D-04	0.000000D+00	0.581810D-01
6	0.000000D+00	0.000000D+00	-0.186030D-04	0.000000D+00	-0.252937D-05

	6
6	0.786399D-02

Test job not archived.
1\1\GINC-C4-31\SP\CASSCF\6-31G(d)\C6H4\MSCHOTT\23-May-1997\0\\#P CAS(6
,6)/6-31G* GEOM=CHECK GUESS=READ SCF=(CONVER=6) # GFINPUT IOP(6/7=3)\\
p-benzyne, ring opening\\0,1\C,0.,1.4726133372,-0.074304751\C,0.,-1.47
26133372,-0.074304751\C,0.,2.1696786672,-1.0506560846\C,0.,-0.66863799
96,1.1032243776\C,0.,0.6686379996,1.1032243776\C,0.,-2.1696786672,-1.0
506560846\H,0.,2.7740558398,-1.9101656044\H,0.,-1.1897361799,2.0405843
53\H,0.,1.1897361799,2.040584353\H,0.,-2.7740558398,-1.9101656044\\Ver
sion=DEC-AXP-OSF/1-G94RevC.3\State=1-A1\HF=-229.4395568\RMSD=0.000e+00
\Dipole=0.,0.,0.052067\PG=C02V [SGV(C6H4)]\\@

MP2=-230.0953024

TS Ene-diyne, CAS(6,6)/3-21g optimized
(benzyne2.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.740961	0.000000			
3	C	1.263521	2.635686	0.000000		
4	C	2.398355	1.411034	2.947611	0.000000	
5	C	1.411034	2.398355	2.451513	1.372180	0.000000
6	C	2.635686	1.263521	1.952000	2.451513	2.947611
7	H	2.207196	3.472027	1.060121	3.977640	3.496503
8	H	3.371582	2.169366	4.014819	1.069831	2.116454
9	H	2.169366	3.371582	3.372652	2.116454	1.069831
10	H	3.472027	2.207196	2.497895	3.496503	3.977640

		6	7	8	9	10
6	C	0.000000				
7	H	2.497895	0.000000			
8	H	3.372652	5.047441	0.000000		
9	H	4.014819	4.371212	2.430322	0.000000	
10	H	1.060121	2.620709	4.371212	5.047441	0.000000

Interatomic angles:

C1-C3-C2= 81.0999	C1-C4-C2= 88.0504	C3-C1-C4=102.7716
C3-C2-C4= 88.0781	C1-C5-C2= 88.0504	C3-C1-C5=132.7934
C2-C5-C3= 65.8277	C1-C5-C4=119.0143	C2-C4-C5=119.0143
C3-C5-C4= 96.7915	C1-C6-C2= 81.0999	C1-C3-C6=108.1923
C2-C6-C3=108.1923	C1-C4-C6= 65.8277	C4-C2-C6=132.7934
C3-C6-C4= 83.2085	C5-C1-C6= 88.0781	C5-C2-C6=102.7716
C5-C3-C6= 83.2085	C5-C4-C6= 96.7915	C2-C1-H7= 88.439
C1-C3-H7=143.4232	C2-C3-H7=135.477	C4-C1-H7=119.4029
C4-C3-H7=164.0602	C5-C1-H7=149.4247	C5-C3-H7=168.407
C1-H7-C6= 67.8111	C2-C6-H7=131.9422	C6-C3-H7=108.3845
C4-C6-H7=106.9583	C5-C6-H7= 79.4255	C1-C2-H8= 85.8943
C3-C2-H8=112.9867	C1-C4-H8=150.603	C2-C4-H8=121.3465
C3-C4-H8=175.3148	C1-C5-H8=145.0763	C2-H8-C5= 68.0437
C3-C5-H8=122.8536	C5-C4-H8=119.6392	C6-C2-H8=157.702
C6-C4-H8=143.5693	C6-C5-H8= 81.7377	C2-C1-H9= 85.8943
C3-C1-H9=157.702	C1-H9-C4= 68.0437	C2-C4-H9=145.0763
C3-C4-H9= 81.7377	C1-C5-H9=121.3465	C2-C5-H9=150.603
C3-C5-H9=143.5693	C4-C5-H9=119.6392	C6-C1-H9=112.9867
C6-C4-H9=122.8536	C6-C5-H9=175.3148	H7-C1-H9=174.3333
C1-H9-H8= 94.1057	C2-H8-H9= 94.1057	H8-C4-H9= 93.5772
H8-C5-H9= 93.5772	C1-C2-H10= 88.439	C1-C3-H10=131.9422
C2-H10-C3= 67.8111	C4-C2-H10=149.4247	C4-C3-H10= 79.4255
C5-C2-H10=119.4029	C5-C3-H10=106.9583	C1-C6-H10=135.477
C2-C6-H10=143.4232	C3-C6-H10=108.3845	C4-C6-H10=168.407
C5-C6-H10=164.0602	C1-H7-H10= 91.561	C2-H10-H7= 91.561
H7-C3-H10= 84.6347	H7-C6-H10= 84.6347	H8-C2-H10=174.3333

****

Population analysis using the SCF density.

****

Orbital Symmetries:

Occupied	(B2)	(A1)	(B2)	(A1)	(B2)	(A1)	(A1)	(B2)	(A1)	(B2)
	(A1)	(B2)	(A1)	(B2)	(A2)	(B1)	(B1)	(A1)	(A1)	(B2)
Virtual	(A1)	(B2)	(B2)	(B1)	(A1)	(A1)	(B2)	(A2)	(B2)	(A2)
	(A1)	(A1)	(B2)	(B2)	(A1)	(A1)	(B1)	(B2)	(A2)	(B1)
	(B2)	(A1)	(A2)	(B1)	(A1)	(B2)	(A2)	(A1)	(B2)	(B2)
	(A1)	(A1)	(B2)	(A1)	(A1)	(B2)	(B2)	(B2)	(A1)	(B2)
	(A1)	(B2)								

The electronic state is 1-A1.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.199036D+01				
2	0.299234D-06	0.193642D+01			
3	0.000000D+00	0.000000D+00	0.169587D+01		
4	-0.803684D-06	-0.603732D-04	0.000000D+00	0.306075D+00	
5	0.000000D+00	0.000000D+00	0.431716D-05	0.000000D+00	0.935712D-02
6	0.000000D+00	0.000000D+00	-0.306780D-04	0.000000D+00	-0.195693D-06

	6
6	0.619166D-01

Zero-point correction= 0.075867 (Hartree/Particle)
Thermal correction to Energy= 0.080221
Thermal correction to Enthalpy= 0.081166
Thermal correction to Gibbs Free Energy= 0.049098
Sum of electronic and zero-point Energies= -228.029040
Sum of electronic and thermal Energies= -228.024686
Sum of electronic and thermal Enthalpies= -228.023742
Sum of electronic and thermal Free Energies= -228.055809

Test job not archived.
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MP2=-228.5214143

TS Ene-diyne, CAS(6,6)/6-31g* (3-21g geometry)
(benzyne2.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.740961	0.000000			
3	C	1.263521	2.635686	0.000000		
4	C	2.398355	1.411034	2.947611	0.000000	
5	C	1.411034	2.398355	2.451513	1.372180	0.000000
6	C	2.635686	1.263521	1.952000	2.451513	2.947611
7	H	2.207196	3.472027	1.060121	3.977640	3.496503
8	H	3.371582	2.169366	4.014819	1.069831	2.116454
9	H	2.169366	3.371582	3.372652	2.116454	1.069831
10	H	3.472027	2.207196	2.497895	3.496503	3.977640

		6	7	8	9	10
6	C	0.000000				
7	H	2.497895	0.000000			
8	H	3.372652	5.047441	0.000000		
9	H	4.014819	4.371212	2.430322	0.000000	
10	H	1.060121	2.620709	4.371212	5.047441	0.000000

Interatomic angles:

C1-C3-C2= 81.0999	C1-C4-C2= 88.0504	C3-C1-C4=102.7716
C3-C2-C4= 88.0781	C1-C5-C2= 88.0504	C3-C1-C5=132.7934
C2-C5-C3= 65.8277	C1-C5-C4=119.0143	C2-C4-C5=119.0143
C3-C5-C4= 96.7915	C1-C6-C2= 81.0999	C1-C3-C6=108.1923
C2-C6-C3=108.1923	C1-C4-C6= 65.8277	C4-C2-C6=132.7934
C3-C6-C4= 83.2085	C5-C1-C6= 88.0781	C5-C2-C6=102.7716
C5-C3-C6= 83.2085	C5-C4-C6= 96.7915	C2-C1-H7= 88.439
C1-C3-H7=143.4232	C2-C3-H7=135.477	C4-C1-H7=119.4029
C4-C3-H7=164.0602	C5-C1-H7=149.4247	C5-C3-H7=168.407
C1-H7-C6= 67.8111	C2-C6-H7=131.9422	C6-C3-H7=108.3845
C4-C6-H7=106.9583	C5-C6-H7= 79.4255	C1-C2-H8= 85.8943
C3-C2-H8=112.9867	C1-C4-H8=150.603	C2-C4-H8=121.3465
C3-C4-H8=175.3148	C1-C5-H8=145.0763	C2-H8-C5= 68.0437
C3-C5-H8=122.8536	C5-C4-H8=119.6392	C6-C2-H8=157.702
C6-C4-H8=143.5693	C6-C5-H8= 81.7377	C2-C1-H9= 85.8943
C3-C1-H9=157.702	C1-H9-C4= 68.0437	C2-C4-H9=145.0763
C3-C4-H9= 81.7377	C1-C5-H9=121.3465	C2-C5-H9=150.603
C3-C5-H9=143.5693	C4-C5-H9=119.6392	C6-C1-H9=112.9867
C6-C4-H9=122.8536	C6-C5-H9=175.3148	H7-C1-H9=174.3333
C1-H9-H8= 94.1057	C2-H8-H9= 94.1057	H8-C4-H9= 93.5772
H8-C5-H9= 93.5772	C1-C2-H10= 88.439	C1-C3-H10=131.9422
C2-H10-C3= 67.8111	C4-C2-H10=149.4247	C4-C3-H10= 79.4255
C5-C2-H10=119.4029	C5-C3-H10=106.9583	C1-C6-H10=135.477
C2-C6-H10=143.4232	C3-C6-H10=108.3845	C4-C6-H10=168.407
C5-C6-H10=164.0602	C1-H7-H10= 91.561	C2-H10-H7= 91.561
H7-C3-H10= 84.6347	H7-C6-H10= 84.6347	H8-C2-H10=174.3333

****

Population analysis using the SCF density.

****

Orbital Symmetries:

Occupied	(B2)	(A1)	(B2)	(A1)	(B2)	(A1)	(A1)	(B2)	(A1)	(B2)
	(A1)	(B2)	(A1)	(B2)	(A2)	(B1)	(B1)	(A1)	(A1)	(A1)
Virtual	(B2)	(B2)	(B2)	(B1)	(A1)	(A1)	(B2)	(A2)	(B2)	(A2)
	(A1)	(A1)	(B2)	(B2)	(A1)	(A1)	(B1)	(B2)	(A2)	(B1)
	(B2)	(A1)	(A2)	(B1)	(A1)	(B2)	(A2)	(A1)	(B2)	(B2)
	(A1)	(A1)	(B2)	(A1)	(A1)	(B2)	(B2)	(B2)	(A1)	(B2)
	(A1)	(B2)	(A1)	(A1)	(A1)	(A1)	(A2)	(A1)	(A1)	(A1)
	(A1)	(A1)	(A2)	(A2)	(A1)	(B2)	(B2)	(B2)	(B2)	(B1)
	(B2)	(B2)	(B2)	(B2)	(B1)	(B1)	(B2)	(A1)	(B2)	(A1)
	(B2)	(A2)	(A2)	(B2)	(A2)	(B1)	(B1)	(B1)		

The electronic state is 1-A1.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.199064D+01				
2	-0.446172D-08	0.193601D+01			
3	0.473497D-04	-0.640988D-05	0.305063D+00		
4	0.000000D+00	0.000000D+00	0.000000D+00	0.169731D+01	
5	0.000000D+00	0.000000D+00	0.000000D+00	0.684900D-05	0.907242D-02
6	0.000000D+00	0.000000D+00	0.000000D+00	-0.597551D-04	0.244695D-06

	6
6	0.619109D-01

Test job not archived.

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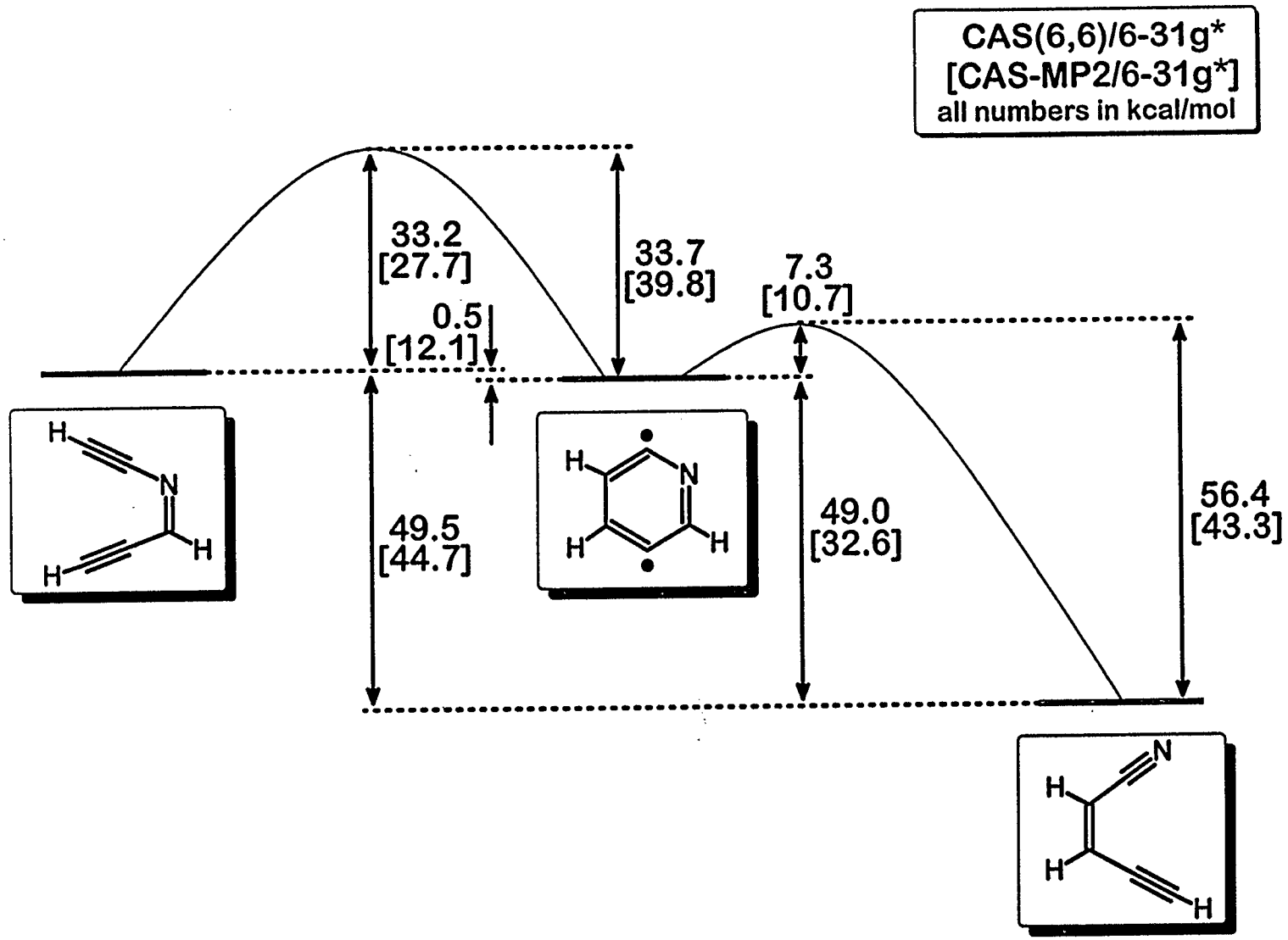
MP2=-230.0397704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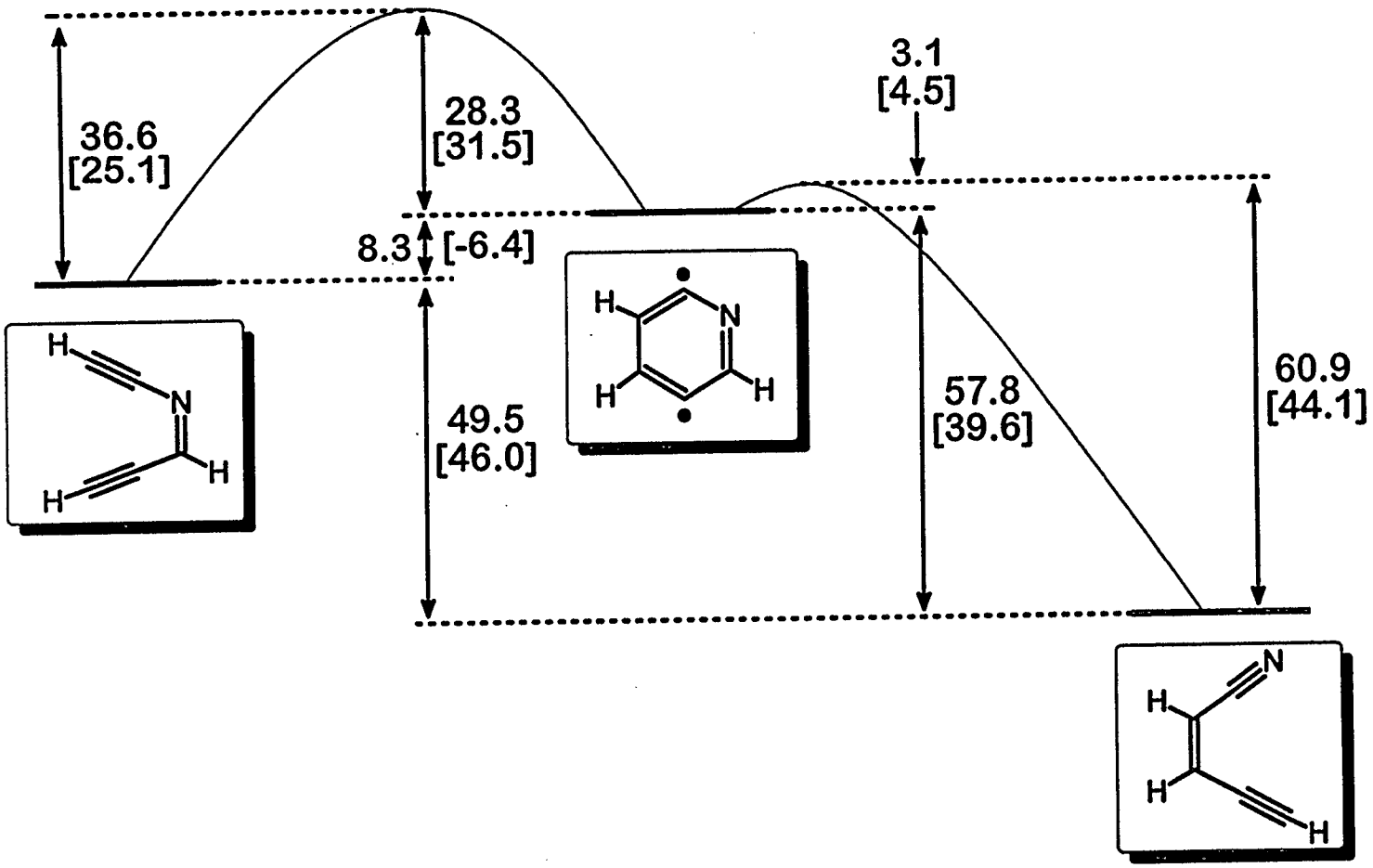
A_E_DY01.CW1

CAS(6,6)/3-21g
[CAS-MP2/3-21g]
all numbers in kcal/mol



Singlet

Pyridyne, CAS(6,6)/3-21g optimized

(scan1.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.643156	0.000000			
3	N	1.269618	2.352531	0.000000		
4	C	2.354421	1.376991	2.754619	0.000000	
5	C	1.380857	2.388748	2.372033	1.408772	0.000000
6	C	2.308232	1.347275	1.407282	2.399889	2.786106
7	H	3.336385	2.147779	3.824966	1.070427	2.150846
8	H	2.162917	3.368346	3.332398	2.165187	1.067877
9	H	3.237966	2.157486	2.106429	3.395131	3.847200

		6	7	8	9
6	C	0.000000			
7	H	3.370444	0.000000		
8	H	3.853913	2.494429	0.000000	
9	H	1.064585	4.294296	4.914417	0.000000

Interatomic angles:

C1-N3-C2= 88.4646	C1-C4-C2= 85.9927	N3-C1-C4= 94.1505
N3-C2-C4= 91.3923	C1-C5-C2= 84.5496	N3-C1-C5=126.9527
C2-N3-C5= 60.741	C1-C5-C4=115.1243	C2-C4-C5=118.0661
N3-C5-C4= 89.8007	C1-C6-C2= 88.5553	C1-N3-C6=119.0574
C2-C6-N3=117.2935	C4-C1-C6= 61.9461	C4-C2-C6=123.506
N3-C6-C4= 88.7107	C5-C1-C6= 94.7483	C5-C2-C6= 92.1468
C5-N3-C6= 91.3338	C5-C4-C6= 90.1549	C1-C2-H7= 87.6388
N3-C2-H7=116.3353	C1-C4-H7=151.8039	C2-C4-H7=122.2034
N3-C4-H7=179.1714	C1-C5-H7=140.7295	C2-H7-C5= 67.5179
N3-C5-H7=115.4058	C5-C4-H7=119.7305	C6-C2-H7=148.449
C6-C4-H7=150.1147	C6-C5-H7= 85.0764	C2-C1-H8= 88.4026
N3-C1-H8=151.2416	C1-H8-C4= 65.9105	C2-C4-H8=142.991
N3-C4-H8= 84.3659	C1-C5-H8=123.5776	C2-C5-H8=151.8728
N3-C5-H8=148.9013	C4-C5-H8=121.2981	C6-C1-H8=119.0372
C6-C4-H8=115.0798	C6-C5-H8=179.2307	C1-H8-H7= 91.2271
C2-H7-H8= 92.7315	H7-C4-H8= 94.8055	H7-C5-H8= 95.6929
C1-C2-H9= 84.1796	C1-N3-H9=146.0222	C2-H9-N3= 66.9592
C4-C2-H9=146.8754	C4-N3-H9= 87.5402	C5-C2-H9=115.5163
C5-N3-H9=118.2986	C1-C6-H9=144.9457	C2-C6-H9=126.499
N3-C6-H9=116.2076	C4-C6-H9=155.0817	C5-C6-H9=174.5444
H7-C2-H9=171.8185		

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Population analysis using the SCF density.

****

Orbital Symmetries:

Occupied	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A")	(A')	(A")	(A")	(A')	(A')	(A')	(A')	(A')
Virtual	(A')	(A')	(A')	(A')	(A')	(A')	(A")	(A')	(A")	(A")
	(A')	(A')	(A')	(A")	(A')	(A')	(A')	(A")	(A")	(A')
	(A')	(A")	(A')	(A')	(A")	(A')	(A')	(A')	(A')	(A')
	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')

The electronic state is 1-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.198945D+01				
2	-0.259679D-07	0.198444D+01			
3	-0.184756D-05	-0.126807D-05	0.139134D+01		
4	-0.486469D-05	-0.276468D-04	0.511189D-06	0.608593D+00	
5	0.222123D-05	0.326618D-06	0.697764D-05	-0.230800D-06	0.105909D-01
6	0.112114D-05	-0.372480D-05	0.337930D-05	0.312159D-05	-0.283066D-07

	6
6	0.155863D-01

Zero-point correction= 0.067471 (Hartree/Particle)
Thermal correction to Energy= 0.071345
Thermal correction to Enthalpy= 0.072289
Thermal correction to Gibbs Free Energy= 0.040420
Sum of electronic and zero-point Energies= -243.977528
Sum of electronic and thermal Energies= -243.973655
Sum of electronic and thermal Enthalpies= -243.972711
Sum of electronic and thermal Free Energies= -244.004579

Test job not archived.
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MP2=-244.4831999

Singlet

Pyridyne, CAS(6,6)/6-31g* (3-21g geometry)

(scan1.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.643156	0.000000			
3	N	1.269618	2.352531	0.000000		
4	C	2.354421	1.376991	2.754619	0.000000	
5	C	1.380857	2.388748	2.372033	1.408772	0.000000
6	C	2.308232	1.347275	1.407282	2.399889	2.786106
7	H	3.336385	2.147779	3.824966	1.070427	2.150846
8	H	2.162917	3.368346	3.332398	2.165187	1.067877
9	H	3.237966	2.157486	2.106429	3.395131	3.847200

		6	7	8	9
6	C	0.000000			
7	H	3.370444	0.000000		
8	H	3.853913	2.494429	0.000000	
9	H	1.064585	4.294296	4.914417	0.000000

Interatomic angles:

C1-N3-C2= 88.4646	C1-C4-C2= 85.9927	N3-C1-C4= 94.1505
N3-C2-C4= 91.3923	C1-C5-C2= 84.5496	N3-C1-C5=126.9527
C2-N3-C5= 60.741	C1-C5-C4=115.1243	C2-C4-C5=118.0661
N3-C5-C4= 89.8007	C1-C6-C2= 88.5553	C1-N3-C6=119.0574
C2-C6-N3=117.2935	C4-C1-C6= 61.9461	C4-C2-C6=123.506
N3-C6-C4= 88.7107	C5-C1-C6= 94.7483	C5-C2-C6= 92.1468
C5-N3-C6= 91.3338	C5-C4-C6= 90.1549	C1-C2-H7= 87.6388
N3-C2-H7=116.3353	C1-C4-H7=151.8039	C2-C4-H7=122.2034
N3-C4-H7=179.1714	C1-C5-H7=140.7295	C2-H7-C5= 67.5179
N3-C5-H7=115.4058	C5-C4-H7=119.7305	C6-C2-H7=148.449
C6-C4-H7=150.1147	C6-C5-H7= 85.0764	C2-C1-H8= 88.4026
N3-C1-H8=151.2416	C1-H8-C4= 65.9105	C2-C4-H8=142.991
N3-C4-H8= 84.3659	C1-C5-H8=123.5776	C2-C5-H8=151.8728
N3-C5-H8=148.9013	C4-C5-H8=121.2981	C6-C1-H8=119.0372
C6-C4-H8=115.0798	C6-C5-H8=179.2307	C1-H8-H7= 91.2271
C2-H7-H8= 92.7315	H7-C4-H8= 94.8055	H7-C5-H8= 95.6929
C1-C2-H9= 84.1796	C1-N3-H9=146.0222	C2-H9-N3= 66.9592
C4-C2-H9=146.8754	C4-N3-H9= 87.5402	C5-C2-H9=115.5163
C5-N3-H9=118.2986	C1-C6-H9=144.9457	C2-C6-H9=126.499
N3-C6-H9=116.2076	C4-C6-H9=155.0817	C5-C6-H9=174.5444
H7-C2-H9=171.8185		

****

Population analysis using the SCF density.

****

Orbital Symmetries:

Occupied	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A")	(A')	(A")	(A")	(A')	(A')	(A')
Virtual	(A')	(A')	(A')	(A")	(A')	(A')	(A')	(A")	(A")	(A')
	(A')	(A')	(A')	(A')	(A")	(A')	(A')	(A")	(A")	(A')
	(A")	(A')	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A')	(A')	(A')	(A")	(A')	(A')	(A')
	(A')	(A")	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A")
	(A')	(A')	(A')	(A")	(A")	(A')	(A")	(A')	(A')	(A")
	(A")	(A')	(A')	(A")	(A")	(A")				

The electronic state is 1-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.198975D+01				
2	0.894061D-06	0.198450D+01			
3	0.162617D-04	-0.100841D-04	0.136564D+01		
4	-0.130364D-04	0.164906D-04	0.217497D-05	0.634326D+00	
5	0.187308D-04	-0.741277D-06	0.797560D-06	-0.478839D-05	0.102661D-01
6	0.306077D-05	0.165131D-04	0.249432D-04	-0.396489D-06	-0.110288D-05

	6
6	0.155171D-01

Test job not archived.

1\1\GINC-C4-31\SP\CASSCF\6-31G(d)\C5H3N1\MSCHOTT\04-May-1997\0\\#P CAS (6,6)/6-31G* GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(6/7=3) TEST\\aza-ene-diyne surface\\0,1\C,0.,1.3148938037,0.\C,-0.1001333553,-1.3263643042,0.\N,-1.1507593249,0.7785321915,0.\C,1.1464894286,-0.7415254569,0.\C,1.2185745137,0.6654007778,0.\C,-1.2505792796,-0.6252053262,0.\H,2.0476338856,-1.3192396304,0.\H,2.1582405809,1.172735507,0.\H,-2.2366670365,-1.0264181822,0.\\Version=DEC-AXP-OSF/1-G94RevC.3\State=1-A'\HF=-245.4234846\RMSD=0.000e+00\Dipole=0.7735025,-0.5447153,0.\PG=CS [SG(C5H3N1)]\\@

MP2=-246.1206479

Tr[redacted]let
P[redacted]dyne, CAS(6,6)/3-21g (singlet geometry)
([redacted]n1.t.com)

```
Di[redacted]matrix (angstroms):
                 1          2          3          4          5
 1 [redacted]  0.000000
 2 [redacted]  2.643156   0.000000
 3 [redacted]  1.269618   2.352531   0.000000
 4 [redacted]  2.354421   1.376991   2.754619   0.000000
 5 [redacted]  1.380857   2.388748   2.372033   1.408772   0.000000
 6 [redacted]  2.308232   1.347275   1.407282   2.399889   2.786106
 7 [redacted]  3.336385   2.147779   3.824966   1.070427   2.150846
 8 [redacted]  2.162917   3.368346   3.332398   2.165187   1.067877
 9 [redacted]  3.237966   2.157486   2.106429   3.395131   3.847200
                 6          7          8          9
 6 [redacted]  0.000000
 7 [redacted]  3.370444   0.000000
 8 [redacted]  3.853913   2.494429   0.000000
 9 [redacted]  1.064585   4.294296   4.914417   0.000000
```

```
                         Interatomic angles:
[redacted]-N3-C2= 88.4646      C1-C4-C2= 85.9927      N3-C1-C4= 94.1505
[redacted]-C2-C4= 91.3923      C1-C5-C2= 84.5496      N3-C1-C5=126.9527
[redacted]-N3-C5= 60.741       C1-C5-C4=115.1243      C2-C4-C5=118.0661
[redacted]-C5-C4= 89.8007      C1-C6-C2= 88.5553      C1-N3-C6=119.0574
[redacted]-C6-N3=117.2935      C4-C1-C6= 61.9461      C4-C2-C6=123.506
[redacted]-C6-C4= 88.7107      C5-C1-C6= 94.7483      C5-C2-C6= 92.1468
[redacted]-N3-C6= 91.3338      C5-C4-C6= 90.1549      C1-C2-H7= 87.6388
[redacted]-C2-H7=116.3353      C1-C4-H7=151.8039      C2-C4-H7=122.2034
[redacted]-C4-H7=179.1714      C1-C5-H7=140.7295      C2-H7-C5= 67.5179
[redacted]-C5-H7=115.4058      C5-C4-H7=119.7305      C6-C2-H7=148.449
[redacted]-C4-H7=150.1147      C6-C5-H7= 85.0764      C2-C1-H8= 88.4026
[redacted]-C1-H8=151.2416      C1-H8-C4= 65.9105      C2-C4-H8=142.991
[redacted]-C4-H8= 84.3659      C1-C5-H8=123.5776      C2-C5-H8=151.8728
[redacted]-C5-H8=148.9013      C4-C5-H8=121.2981      C6-C1-H8=119.0372
[redacted]-C4-H8=115.0798      C6-C5-H8=179.2307      C1-H8-H7= 91.2271
[redacted]7-H8= 92.7315        H7-C4-H8= 94.8055      H7-C5-H8= 95.6929
[redacted]C2-H9= 84.1796       C1-N3-H9=146.0222      C2-H9-N3= 66.9592
[redacted]C2-H9=146.8754       C4-N3-H9= 87.5402      C5-C2-H9=115.5163
[redacted]3-H9=118.2986        C1-C6-H9=144.9457      C2-C6-H9=126.499
[redacted]-C6-H9=116.2076      C4-C6-H9=155.0817      C5-C6-H9=174.5444
[redacted]-C2-H9=171.8185
```

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*************************************************************************
[redacted]**************************************************************
           Population analysis using the SCF density.
*************************************************************************
[redacted]**************************************************************

Or[redacted]metries:
  [redacted]upied  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                   (A') (A') (A') (A") (A') (A") (A") (A') (A') (A')
                   (A')
  [redacted]tual   (A') (A') (A") (A') (A') (A') (A") (A") (A') (A')
                   (A') (A') (A') (A") (A') (A') (A") (A") (A') (A")
                   (A') (A') (A") (A') (A') (A') (A') (A') (A') (A')
                   (A") (A') (A') (A') (A') (A') (A') (A') (A')
[redacted]tronic state is 3-A'.
```

```
Fin[redacted]electron symbolic density matrix:
                 1              2              3              4              5
 [redacted]965D+01
 [redacted]7697D-06   0.198536D+01
 [redacted]0947D-06   0.156041D-04   0.999421D+00
 [redacted]3566D-06   0.248477D-04   0.153812D-02   0.100016D+01
 [redacted]9999D-04  -0.585632D-05  -0.943435D-05   0.910108D-05   0.104879D-01
 [redacted]3619D-05  -0.140306D-05   0.138720D-04  -0.251884D-04   0.749847D-06
                 6
 [redacted]149225D-01
```

```
Te[redacted] not archived.
 1[redacted]-C4-31\SP\CASSCF\3-21G\C5H3N1(3)\MSCHOTT\21-May-1997\0\\#P CAS
 ([redacted]-21G GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(6/7=3)
 T[redacted]a-ene-diyne surface\\0,3\C,0.,1.3148938037,0.\C,-0.1001333553,
 -[redacted]643042,0.\N,-1.1507593249,0.7785321915,0.\C,1.1464894286,-0.741
 5[redacted].0.\C,1.2185745137,0.6654007778,0.\C,-1.2505792796,-0.625205326
 2[redacted]2.0476338856,-1.3192396304,0.\H,2.1582405809,1.172735507,0.\H,-
 2[redacted]0365,-1.0264181822,0.\\Version=DEC-AXP-OSF/1-G94RevC.3\State=3
 -[redacted]244.0328382\RMSD=0.000e+00\Dipole=0.7830539,-0.620028,0.\PG=CS
  [redacted]3N1)]\\@
```

MP2-[redacted].4688041

Pyridyne, CAS(6,6)/3-21g (triplet geometry)
(scan1.t.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.617754	0.000000			
3	N	1.293538	2.352550	0.000000		
4	C	2.355536	1.383213	2.794435	0.000000	
5	C	1.387024	2.365405	2.407620	1.395602	0.000000
6	C	2.273350	1.364220	1.369372	2.424274	2.772508
7	H	3.348758	2.148264	3.864746	1.070454	2.158661
8	H	2.151618	3.357973	3.354225	2.165312	1.068136
9	H	3.227461	2.147813	2.089020	3.402942	3.838638

		6	7	8	9
6	C	0.000000			
7	H	3.390789	0.000000		
8	H	3.839280	2.529971	0.000000	
9	H	1.066689	4.288855	4.904724	0.000000

Interatomic angles:

C1-N3-C2= 86.6552 C1-C4-C2= 84.6358 N3-C1-C4= 95.5283
N3-C2-C4= 93.1806 C1-C5-C2= 84.1716 N3-C1-C5=127.805
N3-C2-C5= 61.3683 C1-C5-C4=115.669 C2-C4-C5=116.6903
N3-C5-C4= 90.5501 C1-C6-C2= 88.3686 C1-N3-C6=117.2065
C2-C6-N3=118.7697 C4-C1-C6= 63.1358 C4-C2-C6=123.8597
N3-C6-C4= 90.4883 C5-C1-C6= 95.4124 C5-C2-C6= 92.0473
C5-N3-C6= 90.1302 C5-C4-C6= 88.8313 C1-C2-H7= 88.7085
N3-C2-H7=118.2662 C1-C4-H7=153.6689 C2-C4-H7=121.6952
N3-C4-H7=178.8959 C1-C5-H7=140.6485 C2-H7-C5= 66.6251
N3-C5-H7=115.5297 C5-C4-H7=121.6145 C6-C2-H7=148.9452
C6-C4-H7=149.5542 C6-C5-H7= 85.9319 C2-C1-H8= 88.9516
N3-C1-H8=152.7388 C1-H8-C4= 66.1374 C2-C4-H8=141.288
N3-C4-H8= 84.0873 C1-C5-H8=121.8753 C2-C5-H8=153.9531
N3-C5-H8=146.9941 C4-C5-H8=122.4558 C6-C1-H8=120.3463
C6-C4-H8=113.4291 C6-C5-H8=176.592 C1-H8-H7= 90.9682
C2-H7-H8= 91.3716 H7-C4-H8= 97.0168 H7-C5-H8= 97.4762
C1-C2-H9= 84.6461 C1-N3-H9=144.1258 C2-H9-N3= 67.4409
C4-C2-H9=148.2691 C4-N3-H9= 87.0893 C5-C2-H9=116.4567
C5-N3-H9=117.0496 C1-C6-H9=147.9464 C2-C6-H9=123.6849
N3-C6-H9=117.5454 C4-C6-H9=151.9663 C5-C6-H9=177.8173
H7-C2-H9=173.3546

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Population analysis using the SCF density.

****

Orbital Symmetries:
Occupied (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A") (A') (A") (A") (A') (A') (A')
(A')
Virtual (A') (A') (A") (A') (A') (A') (A") (A") (A') (A')
(A') (A') (A') (A") (A') (A') (A") (A") (A') (A")
(A') (A') (A") (A') (A') (A') (A') (A') (A') (A')
(A") (A') (A') (A') (A') (A') (A') (A') (A')
The electronic state is 3-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.199015D+01				
2	0.563267D-07	0.198717D+01			
3	0.338081D-05	0.107983D-05	0.999404D+00		
4	-0.395602D-05	-0.146917D-04	0.108013D-02	0.100023D+01	
5	0.411071D-05	0.362668D-06	0.789387D-06	0.288144D-05	0.998643D-02
6	0.777947D-06	0.586452D-05	-0.109334D-05	-0.335134D-05	-0.100820D-06

	6
6	0.130536D-01

Zero-point correction= 0.068238 (Hartree/Particle)
Thermal correction to Energy= 0.072102
Thermal correction to Enthalpy= 0.073046
Thermal correction to Gibbs Free Energy= 0.040135
Sum of electronic and zero-point Energies= -243.967167
Sum of electronic and thermal Energies= -243.963304
Sum of electronic and thermal Enthalpies= -243.962359
Sum of electronic and thermal Free Energies= -243.995270

Test job not archived.
1\1\GINC-C4-31\Freq\CASSCF\3-21G\C5H3N1(3)\MSCHOTT\21-May-1997\0\\#P C
AS(6,6)/3-21G FREQ GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(
6/7=3) TEST\\aza-ene-diyne surface\\0,3\C,0.,1.301832871,0.\C,-0.09288
42381,-1.3142724156,0.\N,-1.1800524018,0.7720061385,0.\C,1.1673470763,
-0.7441017774,0.\C,1.224491492,0.6503302505,0.\C,-1.2523657614,-0.5954
548843,0.\H,2.0551992255,-1.3420911594,0.\H,2.1485059195,1.1861582764,
0.\H,-2.2228697448,-1.038114351,0.\\Version=DEC-AXP-OSF/1-G94RevC.3\St
ate=3-A'\HF=-244.0354053\RMSD=0.000e+00\RMSF=3.304e-04\PG=CS [SG(C5H3N
1)]\NImag=0

MP2=-244.4726243

Triplet

Pyridyne, CAS(6,6)/6-31g* (singlet geometry)

(scan1.t.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.643156	0.000000			
3	N	1.269618	2.352531	0.000000		
4	C	2.354421	1.376991	2.754619	0.000000	
5	C	1.380857	2.388748	2.372033	1.408772	0.000000
6	C	2.308232	1.347275	1.407282	2.399889	2.786106
7	H	3.336385	2.147779	3.824966	1.070427	2.150846
8	H	2.162917	3.368346	3.332398	2.165187	1.067877
9	H	3.237966	2.157486	2.106429	3.395131	3.847200
		6	7	8	9	
6	C	0.000000				
7	H	3.370444	0.000000			
8	H	3.853913	2.494429	0.000000		
9	H	1.064585	4.294296	4.914417	0.000000	

Interatomic angles:

C1-N3-C2= 88.4646	C1-C4-C2= 85.9927	N3-C1-C4= 94.1505
N3-C2-C4= 91.3923	C1-C5-C2= 84.5496	N3-C1-C5=126.9527
C2-N3-C5= 60.741	C1-C5-C4=115.1243	C2-C4-C5=118.0661
N3-C5-C4= 89.8007	C1-C6-C2= 88.5553	C1-N3-C6=119.0574
C2-C6-N3=117.2935	C4-C1-C6= 61.9461	C4-C2-C6=123.506
N3-C6-C4= 88.7107	C5-C1-C6= 94.7483	C5-C2-C6= 92.1468
C5-N3-C6= 91.3338	C5-C4-C6= 90.1549	C1-C2-H7= 87.6388
N3-C2-H7=116.3353	C1-C4-H7=151.8039	C2-C4-H7=122.2034
N3-C4-H7=179.1714	C1-C5-H7=140.7295	C2-H7-C5= 67.5179
N3-C5-H7=115.4058	C5-C4-H7=119.7305	C6-C2-H7=148.449
C6-C4-H7=150.1147	C6-C5-H7= 85.0764	C2-C1-H8= 88.4026
N3-C1-H8=151.2416	C1-H8-C4= 65.9105	C2-C4-H8=142.991
N3-C4-H8= 84.3659	C1-C5-H8=123.5776	C2-C5-H8=151.8728
N3-C5-H8=148.9013	C4-C5-H8=121.2981	C6-C1-H8=119.0372
C6-C4-H8=115.0798	C6-C5-H8=179.2307	C1-H8-H7= 91.2271
C2-H7-H8= 92.7315	H7-C4-H8= 94.8055	H7-C5-H8= 95.6929
C1-C2-H9= 84.1796	C1-N3-H9=146.0222	C2-H9-N3= 66.9592
C4-C2-H9=146.8754	C4-N3-H9= 87.5402	C5-C2-H9=115.5163
C5-N3-H9=118.2986	C1-C6-H9=144.9457	C2-C6-H9=126.499
N3-C6-H9=116.2076	C4-C6-H9=155.0817	C5-C6-H9=174.5444
H7-C2-H9=171.8185		

****

Population analysis using the SCF density.

****

Orbital Symmetries:

Occupied	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A")	(A')	(A")	(A")	(A')	(A')	(A')
	(A')									
Virtual	(A')	(A')	(A")	(A')	(A')	(A')	(A")	(A")	(A')	(A')
	(A')	(A')	(A')	(A")	(A')	(A')	(A")	(A")	(A')	(A")
	(A')	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A')	(A')	(A")	(A')	(A')	(A')	(A')
	(A")	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A")	(A')
	(A')	(A')	(A")	(A")	(A')	(A")	(A')	(A')	(A")	(A")
	(A')	(A')	(A")	(A")	(A")					

The electronic state is 3-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.198998D+01				
2	-0.381873D-06	0.198547D+01			
3	-0.689909D-05	0.603679D-04	0.999495D+00		
4	-0.865936D-05	0.211739D-05	0.135227D-02	0.100014D+01	
5	-0.170479D-04	0.105833D-05	0.218807D-05	-0.867867D-06	0.101471D-01
6	-0.247576D-07	-0.661985D-04	-0.326574D-04	0.346850D-04	0.621177D-06
	6				
6	0.147730D-01				

Test job not archived.

1\1\GINC-C4-31\SP\CASSCF\6-31G(d)\C5H3N1(3)\MSCHOTT\21-May-1997\0\\#P CAS(6,6)/6-31G* GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(6/7 =3) TEST\\aza-ene-diyne surface\\0,3\C,0.,1.3148938037,0.\C,-0.1001333 553,-1.3263643042,0.\N,-1.1507593249,0.7785321915,0.\C,1.1464894286,-0 .7415254569,0.\C,1.2185745137,0.6654007778,0.\C,-1.2505792796,-0.62520 53262,0.\H,2.0476338856,-1.3192396304,0.\H,2.1582405809,1.172735507,0. \H,-2.2366670365,-1.0264181822,0.\\Version=DEC-AXP-OSF/1-G94RevC.3\Sta te=3-A'\HF=-245.4134308\RMSD=0.000e+00\Dipole=0.751762,-0.5802509,0.\P G=CS [SG(C5H3N1)]\\@

MP2=-246.1075771

Pyridyne, CAS(6,6)/6-31g* (triplet geometry)
(scan1.t.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.617754	0.000000			
3	N	1.293538	2.352550	0.000000		
4	C	2.355536	1.383213	2.794435	0.000000	
5	C	1.387024	2.365405	2.407620	1.395602	0.000000
6	C	2.273350	1.364220	1.369372	2.424274	2.772508
7	H	3.348758	2.148264	3.864746	1.070454	2.158661
8	H	2.151618	3.357973	3.354225	2.165312	1.068136
9	H	3.227461	2.147813	2.089020	3.402942	3.838638

		6	7	8	9
6	C	0.000000			
7	H	3.390789	0.000000		
8	H	3.839280	2.529971	0.000000	
9	H	1.066689	4.288855	4.904724	0.000000

Interatomic angles:

C1-N3-C2= 86.6552	C1-C4-C2= 84.6358	N3-C1-C4= 95.5283
N3-C2-C4= 93.1806	C1-C5-C2= 84.1716	N3-C1-C5=127.805
N3-C2-C5= 61.3683	C1-C5-C4=115.669	C2-C4-C5=116.6903
N3-C5-C4= 90.5501	C1-C6-C2= 88.3686	C1-N3-C6=117.2065
C2-C6-N3=118.7697	C4-C1-C6= 63.1358	C4-C2-C6=123.8597
N3-C6-C4= 90.4883	C5-C1-C6= 95.4124	C5-C2-C6= 92.0473
C5-N3-C6= 90.1302	C5-C4-C6= 88.8313	C1-C2-H7= 88.7085
N3-C2-H7=118.2662	C1-C4-H7=153.6689	C2-C4-H7=121.6952
N3-C4-H7=178.8959	C1-C5-H7=140.6485	C2-H7-C5= 66.6251
N3-C5-H7=115.5297	C5-C4-H7=121.6145	C6-C2-H7=148.9452
C6-C4-H7=149.5542	C6-C5-H7= 85.9319	C2-C1-H8= 88.9516
N3-C1-H8=152.7388	C1-H8-C4= 66.1374	C2-C4-H8=141.288
N3-C4-H8= 84.0873	C1-C5-H8=121.8753	C2-C5-H8=153.9531
N3-C5-H8=146.9941	C4-C5-H8=122.4558	C6-C1-H8=120.3463
C6-C4-H8=113.4291	C6-C5-H8=176.592	C1-H8-H7= 90.9682
C2-H7-H8= 91.3716	H7-C4-H8= 97.0168	H7-C5-H8= 97.4762
C1-C2-H9= 84.6461	C1-N3-H9=144.1258	C2-H9-N3= 67.4409
C4-C2-H9=148.2691	C4-N3-H9= 87.0893	C5-C2-H9=116.4567
C5-N3-H9=117.0496	C1-C6-H9=147.9464	C2-C6-H9=123.6849
N3-C6-H9=117.5454	C4-C6-H9=151.9663	C5-C6-H9=177.8173
H7-C2-H9=173.3546		

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Population analysis using the SCF density.

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Orbital Symmetries:

Occupied (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A") (A') (A") (A") (A') (A') (A')
(A')

Virtual (A') (A') (A") (A') (A') (A') (A") (A") (A') (A')
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(A') (A') (A") (A") (A")

The electronic state is 3-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.199048D+01				
2	0.786941D-06	0.198738D+01			
3	0.172169D-04	-0.141354D-04	0.999399D+00		
4	0.167593D-04	-0.163772D-04	0.787709D-03	0.100028D+01	
5	0.227010D-04	0.106772D-05	0.160235D-04	-0.822848D-05	0.965210D-02
6	0.151022D-05	-0.234847D-06	-0.124572D-04	0.155189D-04	-0.102582D-05

	6
6	0.128144D-01

Test job not archived.
1\1\GINC-C4-31\SP\CASSCF\6-31G(d)\C5H3N1(3)\MSCHOTT\21-May-1997\0\\#P
CAS(6,6)/6-31G* GEOM=CHECK.GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(6/7
=3) TEST\\aza-ene-diyne surface\\0,3\C,0.,1.301832871,0.\C,-0.09288423
81,-1.3142724156,0.\N,-1.1800524018,0.7720061385,0.\C,1.1673470763,-0.
7441017774,0.\C,1.224491492,0.6503302505,0.\C,-1.2523657614,-0.5954548
843,0.\H,2.0551992255,-1.3420911594,0.\H,2.1485059195,1.1861582764,0.\
H,-2.2228697448,-1.038114351,0.\\Version=DEC-AXP-OSF/1-G94RevC.3\State
=3-A'\HF=-245.4170952\RMSD=0.000e+00\Dipole=0.7760545,-0.5631598,0.\PG
=CS [SG(C5H3N1)]\\@

MP2=-246.11354

Nitrile, CAS(6,6)/3-21g optimized
(scan2.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.925596	0.000000			
3	N	1.151217	3.700276	0.000000		
4	C	2.432261	1.424257	3.499965	0.000000	
5	C	1.423568	2.439516	2.574749	1.335131	0.000000
6	C	3.739682	1.198913	4.258191	2.623139	3.553972
7	H	3.390076	2.134987	4.503854	1.072368	2.077646
8	H	2.128321	3.400929	3.194636	2.087083	1.070873
9	H	4.585613	2.250035	4.926961	3.674289	4.562440

		6	7	8	9
6	C	0.000000			
7	H	3.248017	0.000000		
8	H	4.561170	2.387725	0.000000	
9	H	1.051191	4.266089	5.588862	0.000000

Interatomic angles:

C2-C1-N3=124.4208	C1-C4-C2= 95.0902	N3-C1-C4=153.4271
C1-C5-C2= 94.801	N3-C1-C5=179.3851	C2-C5-N3= 95.076
C1-C5-C4=123.6573	C2-C4-C5=124.2451	N3-C5-C4=123.9322
C1-C2-C6=124.6522	C1-C4-C6= 95.3441	C4-C2-C6=179.4444
C5-C2-C6=153.657	C5-C4-C6=124.4991	C1-C2-H7= 82.5273
C1-C4-H7=148.0591	C2-C4-H7=116.8507	C1-C5-H7=150.5197
C2-H7-C5= 70.7589	N3-C5-H7=150.7946	C5-C4-H7=118.9041
C6-C2-H7=152.8206	C6-C4-H7=116.5968	C2-C1-H8= 82.9774
N3-C1-H8=152.6018	C1-H8-C4= 70.471	C2-C4-H8=150.6482
C1-C5-H8=116.4163	C2-C5-H8=148.7827	N3-C5-H8=116.1414
C4-C5-H8=119.9264	C6-C4-H8=150.9021	C1-H8-H7= 97.1306
C2-H7-H8= 97.3647	H7-C4-H8= 92.5011	H7-C5-H8= 93.064
C1-C2-H9=124.2318	C4-C2-H9=179.8647	C5-C2-H9=153.2366
C2-C6-H9=179.1002	C4-C6-H9=179.4019	H7-C2-H9=153.2409

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Population analysis using the SCF density.

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Orbital Symmetries:

Occupied	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A")	(A')	(A")	(A")	(A')	(A')	(A')
Virtual	(A')	(A')	(A')	(A")	(A')	(A')	(A')	(A")	(A")	(A')
	(A')	(A')	(A')	(A')	(A")	(A')	(A")	(A')	(A")	(A')
	(A')	(A")	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')

The electronic state is 1-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.199186D+01				
2	0.705984D-06	0.193950D+01			
3	0.190773D-06	-0.386116D-06	0.193413D+01		
4	-0.250306D-05	0.998618D-06	0.493695D-06	0.610177D-01	
5	0.362311D-06	-0.958881D-06	0.263375D-06	0.960119D-06	0.654631D-01
6	0.645047D-06	-0.289549D-05	-0.169157D-05	0.197334D-05	0.926600D-07

	6
6	0.803260D-02

Zero-point correction= 0.065234 (Hartree/Particle)
Thermal correction to Energy= 0.070794
Thermal correction to Enthalpy= 0.071738
Thermal correction to Gibbs Free Energy= 0.036019
Sum of electronic and zero-point Energies= -244.071837
Sum of electronic and thermal Energies= -244.066277
Sum of electronic and thermal Enthalpies= -244.065333
Sum of electronic and thermal Free Energies= -244.101051

Test job not archived.
1\1\GINC-C4-31\Freq\CASSCF\3-21G\C5H3N1\MSCHOTT\26-Apr-1997\0\\#P CAS(6,6)/3-21G FREQ GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(6/7=3) TEST\\aza-ene-diyne surface\\0,1\C,-1.2204351048,-0.8455998838,0.\C,1.29053134,0.6557849954,0.\N,-1.2916032844,-1.9946151645,0.\C,0.,1.2583093387,0.\C,-1.1476834886,0.5761083634,0.\C,2.3817444342,0.1591500452,0.\H,-0.0341286102,2.3301345655,0.\H,-2.0811404593,1.1009188391,0.\H,3.3315489754,-0.2912644057,0.\\Version=DEC-AXP-OSF/1-G94RevC.3\State=1-A'\HF=-244.1370707\RMSD=0.000e+00\RMSF=7.328e-05\PG=CS [SG(C5H3N1)]\NImag=0

MP2=-244.546306

(scan2.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.925596	0.000000			
3	N	1.151217	3.700276	0.000000		
4	C	2.432261	1.424257	3.499965	0.000000	
5	C	1.423568	2.439516	2.574749	1.335131	0.000000
6	C	3.739682	1.198913	4.258191	2.623139	3.553972
7	H	3.390076	2.134987	4.503854	1.072368	2.077646
8	H	2.128321	3.400929	3.194636	2.087083	1.070873
9	H	4.585613	2.250035	4.926961	3.674289	4.562440

		6	7	8	9
6	C	0.000000			
7	H	3.248017	0.000000		
8	H	4.561170	2.387725	0.000000	
9	H	1.051191	4.266089	5.588862	0.000000

Interatomic angles:

C2-C1-N3=124.4208	C1-C4-C2= 95.0902	N3-C1-C4=153.4271
C1-C5-C2= 94.801	N3-C1-C5=179.3851	C2-C5-N3= 95.076
C1-C5-C4=123.6573	C2-C4-C5=124.2451	N3-C5-C4=123.9322
C1-C2-C6=124.6522	C1-C4-C6= 95.3441	C4-C2-C6=179.4444
C5-C2-C6=153.657	C5-C4-C6=124.4991	C1-C2-H7= 82.5273
C1-C4-H7=148.0591	C2-C4-H7=116.8507	C1-C5-H7=150.5197
C2-H7-C5= 70.7589	N3-C5-H7=150.7946	C5-C4-H7=118.9041
C6-C2-H7=152.8206	C6-C4-H7=116.5968	C2-C1-H8= 82.9774
N3-C1-H8=152.6018	C1-H8-C4= 70.471	C2-C4-H8=150.6482
C1-C5-H8=116.4163	C2-C5-H8=148.7827	N3-C5-H8=116.1414
C4-C5-H8=119.9264	C6-C4-H8=150.9021	C1-H8-H7= 97.1306
C2-H7-H8= 97.3647	H7-C4-H8= 92.5011	H7-C5-H8= 93.064
C1-C2-H9=124.2318	C4-C2-H9=179.8647	C5-C2-H9=153.2366
C2-C6-H9=179.1002	C4-C6-H9=179.4019	H7-C2-H9=153.2409

****

Population analysis using the SCF density.

****

Orbital Symmetries:

Occupied	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A")	(A')	(A")	(A")	(A')	(A')	(A')
Virtual	(A')	(A')	(A')	(A")	(A')	(A')	(A')	(A")	(A")	(A')
	(A')	(A')	(A')	(A')	(A")	(A')	(A")	(A')	(A")	(A')
	(A')	(A")	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')
	(A")	(A")	(A')	(A')	(A")	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A")	(A")	(A')	(A')	(A')	(A")	(A")	(A')
	(A')	(A")	(A')	(A")	(A")	(A")				

The electronic state is 1-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.199211D+01				
2	-0.262087D-04	0.586448D-01			
3	0.251240D-04	-0.178126D-05	0.613801D-01		
4	-0.104304D-05	-0.601623D-04	0.565557D-04	0.194210D+01	
5	-0.151625D-05	0.233081D-05	-0.141478D-03	0.363982D-05	0.193799D+01
6	0.346834D-04	-0.191588D-05	-0.407108D-05	0.149383D-04	-0.129735D-05

	6
6	0.778554D-02

Test job not archived.

1\1\GINC-C4-31\SP\CASSCF\6-31G(d)\C5H3N1\MSCHOTT\04-May-1997\0\\#P CAS (6,6)/6-31G* GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(6/7=3) TEST\\aza-ene-diyne surface\\0,1\C,-1.2204351048,-0.8455998838,0.\C,1.29053134,0.6557849954,0.\N,-1.2916032844,-1.9946151645,0.\C,0.,1.2583093387,0.\C,-1.1476834886,0.5761083634,0.\C,2.3817444342,0.1591500452,0.\H,-0.0341286102,2.3301345655,0.\H,-2.0811404593,1.1009188391,0.\H,3.3315489754,-0.2912644057,0.\\Version=DEC-AXP-OSF/1-G94RevC.3\State=1-A'\HF=-245.5016189\RMSD=0.000e+00\Dipole=0.381391,1.4927719,0.\PG=CS [SG(C5H3N1)]\\@

MP2=-246.1726367

TS Nitrile, CAS(6,6)/3-21g optimized (scan22.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.655743	0.000000			
3	N	1.224153	2.456866	0.000000		
4	C	2.349443	1.402084	2.814489	0.000000	
5	C	1.403385	2.401239	2.395286	1.384108	0.000000
6	C	2.409685	1.294701	1.632498	2.412092	2.855377
7	H	3.333726	2.164010	3.884120	1.070294	2.124799
8	H	2.180594	3.383917	3.333261	2.147350	1.067338
9	H	3.273830	2.184957	2.233511	3.442187	3.895921

		6	7	8	9
6	C	0.000000			
7	H	3.360816	0.000000		
8	H	3.922649	2.471449	0.000000	
9	H	1.059529	4.336764	4.962343	0.000000

Interatomic angles:

C1-N3-C2= 85.4061	C1-C4-C2= 86.2338	N3-C1-C4= 99.0311
N3-C2-C4= 89.329	C1-C5-C2= 84.1882	N3-C1-C5=131.3365
C2-C5-N3= 61.6232	C1-C5-C4=114.8832	C2-C4-C5=119.0452
N3-C5-C4= 92.3181	C1-C6-C2= 86.0496	C1-N3-C6=114.2719
C2-C6-N3=113.6375	C4-C1-C6= 60.8908	C4-C2-C6=126.8257
N3-C6-C4= 85.9087	C5-C1-C6= 93.1962	C5-C2-C6= 96.5659
C5-N3-C6= 88.1735	C5-C4-C6= 93.5997	C1-C2-H7= 86.897
N3-C2-H7=114.2496	C1-C4-H7=152.19	C2-C4-H7=121.5762
N3-C4-H7=177.6293	C1-C5-H7=140.9192	C2-H7-C5= 68.0886
N3-C5-H7=118.3542	C5-C4-H7=119.3785	C6-C2-H7=151.7463
C6-C4-H7=147.0217	C6-C5-H7= 83.5037	C2-C1-H8= 88.2333
N3-C1-H8=155.4746	C1-H8-C4= 65.7511	C2-C4-H8=144.0392
N3-C4-H8= 83.2447	C1-C5-H8=123.3352	C2-C5-H8=152.4765
N3-C5-H8=145.9003	C4-C5-H8=121.7816	C6-C1-H8=117.3344
C6-C4-H8=118.5937	C6-C5-H8=179.2492	C1-H8-H7= 91.3327
C2-H7-H8= 93.537	H7-C4-H8= 94.3846	H7-C5-H8= 95.7455
C1-C2-H9= 84.5163	C1-N3-H9=140.6874	C2-H9-N3= 67.5551
C4-C2-H9=146.4927	C4-N3-H9= 85.1578	C5-C2-H9=116.2329
C5-N3-H9=114.5889	C1-C6-H9=137.9009	C2-C6-H9=136.0494
N3-C6-H9=110.3131	C4-C6-H9=163.7782	C5-C6-H9=167.2891
H7-C2-H9=171.4133		

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Population analysis using the SCF density.

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Orbital Symmetries:

Occupied	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A")	(A')	(A")	(A")	(A')	(A')	(A')
Virtual	(A')	(A')	(A')	(A")	(A')	(A')	(A')	(A")	(A")	(A')
	(A')	(A')	(A')	(A')	(A")	(A')	(A')	(A")	(A")	(A')
	(A")	(A')	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')

The electronic state is 1-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.199002D+01				
2	-0.102822D-07	0.196082D+01			
3	0.829832D-07	0.144729D-07	0.161597D+01		
4	0.183357D-05	0.209196D-05	-0.101076D-05	0.385016D+00	
5	0.107988D-06	-0.493738D-06	0.741791D-06	0.889601D-07	0.980711D-02
6	-0.616251D-06	0.345316D-05	-0.649699D-05	-0.106998D-05	-0.794820D-08

	6
6	0.383640D-01

Zero-point correction= 0.065430 (Hartree/Particle)
Thermal correction to Energy= 0.069346
Thermal correction to Enthalpy= 0.070291
Thermal correction to Gibbs Free Energy= 0.038294
Sum of electronic and zero-point Energies= -243.974605
Sum of electronic and thermal Energies= -243.970689
Sum of electronic and thermal Enthalpies= -243.969745
Sum of electronic and thermal Free Energies= -244.001741

Test job not archived.
1\1\GINC-C4-31\Freq\CASSCF\3-21G\C5H3N1\MSCHOTT\28-Apr-1997\0\\#P CAS(
6,6)/3-21G FREQ GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(6/7
=3) TEST\\aza-ene-diyne surface\\0,1\C,0.0000641956,1.3160778483,0.\C,
-0.1126767525,-1.3372710521,0.\N,-1.1478654073,0.8908610707,0.\C,1.151
8683219,-0.7316595182,0.\C,1.2352732161,0.6499329923,0.\C,-1.260215839
5,-0.7377667466,0.\H,2.0511856647,-1.3119683112,0.\H,2.1748029021,1.15
63867782,0.\H,-2.2768095645,-1.0363271033,0.\\Version=DEC-AXP-OSF/1-G9
4RevC.3\State=1-A'\HF=-244.0400355\RMSD=0.000e+00\RMSF=9.083e-05\PG=CS
[SG(C5H3N1)]\NImag=1 (-751 cm-1)

MP2=-244.4759499

TS Nitrile, CAS(6,6)/6-31g* (3-21g geometry)
(scan22.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.655743	0.000000			
3	N	1.224153	2.456866	0.000000		
4	C	2.349443	1.402084	2.814489	0.000000	
5	C	1.403385	2.401239	2.395286	1.384108	0.000000
6	C	2.409685	1.294701	1.632498	2.412092	2.855377
7	H	3.333726	2.164010	3.884120	1.070294	2.124799
8	H	2.180594	3.383917	3.333261	2.147350	1.067338
9	H	3.273830	2.184957	2.233511	3.442187	3.895921

		6	7	8	9
6	C	0.000000			
7	H	3.360816	0.000000		
8	H	3.922649	2.471449	0.000000	
9	H	1.059529	4.336764	4.962343	0.000000

Interatomic angles:

C1-N3-C2= 85.4061	C1-C4-C2= 86.2338	N3-C1-C4= 99.0311
N3-C2-C4= 89.329	C1-C5-C2= 84.1882	N3-C1-C5=131.3365
C2-C5-N3= 61.6232	C1-C5-C4=114.8832	C2-C4-C5=119.0452
N3-C5-C4= 92.3181	C1-C6-C2= 86.0496	C1-N3-C6=114.2719
C2-C6-N3=113.6375	C4-C1-C6= 60.8908	C4-C2-C6=126.8257
N3-C6-C4= 85.9087	C5-C1-C6= 93.1962	C5-C2-C6= 96.5659
C5-N3-C6= 88.1735	C5-C4-C6= 93.5997	C1-C2-H7= 86.897
N3-C2-H7=114.2496	C1-C4-H7=152.19	C2-C4-H7=121.5762
N3-C4-H7=177.6293	C1-C5-H7=140.9192	C2-H7-C5= 68.0886
N3-C5-H7=118.3542	C5-C4-H7=119.3785	C6-C2-H7=151.7463
C6-C4-H7=147.0217	C6-C5-H7= 83.5037	C2-C1-H8= 88.2333
N3-C1-H8=155.4746	C1-H8-C4= 65.7511	C2-C4-H8=144.0392
N3-C4-H8= 83.2447	C1-C5-H8=123.3352	C2-C5-H8=152.4765
N3-C5-H8=145.9003	C4-C5-H8=121.7816	C6-C1-H8=117.3344
C6-C4-H8=118.5937	C6-C5-H8=179.2492	C1-H8-H7= 91.3327
C2-H7-H8= 93.537	H7-C4-H8= 94.3846	H7-C5-H8= 95.7455
C1-C2-H9= 84.5163	C1-N3-H9=140.6874	C2-H9-N3= 67.5551
C4-C2-H9=146.4927	C4-N3-H9= 85.1578	C5-C2-H9=116.2329
C5-N3-H9=114.5889	C1-C6-H9=137.9009	C2-C6-H9=136.0494
N3-C6-H9=110.3131	C4-C6-H9=163.7782	C5-C6-H9=167.2891
H7-C2-H9=171.4133		

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Population analysis using the SCF density.

****

Orbital Symmetries:

Occupied	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A")	(A')	(A")	(A")	(A')	(A')	(A')
Virtual	(A')	(A')	(A')	(A")	(A')	(A')	(A')	(A")	(A")	(A')
	(A')	(A')	(A')	(A')	(A")	(A')	(A')	(A")	(A")	(A')
	(A")	(A')	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A')	(A')	(A')	(A")	(A')	(A')	(A')
	(A')	(A")	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A")
	(A')	(A')	(A')	(A")	(A")	(A')	(A')	(A')	(A")	(A")
	(A')	(A')	(A")	(A")	(A")	(A")				

The electronic state is 1-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.199030D+01				
2	0.148853D-05	0.196016D+01			
3	0.124497D-04	0.278271D-04	0.159732D+01		
4	-0.266700D-04	-0.226460D-04	0.607204D-04	0.403599D+00	
5	0.187740D-04	-0.463406D-05	-0.460392D-05	-0.858995D-05	0.951023D-02
6	0.822677D-05	0.142955D-04	0.110151D-03	0.531001D-05	-0.164962D-05

	6
6	0.391087D-01

Test job not archived.

1\1\GINC-C4-31\SP\CASSCF\6-31G(d)\C5H3N1\MSCHOTT\04-May-1997\0\\#P CAS
(6,6)/6-31G* GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(6/7=3)
TEST\\aza-ene-diyne surface\\0,1\C,0.0000641956,1.3160778483,0.\C,-0.
1126767525,-1.3372710521,0.\N,-1.1478654073,0.8908610707,0.\C,1.151868
3219,-0.7316595182,0.\C,1.2352732161,0.6499329923,0.\C,-1.2602158395,-
0.7377667466,0.\H,2.0511856647,-1.3119683112,0.\H,2.1748029021,1.15638
67782,0.\H,-2.2768095645,-1.0363271033,0.\\Version=DEC-AXP-OSF/1-G94Re
vC.3\State=1-A'\HF=-245.4117963\RMSD=0.000e+00\Dipole=0.8452956,-0.438
4072,0.\PG=CS [SG(C5H3N1)]\\@

MP2=-246.103629

Aza-ene-diyne, CAS(6/6/3) Eig Optimized (scan3.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.887795	0.000000			
3	N	1.346802	2.418809	0.000000		
4	C	3.734450	1.198778	3.539672	0.000000	
5	C	1.197459	3.724461	2.543526	4.319348	0.000000
6	C	2.321998	1.431205	1.277936	2.629981	3.449042
7	H	4.605329	2.250077	4.554448	1.051303	5.018911
8	H	2.247162	4.587413	3.593122	5.009161	1.049718
9	H	3.260863	2.139815	2.003733	3.257627	4.434052

		6	7	8	9
6	C	0.000000			
7	H	3.681273	0.000000		
8	H	4.465615	5.564966	0.000000	
9	H	1.071057	4.275132	5.470062	0.000000

Interatomic angles:

C1-N3-C2= 95.9453 C1-C2-C4=127.0303 N3-C2-C4=154.6674
C2-C1-C5=126.3407 N3-C1-C5=177.2417 C2-N3-C5= 97.2435
C1-C6-C2= 97.7765 C1-N3-C6=124.3984 C2-C6-N3=126.3699
C1-C6-C4= 97.7056 C4-C2-C6=179.8444 N3-C6-C4=126.299
C5-C1-C6=155.7501 C5-N3-C6=125.6966 C1-C2-H7=126.9225
N3-C2-H7=154.5595 C2-C4-H7=179.7691 C6-C2-H7=179.7365
C6-C4-H7=179.6844 C2-C1-H8=126.1452 N3-C1-H8=177.4372
C1-C5-H8=179.5815 N3-C5-H8=178.9584 C6-C1-H8=155.5546
C1-C2-H9= 79.3456 C1-N3-H9=152.893 C2-H9-N3= 71.3438
C4-C2-H9=153.6241 C5-N3-H9=154.1912 C1-C6-H9=145.4026
C2-C6-H9=116.8209 N3-C6-H9=116.8092 C4-C6-H9=116.8918
H7-C2-H9=153.732

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Population analysis using the SCF density.

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Orbital Symmetries:

Occupied (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A") (A') (A") (A") (A') (A') (A') (A") (A')
Virtual (A') (A') (A') (A') (A') (A') (A") (A') (A") (A")
(A') (A') (A') (A") (A') (A') (A') (A") (A") (A')
(A') (A") (A') (A') (A") (A') (A') (A') (A') (A')
(A") (A') (A') (A') (A') (A') (A') (A') (A') (A')

The electronic state is 1-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.199036D+01				
2	0.569615D-06	0.194434D+01			
3	0.122252D-05	-0.143856D-06	0.193785D+01		
4	-0.319813D-05	-0.185254D-04	0.400604D-05	0.559304D-01	
5	-0.118484D-04	-0.546498D-05	-0.659887D-05	0.468328D-06	0.619613D-01
6	0.111231D-04	0.102580D-04	0.358020D-05	-0.818831D-06	-0.892553D-06

	6
6	0.955401D-02

Zero-point correction= 0.064152 (Hartree/Particle)
Thermal correction to Energy= 0.069760
Thermal correction to Enthalpy= 0.070705
Thermal correction to Gibbs Free Energy= 0.034978
Sum of electronic and zero-point Energies= -243.994021
Sum of electronic and thermal Energies= -243.988413
Sum of electronic and thermal Enthalpies= -243.987469
Sum of electronic and thermal Free Energies= -244.023195

Test job not archived.
1\1\GINC-C4-31\Freq\CASSCF\3-21G\C5H3N1\MSCHOTT\26-Apr-1997\0\\#P CAS(
6,6)/3-21G FREQ GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(6/7
=3) TEST\\aza-ene-diyne surface\\0,1\C,-1.2487844577,-0.7124568809,0.\
C,1.2996569623,0.645779506,0.\N,-1.1190868607,0.6280853629,0.\C,2.3868
829716,0.1407948613,0.\C,-1.4213246221,-1.8974203917,0.\C,0.,1.2451462
775,0.\H,3.3385646818,-0.3059051154,0.\H,-1.5649857591,-2.9372613166,0
.\H,-0.0385560222,2.315508659,0.\\Version=DEC-AXP-OSF/1-G94RevC.3\Stat
e=1-A'\HF=-244.0581733\RMSD=0.000e+00\RMSF=7.392e-05\PG=CS [SG(C5H3N1)
]\NImag=0

MP2=-244.4729651

(scan3.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.887795	0.000000			
3	N	1.346802	2.418809	0.000000		
4	C	3.734450	1.198778	3.539672	0.000000	
5	C	1.197459	3.724461	2.543526	4.319348	0.000000
6	C	2.321998	1.431205	1.277936	2.629981	3.449042
7	H	4.605329	2.250077	4.554448	1.051303	5.018911
8	H	2.247162	4.587413	3.593122	5.009161	1.049718
9	H	3.260863	2.139815	2.003733	3.257627	4.434052

		6	7	8	9
6	C	0.000000			
7	H	3.681273	0.000000		
8	H	4.465615	5.564966	0.000000	
9	H	1.071057	4.275132	5.470062	0.000000

Interatomic angles:

C1-N3-C2= 95.9453	C1-C2-C4=127.0303	N3-C2-C4=154.6674
C2-C1-C5=126.3407	N3-C1-C5=177.2417	C2-N3-C5= 97.2435
C1-C6-C2= 97.7765	C1-N3-C6=124.3984	C2-C6-N3=126.3699
C1-C6-C4= 97.7056	C4-C2-C6=179.8444	N3-C6-C4=126.299
C5-C1-C6=155.7501	C5-N3-C6=125.6966	C1-C2-H7=126.9225
N3-C2-H7=154.5595	C2-C4-H7=179.7691	C6-C2-H7=179.7365
C6-C4-H7=179.6844	C2-C1-H8=126.1452	N3-C1-H8=177.4372
C1-C5-H8=179.5815	N3-C5-H8=178.9584	C6-C1-H8=155.5546
C1-C2-H9= 79.3456	C1-N3-H9=152.893	C2-H9-N3= 71.3438
C4-C2-H9=153.6241	C5-N3-H9=154.1912	C1-C6-H9=145.4026
C2-C6-H9=116.8209	N3-C6-H9=116.8092	C4-C6-H9=116.8918
H7-C2-H9=153.732		

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Population analysis using the SCF density.

****

Orbital Symmetries:

Occupied	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A")	(A')	(A")	(A")	(A')	(A')	(A')
Virtual	(A')	(A')	(A')	(A")	(A')	(A')	(A')	(A")	(A")	(A')
	(A')	(A')	(A')	(A')	(A')	(A")	(A")	(A')	(A")	(A')
	(A')	(A')	(A")	(A")	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')
	(A")	(A")	(A')	(A')	(A')	(A")	(A')	(A')	(A')	(A')
	(A')	(A')	(A")	(A")	(A')	(A')	(A')	(A')	(A")	(A")
	(A")	(A')	(A")	(A")	(A')	(A")				

The electronic state is 1-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.199047D+01				
2	0.412249D-05	0.194353D+01			
3	-0.163815D-04	-0.191968D-05	0.595638D-01		
4	-0.405946D-06	0.332786D-04	-0.346145D-05	0.529833D-01	
5	0.491772D-06	0.706178D-02	-0.152297D-04	0.103176D-04	0.194403D+01
6	-0.127241D-04	0.662413D-05	0.125887D-05	-0.626067D-05	-0.203026D-04

	6
6	0.942011D-02

Test job not archived.

1\1\GINC-C4-31\SP\CASSCF\6-31G(d)\C5H3N1\MSCHOTT\04-May-1997\0\\#P CAS (6,6)/6-31G* GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(6/7=3) TEST\\aza-ene-diyne surface\\0,1\C,-1.2487844577,-0.7124568809,0.\C,1.2996569623,0.645779506,0.\N,-1.1190868607,0.6280853629,0.\C,2.3868829716,0.1407948613,0.\C,-1.4213246221,-1.8974203917,0.\C,0.,1.2451462775,0.\H,3.3385646818,-0.3059051154,0.\H,-1.5649857591,-2.9372613166,0.\H,-0.0385560222,2.315508659,0.\\Version=DEC-AXP-OSF/1-G94RevC.3\State=1-A'\HF=-245.4227317\RMSD=0.000e+00\Dipole=1.0282008,-0.0887018,0.\PG=CS [SG(C5H3N1)]\\@

MP2=-246.1013732

(scan33.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.684216	0.000000			
3	N	1.326169	2.367708	0.000000		
4	C	2.589050	1.265784	2.899903	0.000000	
5	C	1.266999	2.667260	2.416301	1.976500	0.000000
6	C	2.288951	1.413444	1.320946	2.433646	2.927933
7	H	3.440478	2.205570	3.930596	1.060494	2.522341
8	H	2.204825	3.548594	3.448799	2.590701	1.059849
9	H	3.240022	2.183066	2.043692	3.371381	3.986859

		6	7	8	9
6	C	0.000000			
7	H	3.480525	0.000000		
8	H	3.973879	2.738904	0.000000	
9	H	1.066632	4.377000	5.037085	0.000000

Interatomic angles:

C1-N3-C2= 88.5424	C1-C4-C2= 80.3351	N3-C1-C4= 89.5622
N3-C2-C4=101.5602	C1-C5-C2= 77.051	N3-C1-C5=137.4212
C2-N3-C5= 67.7624	C1-C5-C4=103.7607	C2-C4-C5=108.7155
N3-C5-C4= 81.9619	C1-C6-C2= 89.7157	C1-N3-C6=119.6961
C2-C6-N3=119.9334	C1-C6-C4= 66.4086	C4-C2-C6=130.4732
N3-C6-C4= 96.6263	C5-C1-C6=107.3349	C5-C2-C6= 85.8984
C5-N3-C6= 98.9161	C5-C4-C6= 82.4958	C1-C2-H7= 88.8741
N3-C2-H7=118.4714	C1-C4-H7=136.8921	C2-C4-H7=142.7727
N3-C4-H7=164.1053	C1-C5-H7=127.2568	C2-H7-C5= 68.3082
N3-C5-H7=105.4579	C5-C4-H7=108.5118	C6-C2-H7=147.3844
C6-C4-H7=168.9924	C6-C5-H7= 78.9897	C2-C1-H8= 92.5482
N3-C1-H8=154.4085	C4-C1-H8= 64.8462	C2-C4-H8=130.7203
N3-C4-H8= 77.5983	C1-C5-H8=142.5706	C2-C5-H8=140.3785
N3-C5-H8=164.3694	C4-C5-H8=113.6688	C6-C1-H8=124.3222
C6-C4-H8=104.5006	C6-C5-H8=169.1624	C1-H8-H7= 87.5041
C2-H7-H8= 91.0736	H7-C4-H8= 86.507	H7-C5-H8= 90.1727
C1-C2-H9= 82.7794	C1-N3-H9=147.3174	C2-H9-N3= 68.043
C4-C2-H9=154.7422	C4-N3-H9= 84.0927	C5-C2-H9=110.1674
C5-N3-H9=126.5374	C1-C6-H9=147.5551	C2-C6-H9=122.7292
N3-C6-H9=117.3374	C4-C6-H9=146.0363	C5-C6-H9=171.9531
H7-C2-H9=171.6534		

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Population analysis using the SCF density.

****

Orbital Symmetries:

Occupied	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A")	(A')	(A")	(A")	(A')	(A')	(A')
Virtual	(A')	(A')	(A')	(A")	(A')	(A')	(A')	(A")	(A")	(A')
	(A')	(A')	(A')	(A')	(A")	(A')	(A')	(A")	(A")	(A')
	(A")	(A')	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')

The electronic state is 1-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.198824D+01				
2	-0.308667D-06	0.193640D+01			
3	-0.484772D-05	-0.149577D-05	0.172984D+01		
4	0.150874D-04	0.184400D-04	0.666891D-05	0.271321D+00	
5	0.391551D-04	0.156931D-04	-0.132775D-04	-0.684213D-05	0.112782D-01
6	0.206198D-04	0.237641D-04	-0.128609D-04	-0.419177D-05	-0.221099D-06

	6
6	0.629207D-01

Zero-point correction= 0.063248 (Hartree/Particle)
Thermal correction to Energy= 0.067438
Thermal correction to Enthalpy= 0.068382
Thermal correction to Gibbs Free Energy= 0.035921
Sum of electronic and zero-point Energies= -243.936599
Sum of electronic and thermal Energies= -243.932409
Sum of electronic and thermal Enthalpies= -243.931465
Sum of electronic and thermal Free Energies= -243.963926

Test job not archived.
1\1\GINC-C4-31\Freq\CASSCF\3-21G\C5H3N1\MSCHOTT\28-Apr-1997\0\\#P CAS(
6,6)/3-21G FREQ GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(6/7
=3) TEST\\aza-ene-diyne surface\\0,1\C,0.,1.3194912777,0.\C,-0.0715923
77,-1.3637696768,0.\N,-1.1856813368,0.7254518041,0.\C,1.1420113405,-1.
004081729,0.\C,1.2181159982,0.9709523752,0.\C,-1.2567636976,-0.5935797
917,0.\H,2.1339230799,-1.3792604283,0.\H,2.2044756204,1.3587351561,0.\
H,-2.2292569273,-1.0317120886,0.\\Version=DEC-AXP-OSF/1-G94RevC.3\Stat
e=1-A'\HF=-243.9998473\RMSD=0.000e+00\RMSF=1.606e-03\PG=CS [SG(C5H3N1)
]\NImag=1 (-774 cm-1)

MP2=-244.4329372

1B aza-ene-diyne) CAS(6,6)/6-31G (5 Deg Geometry)
(scan33.s.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.684216	0.000000			
3	N	1.326169	2.367708	0.000000		
4	C	2.589050	1.265784	2.899903	0.000000	
5	C	1.266999	2.667260	2.416301	1.976500	0.000000
6	C	2.288951	1.413444	1.320946	2.433646	2.927933
7	H	3.440478	2.205570	3.930596	1.060494	2.522341
8	H	2.204825	3.548594	3.448799	2.590701	1.059849
9	H	3.240022	2.183066	2.043692	3.371381	3.986859

		6	7	8	9
6	C	0.000000			
7	H	3.480525	0.000000		
8	H	3.973879	2.738904	0.000000	
9	H	1.066632	4.377000	5.037085	0.000000

Interatomic angles:

C1-N3-C2= 88.5424	C1-C4-C2= 80.3351	N3-C1-C4= 89.5622
N3-C2-C4=101.5602	C1-C5-C2= 77.051	N3-C1-C5=137.4212
C2-N3-C5= 67.7624	C1-C5-C4=103.7607	C2-C4-C5=108.7155
N3-C5-C4= 81.9619	C1-C6-C2= 89.7157	C1-N3-C6=119.6961
C2-C6-N3=119.9334	C1-C6-C4= 66.4086	C4-C2-C6=130.4732
N3-C6-C4= 96.6263	C5-C1-C6=107.3349	C5-C2-C6= 85.8984
C5-N3-C6= 98.9161	C5-C4-C6= 82.4958	C1-C2-H7= 88.8741
N3-C2-H7=118.4714	C1-C4-H7=136.8921	C2-C4-H7=142.7727
N3-C4-H7=164.1053	C1-C5-H7=127.2568	C2-H7-C5= 68.3082
N3-C5-H7=105.4579	C5-C4-H7=108.5118	C6-C2-H7=147.3844
C6-C4-H7=168.9924	C6-C5-H7= 78.9897	C2-C1-H8= 92.5482
N3-C1-H8=154.4085	C4-C1-H8= 64.8462	C2-C4-H8=130.7203
N3-C4-H8= 77.5983	C1-C5-H8=142.5706	C2-C5-H8=140.3785
N3-C5-H8=164.3694	C4-C5-H8=113.6688	C6-C1-H8=124.3222
C6-C4-H8=104.5006	C6-C5-H8=169.1624	C1-H8-H7= 87.5041
C2-H7-H8= 91.0736	H7-C4-H8= 86.507	H7-C5-H8= 90.1727
C1-C2-H9= 82.7794	C1-N3-H9=147.3174	C2-H9-N3= 68.043
C4-C2-H9=154.7422	C4-N3-H9= 84.0927	C5-C2-H9=110.1674
C5-N3-H9=126.5374	C1-C6-H9=147.5551	C2-C6-H9=122.7292
N3-C6-H9=117.3374	C4-C6-H9=146.0363	C5-C6-H9=171.9531
H7-C2-H9=171.6534		

****

Population analysis using the SCF density.

****

Orbital Symmetries:

Occupied	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A")	(A')	(A")	(A")	(A')	(A')	(A')
Virtual	(A')	(A')	(A')	(A")	(A')	(A')	(A')	(A")	(A")	(A')
	(A')	(A')	(A')	(A')	(A")	(A')	(A')	(A")	(A")	(A')
	(A")	(A')	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A')	(A')	(A')	(A")	(A')	(A')	(A')
	(A')	(A")	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A")
	(A')	(A')	(A')	(A')	(A")	(A")	(A')	(A')	(A")	(A')
	(A")	(A")	(A')	(A")	(A")	(A")				

The electronic state is 1-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.193565D+01				
2	0.304129D-05	0.273560D+00			
3	0.613733D-05	0.216778D-04	0.172805D+01		
4	-0.406995D-04	0.740137D-05	0.310982D-04	0.631913D-01	
5	-0.187196D-05	-0.376324D-05	0.176384D-04	0.159183D-05	0.112119D-01
6	0.747311D-06	-0.11"577D-04	-0.990552D-06	-0.392446D-05	-0.105751D-04

	6
6	0.198834D+01

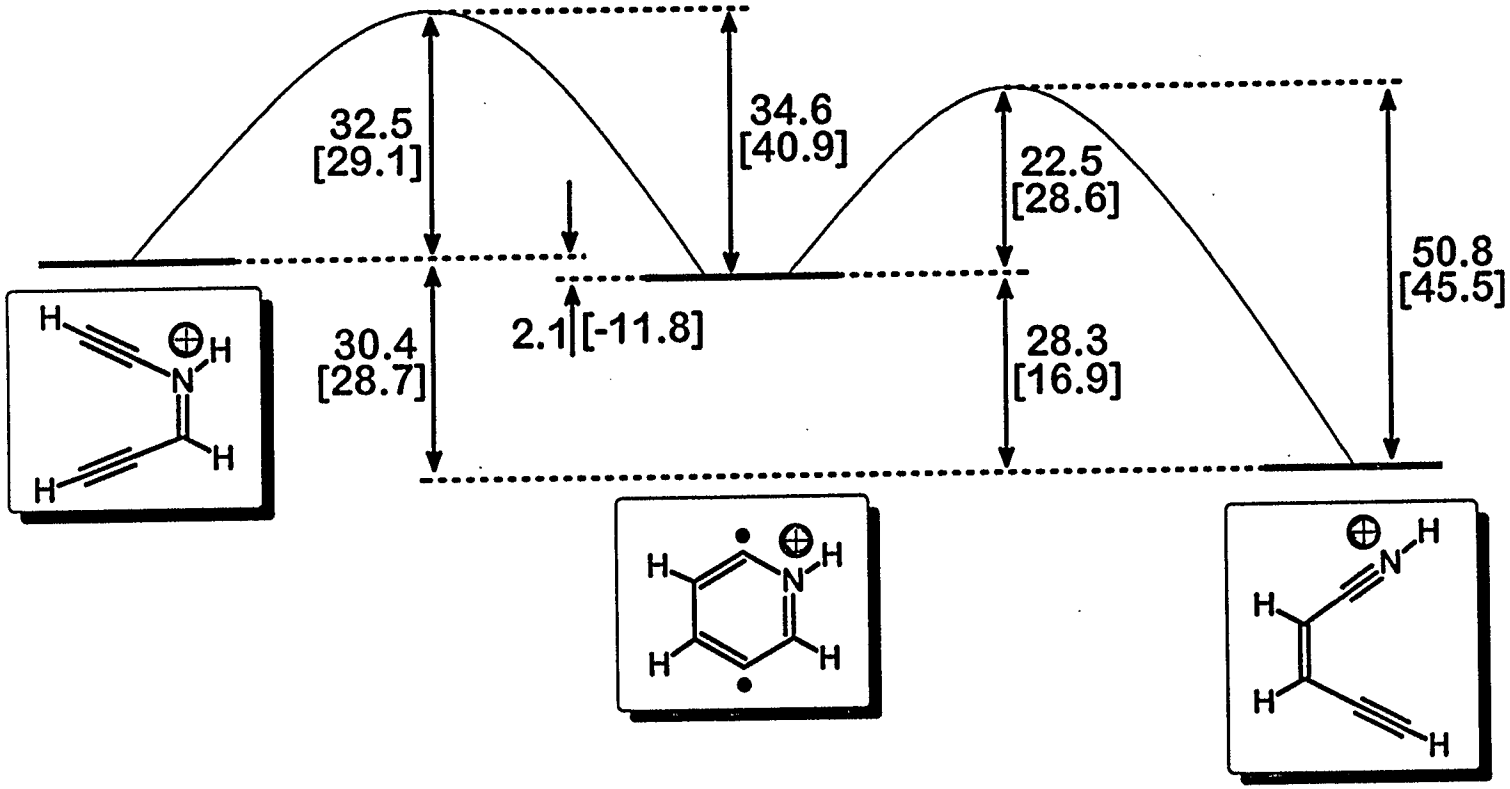
Test job not archived.

1\1\GINC-C4-31\SP\CASSCF\6-31G(d)\C5H3N1\MSCHOTT\05-May-1997\0\\#P CAS (6,6)/6-31G* GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(6/7=3) TEST\\aza-ene-diyne surface\\0,1\C,0.,1.3194912777,0.\C,-0.071592377,-1.3637696768,0.\N,-1.1856813368,0.7254518041,0.\C,1.1420113405,-1.004081729,0.\C,1.2181159982,0.9709523752,0.\C,-1.2567636976,-0.5935797917,0.\H,2.1339230799,-1.3792604283,0.\H,2.2044756204,1.3587351561,0.\H,-2.2292569273,-1.0317120886,0.\\Version=DEC-AXP-OSF/1-G94RevC.3\State=1-A'\HF=-245.3697916\RMSD=0.000e+00\Dipole=0.7443076,-0.5430236,0.\PG=CS [SG(C5H3N1)]\\@

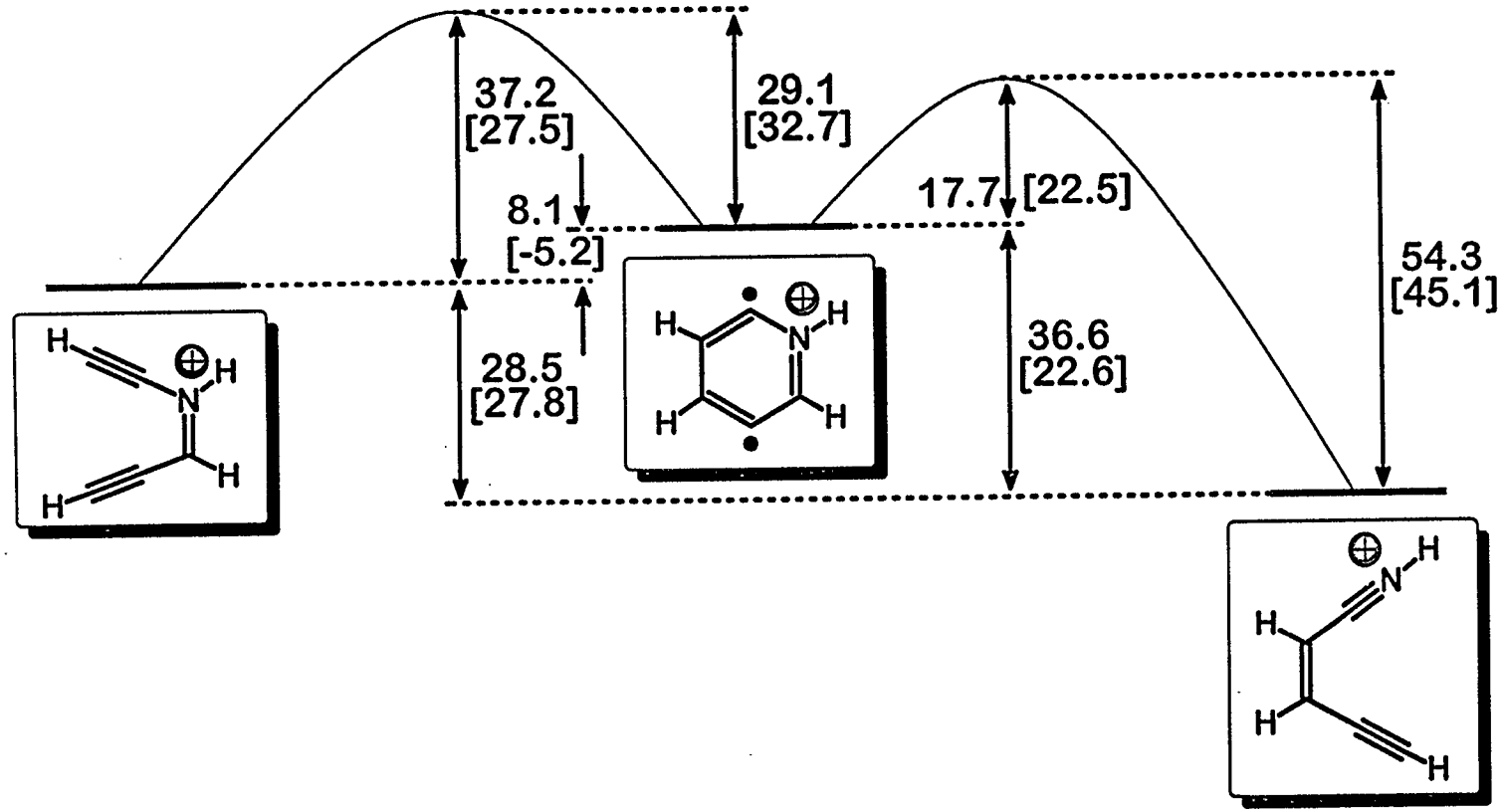
MP2=-246.0571792

A_E_DY04.CW2

CAS(6,6)/6-31g*
[CAS-MP2/6-31g*]
all numbers in kcal/mol



CAS(6,6)/3-21g
[CAS-MP2/3-21g]
all numbers in kcal/mol



Protonated, Singlet Pyridyne, CAS(6,6)/3-21g optimized (scan1.p.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.663179	0.000000			
3	N	1.314187	2.330029	0.000000		
4	C	2.356424	1.377639	2.740366	0.000000	
5	C	1.361362	2.396614	2.371423	1.416603	0.000000
6	C	2.356085	1.344476	1.398388	2.405551	2.803826
7	H	3.334518	2.147539	3.811450	1.071092	2.159429
8	H	2.132072	3.378172	3.334723	2.176742	1.068010
9	H	3.294621	2.158138	2.111313	3.402322	3.868325
10	H	2.025484	3.242109	1.008999	3.749365	3.277126

		6	7	8	9	10
6	C	0.000000				
7	H	3.373258	0.000000			
8	H	3.871761	2.510829	0.000000		
9	H	1.067662	4.296698	4.935702	0.000000	
10	H	2.080115	4.820448	4.153949	2.370232	0.000000

Interatomic angles:

C1-N3-C2= 89.405	C1-C4-C2= 86.8382	N3-C1-C4= 92.1262
N3-C2-C4= 91.6306	C1-C5-C2= 85.5654	N3-C1-C5=124.8223
C2-N3-C5= 61.2883	C1-C5-C4=116.0307	C2-C4-C5=118.1114
N3-C5-C4= 88.9698	C1-C6-C2= 87.5916	C1-N3-C6=120.5562
C2-C6-N3=116.2982	C4-C1-C6= 61.3891	C4-C2-C6=124.1811
N3-C6-C4= 88.0191	C5-C1-C6= 94.0852	C5-C2-C6= 92.7578
C5-N3-C6= 92.4395	C5-C4-C6= 90.5717	C1-C2-H7= 87.0663
N3-C2-H7=116.6331	C1-C4-H7=151.0949	C2-C4-H7=122.0669
N3-C4-H7=179.7304	C1-C5-H7=141.5189	C2-H7-C5= 67.6207
N3-C5-H7=114.4579	C5-C4-H7=119.8218	C6-C2-H7=149.1836
C6-C4-H7=149.6066	C6-C5-H7= 84.5709	C2-C1-H8= 88.8586
N3-C1-H8=149.8868	C1-H8-C4= 66.2976	C2-C4-H8=142.78
N3-C4-H8= 84.5773	C1-C5-H8=122.252	C2-C5-H8=152.1826
N3-C5-H8=149.313	C4-C5-H8=121.7173	C6-C1-H8=119.1497
C6-C4-H8=115.2403	C6-C5-H8=179.2	C1-H8-H7= 91.4398
C2-H7-H8= 92.6354	H7-C4-H8= 95.1531	H7-C5-H8= 96.2291
C1-C2-H9= 85.5317	C1-N3-H9=147.2997	C2-H9-N3= 66.1405
C4-C2-H9=147.5954	C4-N3-H9= 88.0614	C5-C2-H9=116.1721
C5-N3-H9=119.1829	C1-C6-H9=145.8495	C2-C6-H9=126.5589
N3-C6-H9=117.1429	C4-C6-H9=154.8381	C5-C6-H9=174.8164
H7-C2-H9=172.5979	C2-C1-H10= 86.3658	C1-N3-H10=120.7867
C2-N3-H10=149.8083	C4-C1-H10=117.4638	C4-N3-H10=179.975
C5-C1-H10=150.16	C5-N3-H10=148.9034	C1-H10-C6= 70.0267
C2-C6-H10=141.4901	C6-N3-H10=118.6571	C4-C6-H10=113.2109
C5-C6-H10= 82.8653	H8-C1-H10=175.2244	C1-H10-H9= 96.7823
C2-H9-H10= 91.3202	H9-N3-H10= 91.9137	H9-C6-H10= 91.951

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Population analysis using the SCF density.

****

Orbital Symmetries:

Occupied	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A')	(A")	(A")	(A")	(A')	(A')	(A')
Virtual	(A')	(A')	(A')	(A")	(A')	(A')	(A")	(A')	(A")	(A')
	(A')	(A')	(A')	(A')	(A')	(A')	(A")	(A')	(A")	(A")
	(A')	(A')	(A")	(A')	(A")	(A')	(A')	(A')	(A')	(A')
	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')								

The electronic state is 1-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.198896D+01				
2	-0.198914D-07	0.198632D+01			
3	-0.682915D-05	-0.845272D-05	0.123769D+01		
4	-0.248162D-05	-0.168835D-04	-0.362984D-05	0.762216D+00	
5	-0.837191D-05	0.369082D-06	-0.727403D-05	0.264581D-05	0.110860D-01
6	-0.119370D-05	-0.322326D-04	0.159478D-04	0.630027D-05	-0.481414D-07

	6
6	0.137334D-01

Zero-point correction= 0.082006 (Hartree/Particle)
Thermal correction to Energy= 0.085940
Thermal correction to Enthalpy= 0.086884
Thermal correction to Gibbs Free Energy= 0.054853
Sum of electronic and zero-point Energies= -244.320598
Sum of electronic and thermal Energies= -244.316664
Sum of electronic and thermal Enthalpies= -244.315720
Sum of electronic and thermal Free Energies= -244.347751

Test job not archived.
1\1\GINC-C4-31\Freq\CASSCF\3-21G\C5H4N1(1+)\MSCHOTT\08-May-1997\0\\#P CAS(6,6)/3-21G FREQ GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP (6/7=3) TEST\\aza-ene-diyne, protonated\\1,1\C,0.,1.3067368797,0.\C,0.0220631447,-1.3563509629,0.\N,-1.1444137829,0.6606686733,0.\C,1.233776505,-0.7008809331,0.\C,1.2263701393,0.7157025218,0.\C,-1.1714968385,-0.7374572318,0.\H,2.1658034839,-1.2286731397,0.\H,2.1319280923,1.281927 8106,0.\H,-2.1308344596,-1.206044598,0.\H,-2.0202783393,1.1616075715,0.\\Version=DEC-AXP-OSF/1-G94RevC.3\State=1-A'\HF=-244.4026047\RMSD=0.000e+00\RMSF=2.299e-04\PG=CS [SG(C5H4N1)]\NImag=0

MP2=-244.8330325

Protonated, Singlet Pyridyne, CAS(6,6)/6-31g* (3-21g geometry) (scan1.p.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.663179	0.000000			
3	N	1.314187	2.330029	0.000000		
4	C	2.356424	1.377639	2.740366	0.000000	
5	C	1.361362	2.396614	2.371423	1.416603	0.000000
6	C	2.356085	1.344476	1.398388	2.405551	2.803826
7	H	3.334518	2.147539	3.811450	1.071092	2.159429
8	H	2.132072	3.378172	3.334723	2.176742	1.068010
9	H	3.294621	2.158138	2.111313	3.402322	3.868325
10	H	2.025484	3.242109	1.008999	3.749365	3.277126

		6	7	8	9	10
6	C	0.000000				
7	H	3.373258	0.000000			
8	H	3.871761	2.510829	0.000000		
9	H	1.067662	4.296698	4.935702	0.000000	
10	H	2.080115	4.820448	4.153949	2.370232	0.000000

Interatomic angles:

C1-N3-C2= 89.405	C1-C4-C2= 86.8382	N3-C1-C4= 92.1262
N3-C2-C4= 91.6306	C1-C5-C2= 85.5654	N3-C1-C5=124.8223
C2-N3-C5= 61.2883	C1-C5-C4=116.0307	C2-C4-C5=118.1114
N3-C5-C4= 88.9698	C1-C6-C2= 87.5916	C1-N3-C6=120.5562
C2-C6-N3=116.2982	C4-C1-C6= 61.3891	C4-C2-C6=124.1811
N3-C6-C4= 88.0191	C5-C1-C6= 94.0852	C5-C2-C6= 92.7578
C5-N3-C6= 92.4395	C5-C4-C6= 90.5717	C1-C2-H7= 87.0663
N3-C2-H7=116.6331	C1-C4-H7=151.0949	C2-C4-H7=122.0669
N3-C4-H7=179.7304	C1-C5-H7=141.5189	C2-H7-C5= 67.6207
N3-C5-H7=114.4579	C5-C4-H7=119.8218	C6-C2-H7=149.1836
C6-C4-H7=149.6066	C6-C5-H7= 84.5709	C2-C1-H8= 88.8586
N3-C1-H8=149.8868	C1-H8-C4= 66.2976	C2-C4-H8=142.78
N3-C4-H8= 84.5773	C1-C5-H8=122.252	C2-C5-H8=152.1826
N3-C5-H8=149.313	C4-C5-H8=121.7173	C6-C1-H8=119.1497
C6-C4-H8=115.2403	C6-C5-H8=179.2	C1-H8-H7= 91.4398
C2-H7-H8= 92.6354	H7-C4-H8= 95.1531	H7-C5-H8= 96.2291
C1-C2-H9= 85.5317	C1-N3-H9=147.2997	C2-H9-N3= 66.1405
C4-C2-H9=147.5954	C4-N3-H9= 88.0614	C5-C2-H9=116.1721
C5-N3-H9=119.1829	C1-C6-H9=145.8495	C2-C6-H9=126.5589
N3-C6-H9=117.1429	C4-C6-H9=154.8381	C5-C6-H9=174.8164
H7-C2-H9=172.5979	C2-C1-H10= 86.3658	C1-N3-H10=120.7867
C2-N3-H10=149.8083	C4-C1-H10=117.4638	C4-N3-H10=179.975
C5-C1-H10=150.16	C5-N3-H10=148.9034	C1-H10-C6= 70.0267
C2-C6-H10=141.4901	C6-N3-H10=118.6571	C4-C6-H10=113.2109
C5-C6-H10= 82.8653	H8-C1-H10=175.2244	C1-H10-H9= 96.7823
C2-H9-H10= 91.3202	H9-N3-H10= 91.9137	H9-C6-H10= 91.951

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Population analysis using the SCF density.

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Orbital Symmetries:

Occupied	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A')	(A")	(A")	(A")	(A')	(A')	(A')
Virtual	(A')	(A')	(A')	(A")	(A')	(A')	(A")	(A')	(A")	(A')
	(A')	(A')	(A')	(A')	(A')	(A')	(A")	(A')	(A")	(A")
	(A')	(A')	(A")	(A')	(A")	(A')	(A')	(A')	(A')	(A')
	(A")	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A")	(A')
	(A')	(A')	(A')	(A")	(A")	(A')	(A')	(A')	(A')	(A')
	(A')	(A")	(A')	(A')	(A')	(A")	(A")	(A')	(A")	(A')
	(A')	(A")	(A")	(A')	(A')	(A")	(A")	(A")		

The electronic state is 1-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.198932D+01				
2	0.435225D-06	0.198643D+01			
3	0.644878D-06	-0.201079D-06	0.121093D+01		
4	0.890151D-05	-0.188488D-04	-0.262083D-06	0.788989D+00	
5	-0.210616D-04	0.514216D-05	-0.282926D-04	-0.173126D-05	0.107167D-01
6	0.461072D-06	-0.132067D-04	-0.220831D-04	0.967976D-05	-0.250617D-06

	6
6	0.136139D-01

Test job not archived.

1\1\GINC-C4-31\SP\CASSCF\6-31G(d)\C5H4N1(1+)\MSCHOTT\09-May-1997\0\\#P CAS(6,6)/6-31G* GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(6/7=3) TEST\\aza-ene-diyne, protonated\\1,1\C,0.,1.3067368797,0.\C,0.0220631447,-1.3563509629,0.\N,-1.1444137829,0.6606686733,0.\C,1.233776505,-0.7008809331,0.\C,1.2263701393,0.7157025218,0.\C,-1.1714968385,-0.7374572318,0.\H,2.1658034839,-1.2286731397,0.\H,2.1319280923,1.2819278106,0.\H,-2.1308344596,-1.206044598,0.\H,-2.0202783393,1.1616075715,0.\\Version=DEC-AXP-OSF/1-G94RevC.3\State=1-A'\HF=-245.7745936\RMSD=0.000e+00\Dipole=-0.5834581,0.3164897,0.\PG=CS [SG(C5H4N1)]\\@

MP2=-246.4582237

Protonated, Triplet Pyridyne, CAS(6,6)/3-21g (singlet geometry) (scan1.pt.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.663179	0.000000			
3	N	1.314187	2.330029	0.000000		
4	C	2.356424	1.377639	2.740366	0.000000	
5	C	1.361362	2.396614	2.371423	1.416603	0.000000
6	C	2.356085	1.344476	1.398388	2.405551	2.803826
7	H	3.334518	2.147539	3.811450	1.071092	2.159429
8	H	2.132072	3.378172	3.334723	2.176742	1.068010
9	H	3.294621	2.158138	2.111313	3.402322	3.868325
10	H	2.025484	3.242109	1.008999	3.749365	3.277126

		6	7	8	9	10
6	C	0.000000				
7	H	3.373258	0.000000			
8	H	3.871761	2.510829	0.000000		
9	H	1.067662	4.296698	4.935702	0.000000	
10	H	2.080115	4.820448	4.153949	2.370232	0.000000

Interatomic angles:

C1-N3-C2= 89.405	C1-C4-C2= 86.8382	N3-C1-C4= 92.1262
N3-C2-C4= 91.6306	C1-C5-C2= 85.5654	N3-C1-C5=124.8223
C2-N3-C5= 61.2883	C1-C5-C4=116.0307	C2-C4-C5=118.1114
N3-C5-C4= 88.9698	C1-C6-C2= 87.5916	C1-N3-C6=120.5562
C2-C6-N3=116.2982	C4-C1-C6= 61.3891	C4-C2-C6=124.1811
N3-C6-C4= 88.0191	C5-C1-C6= 94.0852	C5-C2-C6= 92.7578
C5-N3-C6= 92.4395	C5-C4-C6= 90.5717	C1-C2-H7= 87.0663
N3-C2-H7=116.6331	C1-C4-H7=151.0949	C2-C4-H7=122.0669
N3-C4-H7=179.7304	C1-C5-H7=141.5189	C2-H7-C5= 67.6207
N3-C5-H7=114.4579	C5-C4-H7=119.8218	C6-C2-H7=149.1836
C6-C4-H7=149.6066	C6-C5-H7= 84.5709	C2-C1-H8= 88.8586
N3-C1-H8=149.8868	C1-H8-C4= 66.2976	C2-C4-H8=142.78
N3-C4-H8= 84.5773	C1-C5-H8=122.252	C2-C5-H8=152.1826
N3-C5-H8=149.313	C4-C5-H8=121.7173	C6-C1-H8=119.1497
C6-C4-H8=115.2403	C6-C5-H8=179.2	C1-H8-H7= 91.4398
C2-H7-H8= 92.6354	H7-C4-H8= 95.1531	H7-C5-H8= 96.2291
C1-C2-H9= 85.5317	C1-N3-H9=147.2997	C2-H9-N3= 66.1405
C4-C2-H9=147.5954	C4-N3-H9= 88.0614	C5-C2-H9=116.1721
C5-N3-H9=119.1829	C1-C6-H9=145.8495	C2-C6-H9=126.5589
N3-C6-H9=117.1429	C4-C6-H9=154.8381	C5-C6-H9=174.8164
H7-C2-H9=172.5979	C2-C1-H10= 86.3658	C1-N3-H10=120.7867
C2-N3-H10=149.8083	C4-C1-H10=117.4638	C4-N3-H10=179.975
C5-C1-H10=150.16	C5-N3-H10=148.9034	C1-H10-C6= 70.0267
C2-C6-H10=141.4901	C6-N3-H10=118.6571	C4-C6-H10=113.2109
C5-C6-H10= 82.8653	H8-C1-H10=175.2244	C1-H10-H9= 96.7823
C2-H9-H10= 91.3202	H9-N3-H10= 91.9137	H9-C6-H10= 91.951

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Population analysis using the SCF density.

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Orbital Symmetries:

Occupied	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A')	(A")	(A")	(A")	(A')	(A')	(A')
	(A')									
Virtual	(A')	(A')	(A")	(A')	(A')	(A")	(A')	(A")	(A')	(A')
	(A')	(A')	(A')	(A')	(A')	(A")	(A')	(A")	(A")	(A')
	(A')	(A")	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A")
	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')									

The electronic state is 3-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.198924D+01				
2	-0.628780D-06	0.198663D+01			
3	-0.200512D-04	-0.879754D-05	0.100015D+01		
4	-0.649672D-05	0.595186D-06	-0.114362D-02	0.999637D+00	
5	0.428123D-04	-0.726006D-05	-0.330606D-05	-0.137898D-04	0.108856D-01
6	-0.733282D-05	-0.299893D-04	0.130407D-04	-0.157721D-05	0.109724D-05

	6
6	0.134650D-01

Test job not archived.

1\1\GINC-C4-32\SP\CASSCF\3-21G\C5H4N1(1+,3)\MSCHOTT\21-May-1997\0\\#P CAS(6,6)/3-21G GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(6/7=3) TEST\\aza-ene-diyne, protonated\\1,3\C,0.,1.3067368797,0.\C,0.0220631447,-1.3563509629,0.\N,-1.1444137829,0.6606686733,0.\C,1.233776505,-0.7008809331,0.\C,1.2263701393,0.7157025218,0.\C,-1.1714968385,-0.7374572318,0.\H,2.1658034839,-1.2286731397,0.\H,2.1319280923,1.2819278106,0.\H,-2.1308344596,-1.206044598,0.\H,-2.0202783393,1.1616075715,0.\\Version=DEC-AXP-OSF/1-G94RevC.3\State=3-A'\HF=-244.3976452\RMSD=0.000e+00\Dipole=-0.6208878,0.334325,0.\PG=CS [SG(C5H4N1)]\\@

MP2=-244.8275941

Protonated, Triplet Pyridyne, CAS(6,6)/3-21g (triplet geometry) (scan1.pt.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.642441	0.000000			
3	N	1.323141	2.321879	0.000000		
4	C	2.349390	1.384563	2.755286	0.000000	
5	C	1.367490	2.385729	2.392246	1.404819	0.000000
6	C	2.340584	1.352793	1.379591	2.424695	2.808104
7	H	3.336540	2.146853	3.825857	1.070753	2.160941
8	H	2.128481	3.376658	3.346923	2.176813	1.067945
9	H	3.291046	2.156134	2.105154	3.413888	3.874446
10	H	2.027853	3.242811	1.008738	3.763806	3.291122

		6	7	8	9	10
6	C	0.000000				
7	H	3.385762	0.000000			
8	H	3.875321	2.534626	0.000000		
9	H	1.067821	4.296389	4.940864	0.000000	
10	H	2.074515	4.834463	4.154213	2.384781	0.000000

Interatomic angles:

C1-N3-C2= 88.5141	C1-C4-C2= 85.997	N3-C1-C4= 92.962
N3-C2-C4= 92.5269	C1-C5-C2= 84.907	N3-C1-C5=125.5133
N3-C2-C5= 61.0656	C1-C5-C4=115.8641	C2-C4-C5=117.5817
N3-C5-C4= 89.107	C1-C6-C2= 87.0502	C1-N3-C6=119.9812
C2-C6-N3=116.3684	C4-C1-C6= 62.2615	C4-C2-C6=124.6913
N3-C6-C4= 88.3656	C5-C1-C6= 94.8128	C5-C2-C6= 93.23
C5-N3-C6= 92.2517	C5-C4-C6= 90.2757	C1-C2-H7= 87.6816
N3-C2-H7=117.7185	C1-C4-H7=152.5887	C2-C4-H7=121.4143
N3-C4-H7=178.7535	C1-C5-H7=140.9964	C2-H7-C5= 67.2576
N3-C5-H7=114.2394	C5-C4-H7=121.004	C6-C2-H7=149.8829
C6-C4-H7=148.7202	C6-C5-H7= 84.8389	C2-C1-H8= 89.4341
N3-C1-H8=150.883	C1-H8-C4= 66.1337	C2-C4-H8=141.9424
N3-C4-H8= 84.6031	C1-C5-H8=121.357	C2-C5-H8=153.7361
N3-C5-H8=148.1141	C4-C5-H8=122.779	C6-C1-H8=120.1825
C6-C4-H8=114.6365	C6-C5-H8=177.5145	C1-H8-H7= 90.9439
C2-H7-H8= 91.9405	H7-C4-H8= 96.6433	H7-C5-H8= 97.6466
C1-C2-H9= 85.972	C1-N3-H9=146.5591	C2-H9-N3= 66.0199
C4-C2-H9=148.4619	C4-N3-H9= 88.1789	C5-C2-H9=117.0007
C5-N3-H9=118.8295	C1-C6-H9=147.4273	C2-C6-H9=125.5225
N3-C6-H9=118.1091	C4-C6-H9=153.5253	C5-C6-H9=176.457
H7-C2-H9=173.6536	C2-C1-H10= 86.9038	C1-N3-H10=120.2291
C2-N3-H10=151.2568	C4-C1-H10=118.4168	C4-N3-H10=178.6093
C5-C1-H10=150.9681	C5-N3-H10=147.9587	C1-H10-C6= 69.5657
C2-C6-H10=141.3291	C6-N3-H10=119.7896	C4-C6-H10=113.3263
C5-C6-H10= 83.3086	H8-C1-H10=176.3378	C1-H10-H9= 96.1228
C2-H9-H10= 91.0014	H9-N3-H10= 93.2118	H9-C6-H10= 93.1484

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Population analysis using the SCF density.

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Orbital Symmetries:

Occupied (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A") (A") (A") (A') (A') (A')
(A')

Virtual (A') (A') (A") (A') (A') (A") (A') (A") (A') (A')
(A') (A') (A') (A') (A') (A") (A') (A") (A") (A')
(A') (A") (A') (A") (A') (A') (A') (A') (A') (A")
(A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A')

The electronic state is 3-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5	6
1	0.104301D-01					
2	-0.197699D-05	0.198748D+01				
3	-0.275968D-05	-0.929796D-05	0.999833D+00			
4	0.218075D-05	0.623644D-06	-0.110554D-02	0.999955D+00		
5	0.225796D-05	0.362639D-07	0.775223D-05	0.295863D-05	0.198969D+01	
6	0.156381D-07	-0.235865D-04	0.922980D-05	0.381732D-05	0.276483D-05	0.126079D-01

Zero-point correction= 0.082494 (Hartree/Particle)
Thermal correction to Energy= 0.086439
Thermal correction to Enthalpy= 0.087383
Thermal correction to Gibbs Free Energy= 0.054287
Sum of electronic and zero-point Energies= -244.315924
Sum of electronic and thermal Energies= -244.311979
Sum of electronic and thermal Enthalpies= -244.311035
Sum of electronic and thermal Free Energies= -244.344131

Test job not archived.
1\1\GINC-C4-32\Freq\CASSCF\3-21G\C5H4N1(1+,3)\MSCHOTT\21-May-1997\0\\#
P CAS(6,6)/3-21G FREQ GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT I
OP(6/7=3) TEST\\aza-ene-diyne, protonated\\1,3\C,0.,1.2959947165,0.\C,
0.0234354976,-1.3463425763,0.\N,-1.1565817295,0.6533281917,0.\C,1.2457
246771,-0.6959404551,0.\C,1.2350204027,0.7088376984,0.\C,-1.1787824638
,-0.7260846594,0.\H,2.1676761672,-1.2404746599,0.\H,2.1284801214,1.293
8478297,0.\H,-2.1286309368,-1.2139681664,0.\H,-2.0238419273,1.16850930
98,0.\\Version=DEC-AXP-OSF/1-G94RevC.3\State=3-A'\HF=-244.398418\RMSD=
0.000e+00\RMSF=2.298e-04\PG=CS [SG(C5H4N1)]\NImag=0

MP2=-244.829551

Protonated, Triplet Pyridyne, CAS(6,6)/6-31g* (singlet geometry) (scan1.pt.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.663179	0.000000			
3	N	1.314187	2.330029	0.000000		
4	C	2.356424	1.377639	2.740366	0.000000	
5	C	1.361362	2.396614	2.371423	1.416603	0.000000
6	C	2.356085	1.344476	1.398388	2.405551	2.803826
7	H	3.334518	2.147539	3.811450	1.071092	2.159429
8	H	2.132072	3.378172	3.334723	2.176742	1.068010
9	H	3.294621	2.158138	2.111313	3.402322	3.868325
10	H	2.025484	3.242109	1.008999	3.749365	3.277126

		6	7	8	9	10
6	C	0.000000				
7	H	3.373258	0.000000			
8	H	3.871761	2.510829	0.000000		
9	H	1.067662	4.296698	4.935702	0.000000	
10	H	2.080115	4.820448	4.153949	2.370232	0.000000

Interatomic angles:

C1-N3-C2= 89.405	C1-C4-C2= 86.8382	N3-C1-C4= 92.1262
N3-C2-C4= 91.6306	C1-C5-C2= 85.5654	N3-C1-C5=124.8223
C2-N3-C5= 61.2883	C1-C5-C4=116.0307	C2-C4-C5=118.1114
N3-C5-C4= 88.9698	C1-C6-C2= 87.5916	C1-N3-C6=120.5562
C2-C6-N3=116.2982	C4-C1-C6= 61.3891	C4-C2-C6=124.1811
N3-C6-C4= 88.0191	C5-C1-C6= 94.0852	C5-C2-C6= 92.7578
C5-N3-C6= 92.4395	C5-C4-C6= 90.5717	C1-C2-H7= 87.0663
N3-C2-H7=116.6331	C1-C4-H7=151.0949	C2-C4-H7=122.0669
N3-C4-H7=179.7304	C1-C5-H7=141.5189	C2-H7-C5= 67.6207
N3-C5-H7=114.4579	C5-C4-H7=119.8218	C6-C2-H7=149.1836
C6-C4-H7=149.6066	C6-C5-H7= 84.5709	C2-C1-H8= 88.8586
N3-C1-H8=149.8868	C1-H8-C4= 66.2976	C2-C4-H8=142.78
N3-C4-H8= 84.5773	C1-C5-H8=122.252	C2-C5-H8=152.1826
N3-C5-H8=149.313	C4-C5-H8=121.7173	C6-C1-H8=119.1497
C6-C4-H8=115.2403	C6-C5-H8=179.2	C1-H8-H7= 91.4398
C2-H7-H8= 92.6354	H7-C4-H8= 95.1531	H7-C5-H8= 96.2291
C1-C2-H9= 85.5317	C1-N3-H9=147.2997	C2-H9-N3= 66.1405
C4-C2-H9=147.5954	C4-N3-H9= 88.0614	C5-C2-H9=116.1721
C5-N3-H9=119.1829	C1-C6-H9=145.8495	C2-C6-H9=126.5589
N3-C6-H9=117.1429	C4-C6-H9=154.8381	C5-C6-H9=174.8164
H7-C2-H9=172.5979	C2-C1-H10= 86.3658	C1-N3-H10=120.7867
C2-N3-H10=149.8083	C4-C1-H10=117.4638	C4-N3-H10=179.975
C5-C1-H10=150.16	C5-N3-H10=148.9034	C1-H10-C6= 70.0267
C2-C6-H10=141.4901	C6-N3-H10=118.6571	C4-C6-H10=113.2109
C5-C6-H10= 82.8653	H8-C1-H10=175.2244	C1-H10-H9= 96.7823
C2-H9-H10= 91.3202	H9-N3-H10= 91.9137	H9-C6-H10= 91.951

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Population analysis using the SCF density.

****

Orbital Symmetries:

Occupied	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A')	(A")	(A")	(A")	(A')	(A')	(A')
	(A')									
Virtual	(A')	(A')	(A")	(A')	(A')	(A")	(A')	(A")	(A')	(A')
	(A')	(A')	(A')	(A')	(A')	(A")	(A')	(A")	(A")	(A')
	(A')	(A")	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A")
	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A")	(A')	(A')
	(A')	(A')	(A")	(A")	(A')	(A')	(A')	(A')	(A')	(A')
	(A")	(A')	(A')	(A')	(A")	(A")	(A')	(A")	(A')	(A')
	(A")	(A")	(A')	(A')	(A")	(A")	(A")			

The electronic state is 3-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.198960D+01				
2	0.470042D-06	0.198673D+01			
3	-0.269174D-05	-0.449062D-05	0.100012D+01		
4	-0.959168D-05	0.543506D-05	-0.101105D-02	0.999686D+00	
5	0.405343D-05	0.208447D-05	0.132955D-04	-0.155268D-05	0.105175D-01
6	0.127468D-05	0.150519D-05	-0.109541D-04	-0.610934D-06	-0.244774D-06

	6
6	0.133514D-01

Test job not archived.

1\1\GINC-C4-31\SP\CASSCF\6-31G(d)\C5H4N1(1+,3)\MSCHOTT\21-May-1997\0\\
#P CAS(6,6)/6-31G* GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(
6/7=3) TEST\\aza-ene-diyne, protonated\\1,3\C,0.,1.3067368797,0.\C,0.0
220631447,-1.3563509629,0.\N,-1.1444137829,0.6606686733,0.\C,1.2337765
05,-0.7008809331,0.\C,1.2263701393,0.7157025218,0.\C,-1.1714968385,-0.
7374572318,0.\H,2.1658034839,-1.2286731397,0.\H,2.1319280923,1.2819278
106,0.\H,-2.1308344596,-1.206044598,0.\H,-2.0202783393,1.1616075715,0.
\\Version=DEC-AXP-OSF/1-G94RevC.3\State=3-A'\HF=-245.7710849\RMSD=0.00
0e+00\Dipole=-0.595757,0.3201607,0.\PG=CS [SG(C5H4N1)]\\@

MP2=-246.4540073

Protonated, Triplet Pyridyne, CAS(6,6)/6-31g* (triplet geometry) (scan1.pt.com)

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	2.642441	0.000000			
3	N	1.323141	2.321879	0.000000		
4	C	2.349390	1.384563	2.755286	0.000000	
5	C	1.367490	2.385729	2.392246	1.404819	0.000000
6	C	2.340584	1.352793	1.379591	2.424695	2.808104
7	H	3.336540	2.146853	3.825857	1.070753	2.160941
8	H	2.128481	3.376658	3.346923	2.176813	1.067945
9	H	3.291046	2.156134	2.105154	3.413888	3.874446
10	H	2.027853	3.242811	1.008738	3.763806	3.291122

		6	7	8	9	10
6	C	0.000000				
7	H	3.385762	0.000000			
8	H	3.875321	2.534626	0.000000		
9	H	1.067821	4.296389	4.940864	0.000000	
10	H	2.074515	4.834463	4.154213	2.384781	0.000000

Interatomic angles:

C1-N3-C2= 88.5141	C1-C4-C2= 85.997	N3-C1-C4= 92.962
N3-C2-C4= 92.5269	C1-C5-C2= 84.907	N3-C1-C5=125.5133
N3-C2-C5= 61.0656	C1-C5-C4=115.8641	C2-C4-C5=117.5817
N3-C5-C4= 89.107	C1-C6-C2= 87.0502	C1-N3-C6=119.9812
C2-C6-N3=116.3684	C4-C1-C6= 62.2615	C4-C2-C6=124.6913
N3-C6-C4= 88.3656	C5-C1-C6= 94.8128	C5-C2-C6= 93.23
C5-N3-C6= 92.2517	C5-C4-C6= 90.2757	C1-C2-H7= 87.6816
N3-C2-H7=117.7185	C1-C4-H7=152.5887	C2-C4-H7=121.4143
N3-C4-H7=178.7535	C1-C5-H7=140.9964	C2-H7-C5= 67.2576
N3-C5-H7=114.2394	C5-C4-H7=121.004	C6-C2-H7=149.8829
C6-C4-H7=148.7202	C6-C5-H7= 84.8389	C2-C1-H8= 89.4341
N3-C1-H8=150.883	C1-H8-C4= 66.1337	C2-C4-H8=141.9424
N3-C4-H8= 84.6031	C1-C5-H8=121.357	C2-C5-H8=153.7361
N3-C5-H8=148.1141	C4-C5-H8=122.779	C6-C1-H8=120.1825
C6-C4-H8=114.6365	C6-C5-H8=177.5145	C1-H8-H7= 90.9439
C2-H7-H8= 91.9405	H7-C4-H8= 96.6433	H7-C5-H8= 97.6466
C1-C2-H9= 85.972	C1-N3-H9=146.5591	C2-H9-N3= 66.0199
C4-C2-H9=148.4619	C4-N3-H9= 88.1789	C5-C2-H9=117.0007
C5-N3-H9=118.8295	C1-C6-H9=147.4273	C2-C6-H9=125.5225
N3-C6-H9=118.1091	C4-C6-H9=153.5253	C5-C6-H9=176.457
H7-C2-H9=173.6536	C2-C1-H10= 86.9038	C1-N3-H10=120.2291
C2-N3-H10=151.2568	C4-C1-H10=118.4168	C4-N3-H10=178.6093
C5-C1-H10=150.9681	C5-N3-H10=147.9587	C1-H10-C6= 69.5657
C2-C6-H10=141.3291	C6-N3-H10=119.7896	C4-C6-H10=113.3263
C5-C6-H10= 83.3086	H8-C1-H10=176.3378	C1-H10-H9= 96.1228
C2-H9-H10= 91.0014	H9-N3-H10= 93.2118	H9-C6-H10= 93.1484

****

Population analysis using the SCF density.

****

Orbital Symmetries:

Occupied	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A')	(A")	(A")	(A')	(A')	(A')	
	(A')									
Virtual	(A')	(A')	(A")	(A')	(A')	(A")	(A')	(A")	(A')	(A')
	(A')	(A')	(A')	(A')	(A')	(A")	(A')	(A")	(A")	(A')
	(A')	(A")	(A')	(A")	(A')	(A')	(A')	(A')	(A')	(A")
	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A')
	(A')	(A')	(A')	(A')	(A')	(A')	(A')	(A")	(A')	(A')
	(A')	(A')	(A")	(A")	(A')	(A')	(A')	(A')	(A')	(A')
	(A")	(A')	(A')	(A')	(A")	(A")	(A')	(A")	(A')	(A')
	(A")	(A")	(A')	(A')	(A")	(A")	(A")			

The electronic state is 3-A'.

Final one electron symbolic density matrix:

	1	2	3	4	5
1	0.199005D+01				
2	-0.283184D-06	0.198761D+01			
3	-0.192596D-04	-0.589819D-05	0.999856D+00		
4	0.179110D-04	0.567721D-05	-0.970506D-03	0.999950D+00	
5	-0.336477D-05	0.527489D-06	-0.123123D-04	-0.121964D-04	0.100663D-01
6	0.296606D-05	0.391962D-05	-0.707412D-05	-0.274718D-05	0.273339D-06

	6
6	0.124648D-01

Test job not archived.

1\1\GINC-C4-32\SP\CASSCF\6-31G(d)\C5H4N1(1+,3)\MSCHOTT\21-May-1997\0\\
#P CAS(6,6)/6-31G* GEOM=CHECK GUESS=READ # SCF=(CONVER=6) GFINPUT IOP(
6/7=3) TEST\\aza-ene-diyne, protonated\\1,3\C,0.,1.2959947165,0.\C,0.0
234354976,-1.3463425763,0.\N,-1.1565817295,0.6533281917,0.\C,1.2457246
771,-0.6959404551,0.\C,1.2350204027,0.7088376984,0.\C,-1.1787824638,-0
.7260846594,0.\H,2.1676761672,-1.2404746599,0.\H,2.1284801214,1.293847
8297,0.\H,-2.1286309368,-1.2139681664,0.\H,-2.0238419273,1.1685093098,
0.\\Version=DEC-AXP-OSF/1-G94RevC.3\State=3-A'\HF=-245.7720467\RMSD=0.
000e+00\Dipole=-0.5979223,0.3376246,0.\PG=CS [SG(C5H4N1)]\\@

MP2=-246.4568635