

Supporting Information for:

Accurate treatment of charge-transfer excitations and thermally activated delayed fluorescence using the particle-particle random phase approximation

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xyz coordinates for B3LYP/ cc-pVDZ optimized geometries

PhCz (1)

S₀ geometry

C	-2.954038	1.691039	0.104831
C	-1.940405	0.724104	0.039747
C	-0.579982	1.133882	0.060688
C	-0.222733	2.484107	0.160481
C	-1.251157	3.425189	0.223688
C	-2.604188	3.037488	0.193333
N	0.238204	0.000005	0.000015
C	1.661766	-0.000055	-0.000056
C	-0.580073	-1.133810	-0.060567
C	2.364958	-0.659498	1.018329
C	3.761845	-0.665313	1.009668
C	4.463979	-0.000188	-0.000178
C	3.761822	0.665000	-1.009967
C	2.364935	0.659312	-1.018510
C	-1.940463	-0.723917	-0.039739
C	-2.954171	-1.690770	-0.104867
C	-2.604425	-3.037251	-0.193297
C	-1.251424	-3.425064	-0.223546
C	-0.222927	-2.484065	-0.160298
H	-4.004370	1.391052	0.089876
H	0.823036	2.792231	0.192433
H	-0.997372	4.484841	0.301179
H	-3.384388	3.799718	0.243532
H	1.810808	-1.157786	1.815616
H	4.303560	-1.182614	1.804643
H	5.556041	-0.000241	-0.000226
H	4.303519	1.182244	-1.804992
H	1.810764	1.157644	-1.815754
H	-4.004479	-1.390696	-0.089979
H	-3.384684	-3.799418	-0.243529
H	-0.997719	-4.484738	-0.301014
H	0.822820	-2.792271	-0.192208

PhCz (1)

T₁ geometry

C	-2.98725000	1.69759200	0.07549000
C	-1.93837700	0.69661600	0.02987200
C	-0.53906800	1.14621000	0.05436100
C	-0.20121100	2.47840700	0.13986400
C	-1.26119400	3.42974000	0.19034700
C	-2.62589000	3.02389000	0.15369500
N	0.26415500	0.01007300	0.00907600
C	1.68712900	-0.00120200	0.00361700
C	-0.56099700	-1.13553400	-0.04478700
C	2.38795200	-0.69011500	1.00416300
C	3.78454200	-0.70627600	0.99074000

C	4.48914900	-0.02490700	-0.00652600
C	3.78899600	0.66808900	-0.99887200
C	2.39227000	0.67508200	-1.00243900
C	-1.94057900	-0.68271100	-0.02682000
C	-3.00691300	-1.67635600	-0.08215800
C	-2.65742200	-3.02208500	-0.16339000
C	-1.31711700	-3.42756500	-0.19093800
C	-0.22592200	-2.45607900	-0.13131300
H	-4.03398100	1.39227100	0.05129200
H	0.83887900	2.80249300	0.17420100
H	-1.02004400	4.49158100	0.26031300
H	-3.40136400	3.79288700	0.19094000
H	1.83269300	-1.20361600	1.79067200
H	4.32443100	-1.24554900	1.77226500
H	5.58115000	-0.03405900	-0.01042600
H	4.33224000	1.19817200	-1.78434900
H	1.84009400	1.19720300	-1.78547800
H	-4.05001100	-1.35920200	-0.06294100
H	-3.44314800	-3.77996000	-0.20642700
H	-1.06873700	-4.48792900	-0.25842200
H	0.81012500	-2.79157800	-0.16460500

NPh₃ (2)

S₀ geometry

C	-1.569507	-3.290421	-0.804833
C	-0.678326	-2.216259	-0.816000
C	-0.908593	-1.093677	-0.000303
C	-2.053512	-1.070315	0.816459
C	-2.947982	-2.141741	0.807487
C	-2.711576	-3.260173	0.001844
N	0.000686	-0.000293	-0.001538
C	-0.492183	1.333684	-0.001417
C	1.402126	-0.240738	-0.001081
C	0.099212	2.314413	0.815208
C	-0.382945	3.624241	0.805817
C	-1.470067	3.977270	-0.000039
C	-2.066123	3.002381	-0.806402
C	-1.579964	1.694063	-0.817128
C	1.955078	-1.245541	0.813367
C	3.330435	-1.482982	0.804415
C	4.180557	-0.716265	0.001151
C	3.634976	0.289178	-0.803398
C	2.258941	0.522578	-0.814646
H	-1.374102	-4.153911	-1.445174
H	0.204265	-2.241141	-1.457091
H	-2.237627	-0.206086	1.456597
H	-3.832019	-2.105613	1.448575
H	-3.410027	-4.099427	0.002588
H	0.939720	2.042814	1.455791
H	0.089292	4.372435	1.446936
H	-1.848865	5.001330	0.000455
H	-2.912054	3.263681	-1.446677
H	-2.042059	0.941388	-1.457858
H	1.299345	-1.839048	1.452377
H	3.741639	-2.267667	1.443960
H	5.256796	-0.900345	0.002118
H	4.284667	0.892298	-1.442139
H	1.838807	1.300235	-1.454400

NPh₃ (2)

T₁ geometry

C	0.90204000	-3.50516000	-0.74399700
C	0.96579400	-2.14345100	-0.74238300
C	-0.03364300	-1.36167600	0.00214000
C	-1.07517300	-2.08782400	0.74602100
C	-1.08875100	-3.45107100	0.74354300
C	-0.11454600	-4.20852300	-0.00155900
N	0.00215400	0.02422800	0.00018900

C	-1.20758700	0.76615700	-0.02774600
C	1.24840900	0.70325600	0.02669400
C	-1.35828700	1.92984000	0.75791400
C	-2.56941400	2.61441100	0.76037100
C	-3.65286100	2.15338300	-0.00386100
C	-3.50666300	0.99436200	-0.77578200
C	-2.29912900	0.29890100	-0.79153300
C	2.31405300	0.18310600	0.79253600
C	3.55491900	0.81716100	0.77741300
C	3.75991200	1.96615500	0.00378900
C	2.70212800	2.47944200	-0.76277600
C	1.45819300	1.85621400	-0.76106000
H	1.62566800	-4.07722700	-1.33005200
H	1.71312600	-1.61549100	-1.33607300
H	-1.79032200	-1.52015900	1.34259400
H	-1.84293900	-3.98286500	1.32900500
H	-0.14501400	-5.29820000	-0.00265000
H	-0.52501500	2.27625800	1.37079700
H	-2.67653200	3.51168100	1.37416300
H	-4.60239600	2.69201400	0.00721500
H	-4.34053000	0.63155800	-1.38107200
H	-2.17497500	-0.59523900	-1.40343100
H	2.14454400	-0.70268100	1.40573900
H	4.36882300	0.41420900	1.38444600
H	4.73521000	2.45662600	-0.00664600
H	2.85487300	3.36906600	-1.37803200
H	0.64404200	2.24275200	-1.37567100

CBP (3)

S₀ geometry

C	-7.840546	-2.323348	-1.964958
C	-8.189460	-1.295180	-1.090756
C	-7.175054	-0.558413	-0.462621
C	-5.815163	-0.875874	-0.723661
C	-5.458851	-1.899557	-1.610034
C	-6.487945	-2.616606	-2.221863
C	-7.175055	0.558415	0.462623
C	-5.815164	0.875870	0.723673
N	-4.996004	0.000000	0.000003
C	-8.189461	1.295186	1.090753
C	-7.840549	2.323349	1.964960
C	-6.487948	2.616601	2.221874
C	-5.458854	1.899549	1.610050
C	-3.575238	0.000001	0.000002
C	-2.864984	1.146533	-0.383500
C	-1.470992	1.144888	-0.374496
C	-0.742506	0.000001	0.000001
C	-1.470992	-1.144887	0.374497
C	-2.864984	-1.146532	0.383503
C	0.742506	0.000001	-0.000001
C	1.470993	1.144888	0.374496
C	2.864985	1.146533	0.383500
C	3.575238	0.000000	-0.000002
C	2.864984	-1.146532	-0.383503
C	1.470992	-1.144887	-0.374497
N	4.996004	0.000000	-0.000003
C	5.815163	0.875872	-0.723670
C	7.175054	0.558414	-0.462626
C	7.175054	-0.558413	0.462620
C	5.815164	-0.875873	0.723663
C	8.189461	-1.295181	1.090753
C	7.840548	-2.323347	1.964957
C	6.487947	-2.616603	2.221866
C	5.458853	-1.899554	1.610038
C	5.458852	1.899552	-1.610045
C	6.487947	2.616603	-2.221873
C	7.840547	2.323348	-1.964963
C	8.189461	1.295182	-1.090758
H	-8.621290	-2.904911	-2.459317

H	-9.239515	-1.062384	-0.899731
H	-4.413621	-2.127801	-1.821810
H	-6.234831	-3.420481	-2.916764
H	-9.239516	1.062393	0.899721
H	-8.621293	2.904915	2.459315
H	-6.234835	3.420475	2.916777
H	-4.413623	2.127791	1.821830
H	-3.411938	2.033666	-0.706982
H	-0.938937	2.039802	-0.703012
H	-0.938936	-2.039800	0.703012
H	-3.411937	-2.033666	0.706984
H	0.938937	2.039802	0.703011
H	3.411939	2.033666	0.706981
H	3.411937	-2.033666	-0.706985
H	0.938936	-2.039800	-0.703012
H	9.239516	-1.062386	0.899726
H	8.621292	-2.904911	2.459316
H	6.234833	-3.420478	2.916768
H	4.413622	-2.127798	1.821815
H	4.413622	2.127796	-1.821824
H	6.234833	3.420477	-2.916775
H	8.621291	2.904912	-2.459321
H	9.239516	1.062388	-0.899730

CBP (3)

T₁ geometry

C	-7.85262000	-2.27095000	2.02166500
C	-8.19886100	-1.25601800	1.12881200
C	-7.18240600	-0.53353000	0.49205100
C	-5.82345000	-0.83773900	0.76890800
C	-5.47057900	-1.87361700	1.64308000
C	-6.50189800	-2.57720700	2.26771300
C	-7.18240600	0.53353200	-0.49205200
C	-5.82344900	0.83774000	-0.76890900
N	-4.99756900	0.00000000	0.00000000
C	-8.19885900	1.25602200	-1.12881300
C	-7.85261700	2.27095300	-2.02166600
C	-6.50189400	2.57720800	-2.26771400
C	-5.47057600	1.87361600	-1.64308100
C	-3.59126800	-0.00000100	0.00000000
C	-2.85807600	-0.01969000	-1.22463000
C	-1.48832400	-0.02227600	-1.23039800
C	-0.70248400	-0.00000200	0.00000000
C	-1.48832500	0.02227200	1.23039800
C	-2.85807600	0.01968700	1.22462900
C	0.70248500	-0.00000200	0.00000000
C	1.48832500	0.02223200	-1.23039800
C	2.85807600	0.01964700	-1.22462900
C	3.59126800	-0.00000200	0.00000100
C	2.85807500	-0.01965200	1.22463100
C	1.48832400	-0.02223700	1.23039900
N	4.99756900	-0.00000200	0.00000100
C	5.82345000	-0.83776300	-0.76888200
C	7.18240600	-0.53354400	-0.49203600
C	7.18240600	0.53354700	0.49203500
C	5.82344900	0.83776300	0.76888400
C	8.19885900	1.25605700	1.12877400
C	7.85261800	2.27101500	2.02159600
C	6.50189500	2.57727700	2.26763500
C	5.47057600	1.87366600	1.64302400
C	5.47057900	-1.87366700	-1.64302200
C	6.50189800	-2.57727600	-2.26763500
C	7.85262000	-2.27101000	-2.02159700
C	8.19886000	-1.25605100	-1.12877600
H	-8.63540900	-2.84058300	2.52649600
H	-9.24803900	-1.03286000	0.92277800
H	-4.42794900	-2.13422200	1.82384900
H	-6.25059000	-3.38703100	2.95606700

H	-9.24803700	1.03286600	-0.92277800
H	-8.63540500	2.84058700	-2.52649700
H	-6.25058600	3.38703200	-2.95606900
H	-4.42794700	2.13422000	-1.82385100
H	-3.40350100	-0.07307900	-2.16830700
H	-0.98052300	-0.07020900	-2.19227900
H	-0.98052400	0.07020600	2.19228000
H	-3.40350100	0.07307700	2.16830700
H	0.98052400	0.07013500	-2.19228100
H	3.40350200	0.07300700	-2.16830800
H	3.40350100	-0.07301200	2.16831000
H	0.98052300	-0.07014000	2.19228200
H	9.24803700	1.03289500	0.92274500
H	8.63540600	2.84066500	2.52641000
H	6.25058600	3.38712100	2.95596600
H	4.42794700	2.13427500	1.82378700
H	4.42794900	-2.13427900	-1.82378300
H	6.25059000	-3.38712100	-2.95596400
H	8.63540900	-2.84065800	-2.52641200
H	9.24803800	-1.03288700	-0.92274900

α -NPD (4)

S₀ geometry

C	2.903142	0.007287	0.992048
C	3.563631	-0.568827	-0.106600
C	2.791079	-0.939768	-1.224702
C	1.412954	-0.748018	-1.231061
C	0.738646	-0.167590	-0.137802
C	1.523281	0.205403	0.968656
C	-0.728793	0.045261	-0.160228
C	-1.592898	-0.847714	-0.819737
C	-2.971218	-0.642097	-0.862202
C	-3.551197	0.468014	-0.224391
C	-2.699267	1.359802	0.456468
C	-1.322925	1.154352	0.474950
N	-4.955401	0.670169	-0.233320
N	4.971798	-0.738905	-0.110161
C	5.566153	-1.916821	-0.643516
C	5.789160	0.142454	0.667582
C	-5.508083	1.973270	-0.387372
C	-5.826909	-0.454655	-0.395605
C	6.812082	-1.836262	-1.291956
C	7.414676	-2.983811	-1.808109
C	6.784432	-4.228227	-1.702358
C	5.544512	-4.311222	-1.061793
C	4.940659	-3.171270	-0.527336
C	5.891641	1.530990	0.314413
C	6.704355	2.388207	1.132316
C	7.406032	1.840918	2.242293
C	7.312417	0.497883	2.536166
C	6.495443	-0.350085	1.752571
C	-6.712146	2.298102	0.263913
C	-7.277777	3.564290	0.111878
C	-6.650655	4.534484	-0.676954
C	-5.452103	4.216472	-1.322515
C	-4.886381	2.946600	-1.190112
C	-5.930985	-1.441904	0.642162
C	-6.800178	-2.566631	0.433384
C	-7.552765	-2.658831	-0.770419
C	-7.454955	-1.678200	-1.733619
C	-6.583634	-0.579445	-1.548836
C	-5.228235	-1.343343	1.875863
C	-5.359449	-2.315974	2.845162
C	-6.197947	-3.438086	2.630432
C	-6.903061	-3.555496	1.452340
C	5.241951	2.090007	-0.821871
C	5.369994	3.429951	-1.123310

C	6.151893	4.281137	-0.303372
C	6.805374	3.767862	0.795897
H	3.475502	0.295396	1.874698
H	3.281766	-1.368874	-2.099718
H	0.850685	-1.020462	-2.126782
H	1.042151	0.631437	1.851624
H	-1.182904	-1.736693	-1.303687
H	-3.606921	-1.356202	-1.386869
H	-3.122376	2.227488	0.964822
H	-0.692221	1.884911	0.985845
H	7.302876	-0.866275	-1.387318
H	8.382106	-2.900546	-2.309113
H	7.255140	-5.123323	-2.113996
H	5.043564	-5.277165	-0.961541
H	3.980058	-3.248841	-0.016333
H	8.026484	2.502295	2.851937
H	7.856183	0.080121	3.386272
H	6.413057	-1.409698	2.000478
H	-7.200030	1.549190	0.890014
H	-8.213102	3.797424	0.626340
H	-7.091951	5.527082	-0.787683
H	-4.954630	4.959246	-1.950855
H	-3.958589	2.704256	-1.709998
H	-8.215221	-3.515985	-0.913609
H	-8.037828	-1.749411	-2.654524
H	-6.499139	0.185807	-2.322349
H	-4.583235	-0.482669	2.049655
H	-4.814440	-2.220319	3.786942
H	-6.288320	-4.204383	3.403653
H	-7.560672	-4.412125	1.283453
H	4.639386	1.443429	-1.458801
H	4.866106	3.838618	-2.002081
H	6.240099	5.341723	-0.549564
H	7.419958	4.414901	1.427139

α -NPD (4)

T₁ geometry

C	2.91946700	0.34895000	1.02053300
C	3.55461200	-0.56316200	0.12565400
C	2.72894800	-1.23238500	-0.83564900
C	1.37816900	-1.01679600	-0.88618100
C	0.69578500	-0.10773100	0.02277800
C	1.56644000	0.56453300	0.97857600
C	-0.69586200	0.10772000	-0.02259400
C	-1.56650500	-0.56427400	-0.97857600
C	-2.91952900	-0.34867900	-1.02046800
C	-3.55467500	0.56313600	-0.12527000
C	-2.72902500	1.23210000	0.83618400
C	-1.37822900	1.01655500	0.88660800
N	-4.94598500	0.74736300	-0.13936500
N	4.94592600	-0.74733800	0.13976200
C	5.51981200	-2.02498900	-0.09962200
C	5.80193400	0.32009300	0.55622800
C	-5.51974400	2.02501400	0.10046900
C	-5.80208000	-0.31980100	-0.55626400
C	6.74406800	-2.12944400	-0.78784200
C	7.31075200	-3.38064800	-1.02543600
C	6.66827600	-4.54781400	-0.59548700
C	5.45076900	-4.44651100	0.08538100
C	4.87893800	-3.19916400	0.33952600
C	5.83534000	1.56136000	-0.16969100
C	6.70563500	2.60218600	0.30630700
C	7.51375700	2.37657600	1.45563500
C	7.47373500	1.16581300	2.11460700
C	6.61315900	0.13945000	1.66800800
C	-6.74383000	2.12939000	0.78897500
C	-7.31035500	3.38059500	1.02698700
C	-6.66786600	4.54780200	0.59717400
C	-5.45051300	4.44656100	-0.08398000

C	-4.87885000	3.19921800	-0.33854000
C	-5.83538600	-1.56149800	0.16893700
C	-6.70580000	-2.60201600	-0.30749300
C	-7.51418600	-2.37571800	-1.45649800
C	-7.47428600	-1.16456600	-2.11475600
C	-6.61355700	-0.13850200	-1.66775300
C	-5.07723000	-1.79955200	1.34956500
C	-5.16115100	-3.00468500	2.01648200
C	-6.00166700	-4.03786300	1.53533400
C	-6.75619600	-3.83618900	0.39976600
C	5.07742400	1.79868300	-1.35061400
C	5.16146800	3.00342100	-2.01824300
C	6.00186500	4.03689000	-1.53754600
C	6.75616100	3.83592300	-0.40168500
H	3.52619200	0.87297500	1.76097900
H	3.19376900	-1.91184100	-1.55206500
H	0.80656800	-1.54095500	-1.65098900
H	1.13807200	1.25794000	1.70088300
H	-1.13813300	-1.25743900	-1.70110900
H	-3.52627300	-0.87245200	-1.76107800
H	-3.19385200	1.91133700	1.55280700
H	-0.80660100	1.54049500	1.65154600
H	7.24195700	-1.22334400	-1.13618200
H	8.25984300	-3.44462500	-1.56277900
H	7.11322400	-5.52599900	-0.78866300
H	4.94368100	-5.34795500	0.43748800
H	3.93870500	-3.12409200	0.88727100
H	8.17158900	3.17729600	1.80185800
H	8.09686700	0.99589600	2.99526500
H	6.57357100	-0.81170200	2.20127000
H	-7.24172700	1.22324900	1.13719900
H	-8.25932200	3.44453200	1.56455400
H	-7.11269000	5.52597800	0.79068000
H	-4.94341500	5.34804400	-0.43597300
H	-3.93872100	3.12418200	-0.88647100
H	-8.17212400	-3.17622000	-1.80302700
H	-8.09761100	-0.99408400	-2.99516800
H	-6.57406000	0.81294900	-2.20048900
H	-4.42110000	-1.01704000	1.72864300
H	-4.57177200	-3.16326200	2.92227000
H	-6.05283900	-4.99019100	2.06784000
H	-7.41447600	-4.62417100	0.02490100
H	4.42138100	1.01593100	-1.72934500
H	4.57227800	3.16144500	-2.92425100
H	6.05314900	4.98889600	-2.07061700
H	7.41433900	4.62415700	-0.02717500

PIC-TRZ (5)

S₀ geometry

N	1.703095	0.920131	-0.753445
N	-0.360366	-0.000015	0.000003
N	1.703099	-0.920156	0.753443
N	-0.329788	1.856896	-1.420357
N	-2.303940	-0.630507	-2.351375
N	-0.329782	-1.856917	1.420373
N	-2.303916	0.630513	2.351358
C	2.327099	-0.000012	-0.000002
C	0.367114	0.878289	-0.698412
C	0.367118	-0.878318	0.698414
C	3.808931	-0.000009	-0.000003
C	4.526388	-0.760042	0.939649
H	3.975088	-1.349535	1.672257
C	5.918595	-0.755233	0.940435
H	6.454064	-1.368119	1.668135
C	6.646367	-0.000004	-0.000005
C	5.918591	0.755223	-0.940443
H	6.454056	1.368112	-1.668143
C	4.526384	0.760026	-0.939656
H	3.975080	1.349518	-1.672263

C	8.132027	-0.000001	-0.000005
C	8.855913	-0.021789	1.207283
H	8.317995	-0.012595	2.157571
C	10.251916	-0.020212	1.207246
H	10.792192	-0.027319	2.156755
C	10.956707	0.000004	-0.000006
H	12.048946	0.000006	-0.000007
C	10.251915	0.020218	-1.207258
H	10.792190	0.027326	-2.156768
C	8.855912	0.021790	-1.207294
H	8.317993	0.012594	-2.157582
C	0.028629	3.236037	-1.345428
C	1.274430	3.832584	-1.132122
H	2.168135	3.225773	-1.017214
C	1.327293	5.229242	-1.078764
H	2.293212	5.715039	-0.923308
C	0.172859	6.014530	-1.232247
H	0.248965	7.103214	-1.192771
C	-1.067353	5.412212	-1.441235
H	-1.967699	6.018554	-1.560844
C	-1.143589	4.013929	-1.496774
C	-2.255127	3.102907	-1.704410
C	-3.625764	3.349703	-1.909592
H	-4.007830	4.371525	-1.883111
C	-4.478102	2.279046	-2.134806
H	-5.548889	2.440875	-2.271478
C	-3.946528	0.980847	-2.240936
C	-4.568547	-0.281243	-2.579410
C	-5.893751	-0.653941	-2.848340
H	-6.698991	0.080763	-2.778225
C	-6.164660	-1.970585	-3.213780
H	-7.191367	-2.277188	-3.424185
C	-5.121968	-2.909472	-3.322225
H	-5.350293	-3.934740	-3.622033
C	-3.796992	-2.561783	-3.055283
H	-2.999765	-3.297680	-3.154239
C	-3.532571	-1.243616	-2.665242
C	-2.555978	0.722293	-2.080556
C	-1.721460	1.792272	-1.702553
C	-1.053790	-1.170826	-2.781591
C	-0.279694	-0.488465	-3.730892
H	-0.629944	0.465361	-4.127668
C	0.930476	-1.034123	-4.166680
H	1.529340	-0.492123	-4.901884
C	1.366018	-2.268866	-3.678090
H	2.310455	-2.694666	-4.023500
C	0.587541	-2.953315	-2.738752
H	0.923191	-3.911984	-2.338191
C	-0.614238	-2.406003	-2.284278
H	-1.204034	-2.921825	-1.525922
C	0.028628	-3.236060	1.345461
C	1.274425	-3.832618	1.132154
H	2.168132	-3.225814	1.017229
C	1.327279	-5.229277	1.078816
H	2.293195	-5.715081	0.923358
C	0.172843	-6.014556	1.232321
H	0.248943	-7.103242	1.192861
C	-1.067364	-5.412228	1.441311
H	-1.967711	-6.018565	1.560938
C	-1.143592	-4.013945	1.496830
C	-2.255124	-3.102914	1.704464
C	-3.625760	-3.349702	1.909664
H	-4.007831	-4.371522	1.883205
C	-4.478091	-2.279037	2.134871
H	-5.548877	-2.440859	2.271558
C	-3.946511	-0.980839	2.240972
C	-4.568521	0.281260	2.579430
C	-5.893721	0.653968	2.848369
H	-6.698965	-0.080735	2.778278
C	-6.164621	1.970620	3.213788

H	-7.191324	2.277230	3.424200
C	-5.121924	2.909505	3.322202
H	-5.350241	3.934779	3.621993
C	-3.796953	2.561807	3.055249
H	-2.999722	3.297703	3.154180
C	-3.532541	1.243631	2.665230
C	-2.555962	-0.722293	2.080571
C	-1.721452	-1.792282	1.702580
C	-1.053758	1.170838	2.781542
C	-0.614211	2.406002	2.284192
H	-1.204017	2.921806	1.525832
C	0.587578	2.953321	2.738631
H	0.923223	3.911979	2.338041
C	1.366069	2.268892	3.677972
H	2.310513	2.694697	4.023356
C	0.930531	1.034162	4.166599
H	1.529406	0.492178	4.901806
C	-0.279647	0.488497	3.730846
H	-0.629894	-0.465319	4.127651

PIC-TRZ (5)

T₁ geometry

N	-1.68619400	0.91329600	0.77939600
N	0.37368100	0.00000700	-0.00012800
N	-1.68616900	-0.91344500	-0.77952000
N	0.34937700	1.84484400	1.44040300
N	2.27357600	-0.67763700	2.37355100
N	0.34943800	-1.84484800	-1.44064400
N	2.27375400	0.67761700	-2.37362200
C	-2.32635400	-0.00009500	-0.00005700
C	-0.35995700	0.87078200	0.71185700
C	-0.35992400	-0.87084400	-0.71204900
C	-3.76443100	-0.00012000	-0.00003200
C	-4.51758900	-0.86053600	-0.88790500
H	-3.96111100	-1.49923900	-1.57269100
C	-5.87728000	-0.85914900	-0.88996400
H	-6.39199300	-1.51859000	-1.58725500
C	-6.66233300	-0.00011100	-0.00003200
C	-5.87727700	0.85886100	0.88995600
H	-6.39198700	1.51823800	1.58730900
C	-4.51758600	0.86025600	0.88788500
H	-3.96110200	1.49892500	1.57269900
C	-8.07954600	-0.00002800	-0.00011100
C	-8.84776300	-0.86351900	-0.86735800
H	-8.33556300	-1.54298600	-1.54628100
C	-10.22899200	-0.85680100	-0.86035500
H	-10.77136300	-1.52649900	-1.53162500
C	-10.94446400	0.00014000	-0.00026700
H	-12.03578700	0.00020100	-0.00032300
C	-10.22898500	0.85700000	0.85989600
H	-10.77135000	1.52676500	1.53110400
C	-8.84775600	0.86355800	0.86704700
H	-8.33554900	1.54297600	1.54601400
C	0.01519500	3.22638200	1.35778600
C	-1.21792300	3.84143900	1.12202600
H	-2.11713700	3.24646600	0.98886900
C	-1.25063600	5.23844800	1.06938200
H	-2.20652400	5.73809200	0.89617900
C	-0.08828800	6.00789300	1.24532500
H	-0.14870100	7.09758900	1.20598900
C	1.13938000	5.38812400	1.47533400
H	2.04582500	5.98191100	1.61121500
C	1.19550500	3.98860500	1.52996900
C	2.28920000	3.06057900	1.75145400
C	3.66160700	3.28390600	1.97145000
H	4.06024500	4.29962000	1.95365900
C	4.49523400	2.19865200	2.19716300
H	5.56720400	2.34272000	2.34415800
C	3.94208900	0.90812700	2.28848000

C	4.54126400	-0.36647400	2.62156400
C	5.85788300	-0.76273900	2.89767400
H	6.67531200	-0.04048700	2.84034900
C	6.10489600	-2.08683400	3.25380200
H	7.12496000	-2.41156900	3.46933200
C	5.04663000	-3.00988000	3.34610300
H	5.25623400	-4.04122200	3.63864100
C	3.72956900	-2.63862300	3.07202200
H	2.91992900	-3.36245700	3.15811100
C	3.48912600	-1.31300200	2.69121100
C	2.54958900	0.67308800	2.11475400
C	1.73360800	1.75804700	1.73737100
C	1.01198800	-1.20063200	2.79217700
C	0.24387400	-0.51225600	3.74191600
H	0.60578400	0.43467500	4.14457200
C	-0.97553900	-1.04296800	4.16997100
H	-1.57001100	-0.49589700	4.90496300
C	-1.42624200	-2.26897700	3.67346300
H	-2.37773000	-2.68346600	4.01336400
C	-0.65414500	-2.95893400	2.73294100
H	-1.00163000	-3.91034200	2.32524400
C	0.55674100	-2.42618200	2.28567300
H	1.14135300	-2.94570000	1.52589800
C	0.01528400	-3.22640900	-1.35803900
C	-1.21786200	-3.84149900	-1.12252600
H	-2.11711600	-3.24654700	-0.98955300
C	-1.25054500	-5.23850900	-1.06986500
H	-2.20645500	-5.73817800	-0.89685000
C	-0.08814000	-6.00792100	-1.24555700
H	-0.14852700	-7.09761900	-1.20621400
C	1.13955600	-5.38811900	-1.47533800
H	2.04604300	-5.98188100	-1.61103800
C	1.19564600	-3.98860000	-1.52998900
C	2.28935900	-3.06055300	-1.75131700
C	3.66180300	-3.28387000	-1.97109400
H	4.06045500	-4.29957600	-1.95318900
C	4.49543700	-2.19860700	-2.19673800
H	5.56743300	-2.34265400	-2.34356500
C	3.94227800	-0.90809900	-2.28820100
C	4.54147300	0.36648800	-2.62128300
C	5.85812000	0.76276400	-2.89724900
H	6.67555900	0.04053400	-2.83976400
C	6.10515200	2.08683800	-3.25343700
H	7.12523800	2.41157900	-3.46885500
C	5.04687700	3.00985500	-3.34595000
H	5.25649800	4.04117900	-3.63853800
C	3.72978800	2.63859100	-3.07202000
H	2.92014200	3.36239900	-3.15827800
C	3.48932400	1.31299300	-2.69113500
C	2.54974100	-0.67307600	-2.11468800
C	1.73373400	-1.75804000	-1.73737900
C	1.01216800	1.20069200	-2.79212600
C	0.55700400	2.42623400	-2.28552700
H	1.14169300	2.94568600	-1.52576500
C	-0.65389400	2.95905000	-2.73268100
H	-1.00132200	3.91044800	-2.32490900
C	-1.42608300	2.26916800	-3.67318500
H	-2.37758100	2.68371000	-4.01299500
C	-0.97545800	1.04317200	-4.16979300
H	-1.57000200	0.49616300	-4.90477300
C	0.24396900	0.51239600	-3.74185400
H	0.60582400	-0.43452300	-4.14458600

DPA-DPS (6)

S₀ geometry

C	1.677759	-1.260356	-1.433290
S	2.553675	-1.920028	0.000000
C	1.677759	-1.260356	1.433290
C	2.082780	-0.045715	1.994631

C	1.416225	0.456609	3.108720
C	0.349053	-0.259531	3.691665
C	-0.026160	-1.496546	3.125347
C	0.631987	-1.992533	2.003760
C	2.082780	-0.045715	-1.994631
C	1.416225	0.456609	-3.108720
C	0.349053	-0.259531	-3.691665
C	-0.026160	-1.496546	-3.125347
C	0.631987	-1.992533	-2.003760
O	3.913754	-1.309550	0.000000
O	2.344219	-3.396133	0.000000
N	-0.322006	0.244765	-4.824893
N	-0.322006	0.244765	4.824893
C	0.379809	1.012232	-5.802733
C	-1.712313	-0.008929	-5.019863
C	-1.712313	-0.008929	5.019863
C	0.379809	1.012232	5.802733
C	1.610886	0.566410	-6.312978
C	2.289171	1.323023	-7.270186
C	1.744234	2.520180	-7.745610
C	0.513636	2.959335	-7.247289
C	-0.163079	2.217737	-6.277003
C	-2.184481	-0.433971	-6.272861
C	-3.547645	-0.662856	-6.469477
C	-4.455610	-0.487640	-5.420584
C	-3.986940	-0.069773	-4.170807
C	-2.627923	0.178198	-3.970097
C	1.610886	0.566410	6.312978
C	2.289171	1.323023	7.270186
C	1.744234	2.520180	7.745610
C	0.513636	2.959335	7.247289
C	-0.163079	2.217737	6.277003
C	-2.184481	-0.433971	6.272861
C	-3.547645	-0.662856	6.469477
C	-4.455610	-0.487640	5.420584
C	-3.986940	-0.069773	4.170807
C	-2.627923	0.178198	3.970097
H	2.922837	0.497764	1.560397
H	1.725354	1.409188	3.539890
H	-0.829142	-2.075860	3.582038
H	0.363090	-2.964119	1.587372
H	2.922837	0.497764	-1.560397
H	1.725354	1.409188	-3.539890
H	-0.829142	-2.075860	-3.582038
H	0.363090	-2.964119	-1.587372
H	2.033097	-0.374176	-5.954939
H	3.245856	0.964519	-7.657009
H	2.274175	3.105590	-8.499728
H	0.078993	3.894803	-7.607108
H	-1.118593	2.567088	-5.882202
H	-1.476966	-0.581225	-7.090476
H	-3.899771	-0.992951	-7.449522
H	-5.520220	-0.673872	-5.575984
H	-4.686799	0.079566	-3.345305
H	-2.267486	0.518038	-2.997689
H	2.033097	-0.374176	5.954939
H	3.245856	0.964519	7.657009
H	2.274175	3.105590	8.499728
H	0.078993	3.894803	7.607108
H	-1.118593	2.567088	5.882202
H	-1.476966	-0.581225	7.090476
H	-3.899771	-0.992951	7.449522
H	-5.520220	-0.673872	5.575984
H	-4.686799	0.079566	3.345305
H	-2.267486	0.518038	2.997689

DPA-DPS (6)

T₁ geometry

C	-2.25501400	1.05601300	-1.37968400
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S	-3.25778000	1.52208700	0.00000000
C	-2.25501400	1.05601300	1.37968400
C	-2.34201100	-0.26364400	1.91285900
C	-1.46628700	-0.66993200	2.89499000
C	-0.46412600	0.21900400	3.39092500
C	-0.39638200	1.54453800	2.86449500
C	-1.27359700	1.95853300	1.88661000
C	-2.34201100	-0.26364400	-1.91285900
C	-1.46628700	-0.66993200	-2.89499000
C	-0.46412600	0.21900400	-3.39092500
C	-0.39638200	1.54453800	-2.86449500
C	-1.27359700	1.95853300	-1.88661000
O	-4.46255300	0.63891900	0.00000000
O	-3.35810300	3.01221200	0.00000000
N	0.42837400	-0.19761400	-4.39945400
N	0.42837400	-0.19761400	4.39945400
C	-0.04274500	-0.99234500	-5.47759300
C	1.79422100	0.17618600	-4.33752300
C	1.79422100	0.17618600	4.33752300
C	-0.04274500	-0.99234500	5.47759300
C	-1.29308700	-0.71680100	-6.06487300
C	-1.76404900	-1.51131900	-7.10910600
C	-1.00256800	-2.58410300	-7.58685500
C	0.24036900	-2.85917800	-7.00395700
C	0.71964300	-2.07689000	-5.95470300
C	2.49076700	0.54768300	-5.50567000
C	3.83071800	0.92255200	-5.43065200
C	4.49723200	0.94460600	-4.19932800
C	3.80538500	0.58214600	-3.03775500
C	2.46684700	0.19864000	-3.09911900
C	-1.29308700	-0.71680100	6.06487300
C	-1.76404900	-1.51131900	7.10910600
C	-1.00256800	-2.58410300	7.58685500
C	0.24036900	-2.85917800	7.00395700
C	0.71964300	-2.07689000	5.95470300
C	2.49076700	0.54768300	5.50567000
C	3.83071800	0.92255200	5.43065200
C	4.49723200	0.94460600	4.19932800
C	3.80538500	0.58214600	3.03775500
C	2.46684700	0.19864000	3.09911900
H	-3.11786000	-0.93357700	1.54154700
H	-1.53237300	-1.68076500	3.30100700
H	0.33341500	2.24415300	3.27597500
H	-1.25900800	2.98489600	1.51917300
H	-3.11786000	-0.93357700	-1.54154700
H	-1.53237300	-1.68076500	-3.30100700
H	0.33341500	2.24415300	-3.27597500
H	-1.25900800	2.98489600	-1.51917300
H	-1.88153600	0.12587900	-5.69970700
H	-2.73195800	-1.28261800	-7.56047200
H	-1.37558900	-3.20265300	-8.40549000
H	0.83815200	-3.70077500	-7.36106200
H	1.67999600	-2.30532400	-5.49045600
H	1.97043600	0.54962700	-6.46432800
H	4.35658900	1.21406900	-6.34259100
H	5.54575200	1.24398000	-4.14599300
H	4.31679000	0.58734300	-2.07255300
H	1.93154300	-0.09631200	-2.19582500
H	-1.88153600	0.12587900	5.69970700
H	-2.73195800	-1.28261800	7.56047200
H	-1.37558900	-3.20265300	8.40549000
H	0.83815200	-3.70077500	7.36106200
H	1.67999600	-2.30532400	5.49045600
H	1.97043600	0.54962700	6.46432800
H	4.35658900	1.21406900	6.34259100
H	5.54575200	1.24398000	4.14599300
H	4.31679000	0.58734300	2.07255300
H	1.93154300	-0.09631200	2.19582500

DTPA-DPS (7)

S₀ geometry

C	-1.420944	0.142133	-2.901614
S	-0.003104	-0.049814	-4.000718
C	1.418403	-0.215910	-2.902484
O	0.158120	1.236861	-4.736793
O	-0.167077	-1.353321	-4.706034
C	1.835997	-1.487265	-2.497087
C	2.941246	-1.617394	-1.661401
C	3.645263	-0.478055	-1.214700
C	3.217242	0.794689	-1.650653
C	2.119334	0.923569	-2.496163
C	-1.828396	1.422386	-2.513722
C	-2.929856	1.572262	-1.676595
C	-3.640822	0.444500	-1.212223
C	-3.223805	-0.837269	-1.631039
C	-2.128532	-0.986346	-2.477107
N	-4.749179	0.598467	-0.355074
N	4.756500	-0.610236	-0.358620
C	-5.843629	-0.315548	-0.411436
C	-4.782882	1.651622	0.606234
C	4.813912	-1.661279	0.603939
C	5.838513	0.318704	-0.424287
C	-3.673474	1.928891	1.416402
C	-3.718017	2.962978	2.355282
C	-4.867770	3.746602	2.541174
C	-5.976797	3.444059	1.728181
C	-5.941105	2.427867	0.775643
C	5.984587	-2.411216	0.775070
C	6.048378	-3.422856	1.737705
C	4.951409	-3.739480	2.553799
C	3.781507	-2.978883	2.363408
C	3.709081	-1.956100	1.420723
C	6.425100	0.659196	-1.650081
C	7.478545	1.576136	-1.704244
C	8.002127	2.171802	-0.545935
C	7.409435	1.805405	0.677698
C	6.347152	0.906656	0.744982
C	-6.429551	-0.665862	-1.635040
C	-7.495118	-1.568880	-1.680977
C	-8.032281	-2.140649	-0.516764
C	-7.440720	-1.764004	0.704179
C	-6.366395	-0.879019	0.763752
C	-4.948253	4.890604	3.568923
C	-3.641559	5.049134	4.367224
C	-6.093109	4.607425	4.569341
C	-9.207172	-3.136085	-0.533194
C	-8.752990	-4.476597	0.089952
C	-9.713136	-3.416576	-1.959859
C	9.164787	3.181334	-0.570982
C	9.671287	3.451352	-1.999440
C	10.344291	2.629255	0.263176
C	4.985540	-4.853531	3.616306
C	3.908053	-5.912629	3.285534
C	4.696015	-4.246670	5.008915
C	6.352051	-5.559892	3.675726
C	8.693176	4.523404	0.035488
C	-10.382362	-2.560852	0.291250
C	-5.229254	6.221660	2.833092
H	1.312724	-2.369972	-2.866809
H	3.277280	-2.609731	-1.359269
H	3.755773	1.684985	-1.325187
H	1.803887	1.906697	-2.847823
H	-1.300386	2.296064	-2.897857
H	-3.257598	2.570952	-1.386428
H	-3.768310	-1.718666	-1.291440
H	-1.820133	-1.976505	-2.815013
H	-2.765581	1.332433	1.310293
H	-2.828380	3.140103	2.959318
H	-6.897246	4.023668	1.826013

H	-6.817323	2.228744	0.156121
H	6.855399	-2.198375	0.152514
H	6.982343	-3.976587	1.832541
H	2.899390	-3.174640	2.976764
H	2.789346	-1.378364	1.313157
H	6.051691	0.206742	-2.570599
H	7.898924	1.810890	-2.681924
H	7.774065	2.240591	1.610679
H	5.905003	0.653762	1.710257
H	-6.045872	-0.232082	-2.560302
H	-7.914006	-1.812056	-2.657245
H	-7.815732	-2.180300	1.641659
H	-5.925417	-0.618616	1.727539
H	-3.744501	5.874951	5.088925
H	-2.786646	5.285917	3.714265
H	-3.395818	4.139692	4.938207
H	-6.166524	5.421209	5.310033
H	-5.917917	3.665269	5.113422
H	-7.068690	4.527143	4.065437
H	-9.584625	-5.200907	0.091804
H	-8.416779	-4.352354	1.130953
H	-7.919584	-4.915201	-0.482127
H	-10.547756	-4.134556	-1.923627
H	-8.927794	-3.854461	-2.596089
H	-10.083662	-2.503477	-2.452097
H	10.496836	4.180023	-1.969361
H	8.882349	3.871955	-2.642832
H	10.054608	2.537296	-2.479938
H	11.185152	3.342883	0.259467
H	10.706017	1.673281	-0.148677
H	10.059183	2.455570	1.312384
H	3.912904	-6.715584	4.041534
H	4.093367	-6.369996	2.300277
H	2.897013	-5.477014	3.267943
H	4.713089	-5.033066	5.781970
H	3.708251	-3.762012	5.049019
H	5.452308	-3.490435	5.274355
H	6.330593	-6.346095	4.446939
H	7.163967	-4.862725	3.936749
H	6.608113	-6.042017	2.719030
H	9.516240	5.257391	0.031074
H	8.355654	4.407365	1.077003
H	7.856238	4.945474	-0.543820
H	-11.231206	-3.264944	0.293466
H	-10.732087	-1.605720	-0.132726
H	-10.098275	-2.378217	1.339210
H	-5.298165	7.053187	3.554334
H	-6.175470	6.187916	2.271153
H	-4.423158	6.454931	2.118907

DTPA-DPS (7)

T₁ geometry

C	-1.29929600	-0.15313100	-3.04205700
S	0.10188200	-0.48586200	-4.12580800
C	1.50595900	-0.57201500	-3.05897000
O	0.26659000	0.72004100	-4.99186900
O	-0.11708300	-1.85009900	-4.69434700
C	1.87734200	-1.83039900	-2.45412100
C	2.87398100	-1.87264800	-1.52336600
C	3.59179600	-0.66323800	-1.15231900
C	3.24823400	0.58516100	-1.81741300
C	2.23917100	0.62905500	-2.73439400
C	-1.63628100	1.16953200	-2.72002900
C	-2.69879000	1.42287200	-1.85915700
C	-3.44223300	0.36078100	-1.30144500
C	-3.09640700	-0.96357500	-1.64324800
C	-2.03961800	-1.21866200	-2.51169400
N	-4.52282900	0.62018100	-0.42613100
N	4.62146700	-0.70721000	-0.20826300

C	-5.70396000	-0.17341200	-0.49011200
C	-4.44603100	1.68148000	0.51823500
C	4.48383000	-1.50955800	0.94895200
C	5.80308600	0.04473600	-0.41675300
C	-3.28078300	1.90198400	1.26690000
C	-3.21545600	2.94555800	2.19367500
C	-4.30455400	3.79957900	2.42865700
C	-5.46811600	3.55946000	1.67288500
C	-5.54300900	2.53404300	0.73344000
C	5.57618000	-2.22732200	1.47325100
C	5.41213300	-3.03969400	2.59267500
C	4.16704700	-3.18336200	3.23355800
C	3.08450900	-2.46166400	2.68853600
C	3.22606200	-1.64438700	1.57361100
C	6.33231500	0.18894200	-1.71286800
C	7.47463500	0.96025300	-1.92510700
C	8.13173400	1.62128200	-0.87334300
C	7.57889000	1.47123600	0.41823500
C	6.44305400	0.70799800	0.65177900
C	-6.28713300	-0.50237900	-1.72171600
C	-7.44486900	-1.28284300	-1.77551200
C	-8.07832400	-1.75186200	-0.61376700
C	-7.48257900	-1.40509400	0.61411800
C	-6.31936700	-0.64210900	0.68320400
C	-4.26764900	4.95012100	3.45182500
C	-2.91557500	5.03617400	4.18259900
C	-5.37465100	4.73486000	4.50998700
C	-9.36142900	-2.60258700	-0.63974900
C	-9.08989300	-3.96633800	0.03734700
C	-9.85504200	-2.86830400	-2.07360100
C	9.39204900	2.47929200	-1.07791900
C	9.84235500	2.51129000	-2.54956000
C	10.54961500	1.90127300	-0.22995300
C	3.95685500	-4.08072600	4.46538600
C	2.91547300	-5.17455600	4.12950800
C	3.43695500	-3.22364300	5.64361300
C	5.25762400	-4.77266600	4.91119300
C	9.10269800	3.93104500	-0.62815600
C	-10.48372900	-1.86516700	0.12736200
C	-4.50916600	6.29380000	2.72513700
H	1.37393600	-2.73931900	-2.78376000
H	3.18821200	-2.82624300	-1.09516000
H	3.79033100	1.49419200	-1.55175200
H	1.97684100	1.55837300	-3.24022200
H	-1.08510100	1.99116100	-3.17910300
H	-2.97539800	2.45178500	-1.62473800
H	-3.67131200	-1.79280000	-1.22854500
H	-1.78491200	-2.24068300	-2.79471600
H	-2.41672200	1.25113100	1.12277900
H	-2.28665300	3.07371000	2.74958800
H	-6.34490500	4.19695700	1.80597600
H	-6.45917400	2.38685700	0.15917700
H	6.55034200	-2.16052100	0.98726000
H	6.28285500	-3.58255100	2.95896900
H	2.09811600	-2.52988200	3.15127100
H	2.37391500	-1.08713200	1.18298400
H	5.85233200	-0.32490500	-2.54650700
H	7.85665500	1.03183400	-2.94289500
H	8.04166300	1.97601800	1.26844300
H	6.03113400	0.63244100	1.65901600
H	-5.83069700	-0.14550500	-2.64657200
H	-7.85846000	-1.51066700	-2.75778100
H	-7.92771500	-1.74800400	1.55069800
H	-5.88063300	-0.40213700	1.65326200
H	-2.93587400	5.86733500	4.90530500
H	-2.08288900	5.22391900	3.48637800
H	-2.69277300	4.11476200	4.74368400
H	-5.36397800	5.55274400	5.24981300
H	-5.22620900	3.78482900	5.04828900
H	-6.37703500	4.70945900	4.05545700

H	-10.00243400	-4.58581200	0.03529400
H	-8.76994800	-3.84890300	1.08439300
H	-8.29981500	-4.52039400	-0.49468300
H	-10.77293400	-3.47674000	-2.04457000
H	-9.11107100	-3.42046200	-2.66929600
H	-10.09497400	-1.93399400	-2.60554200
H	10.74664900	3.13236400	-2.64669100
H	9.07201700	2.94461700	-3.20671100
H	10.08957600	1.50608800	-2.92590600
H	11.45900000	2.51133700	-0.35849100
H	10.78559800	0.86896600	-0.53466300
H	10.30688900	1.88789100	0.84386000
H	2.74794900	-5.82479000	5.00415200
H	3.26024200	-5.80657100	3.29539200
H	1.94377600	-4.74277300	3.84416000
H	3.27656000	-3.85500000	6.53322100
H	2.47976700	-2.73430900	5.40644500
H	4.16103400	-2.43682500	5.90971500
H	5.06023100	-5.40000700	5.79453600
H	6.03596200	-4.04479900	5.19032100
H	5.66569200	-5.42800500	4.12553300
H	9.99949500	4.55820600	-0.76318400
H	8.81575200	3.98372800	0.43345600
H	8.28530400	4.37267300	-1.22040800
H	-11.41101800	-2.46233300	0.12093700
H	-10.70258600	-0.88973900	-0.33626800
H	-10.21165600	-1.68328100	1.17862300
H	-4.49331800	7.12925100	3.44515600
H	-5.48332100	6.31413500	2.21249500
H	-3.72879200	6.47900700	1.96953300

ACRFLCN (8)

S₀ geometry

C	1.467854	-0.005566	1.226092
C	0.057544	-0.003465	1.270441
C	-0.801310	0.000065	0.000000
C	0.057544	-0.003440	-1.270440
C	1.467855	-0.005545	-1.226091
N	2.155684	-0.005479	0.000001
C	-1.783145	1.186586	0.000011
C	-3.122135	0.744351	0.000005
C	-3.128465	-0.724159	-0.000010
C	-1.793335	-1.177903	-0.000011
C	2.188471	-0.007677	2.442293
C	1.529448	-0.007776	3.666320
C	0.132065	-0.005795	3.716598
C	-0.579882	-0.003662	2.521194
C	-0.579881	-0.003607	-2.521194
C	0.132066	-0.005714	-3.716597
C	1.529450	-0.007699	-3.666319
C	2.188472	-0.007628	-2.442291
C	-4.191699	-1.635839	-0.000020
C	-3.911677	-3.001011	-0.000032
C	-2.575777	-3.454691	-0.000035
C	-1.507077	-2.535776	-0.000022
C	-1.485314	2.541961	0.000025
C	-2.546093	3.470013	0.000035
C	-3.885839	3.027851	0.000026
C	-4.177507	1.665117	0.000012
C	-2.263001	4.878208	0.000056
C	-2.304821	-4.865274	-0.000055
C	3.594755	-0.007271	0.000001
C	4.293285	-1.220541	-0.000005
C	5.691064	-1.220284	-0.000005
C	6.392608	-0.010469	0.000001
C	5.693846	1.200944	0.000007
C	4.296065	1.204373	0.000007
N	-2.034217	6.020050	0.000038
N	-2.085945	-6.009056	-0.000036

H	3.276717	-0.009275	2.420491
H	2.116586	-0.009442	4.587287
H	-0.394713	-0.005861	4.672233
H	-1.671548	-0.001986	2.550436
H	-1.671547	-0.001927	-2.550436
H	-0.394711	-0.005756	-4.672233
H	2.116588	-0.009343	-4.587286
H	3.276718	-0.009226	-2.420489
H	-5.227789	-1.291595	-0.000020
H	-4.721988	-3.731110	-0.000041
H	-0.477400	-2.895945	-0.000024
H	-0.452623	2.893416	0.000030
H	-4.689866	3.764860	0.000033
H	-5.216506	1.329744	0.000008
H	3.735158	-2.158638	-0.000009
H	6.232944	-2.168513	-0.000009
H	7.484768	-0.011727	0.000001
H	6.237881	2.147937	0.000011
H	3.740070	2.143731	0.000011

ACRFLCN (8)

T₁ geometry

C	1.49096000	-0.03337400	1.22711400
C	0.08155800	-0.02092800	1.27561000
C	-0.78002500	-0.00070900	0.01185000
C	0.06859300	-0.01926100	-1.26065200
C	1.48179200	-0.03179900	-1.22509800
N	2.17369800	-0.03322300	-0.00352200
C	-1.73778100	1.20767900	0.00522700
C	-3.12584600	0.75101400	-0.01084600
C	-3.15938800	-0.63822400	-0.01128000
C	-1.79505400	-1.16129500	0.00455700
C	2.21579200	-0.04618300	2.43944200
C	1.55982200	-0.04699500	3.66709900
C	0.16405700	-0.03531000	3.72122400
C	-0.55296600	-0.02236900	2.52640000
C	-0.57725800	-0.01910300	-2.50892500
C	0.12830200	-0.03045600	-3.70692900
C	1.52685500	-0.04220500	-3.66434600
C	2.19490000	-0.04293800	-2.44531600
C	-4.26643000	-1.56702900	-0.02051300
C	-4.01136200	-2.90974800	-0.01456700
C	-2.65873000	-3.41716600	0.00191000
C	-1.55153700	-2.50506700	0.00773700
C	-1.42997100	2.53815100	0.00913000
C	-2.49189300	3.50261000	0.00395700
C	-3.86749100	3.06107500	-0.01253100
C	-4.18684000	1.73221200	-0.01925300
C	-2.20044200	4.88733800	0.02097400
C	-2.43444900	-4.81441100	0.01806300
C	3.61320000	-0.04060100	-0.00942000
C	4.30669600	-1.25667100	-0.01300600
C	5.70445600	-1.26109500	-0.01853000
C	6.41014900	-0.05368100	-0.02051300
C	5.71582200	1.16026000	-0.01701500
C	4.31807000	1.16883300	-0.01148300
N	-1.96152500	6.03385400	0.03424300
N	-2.25119200	-5.97112300	0.03059500
H	3.30397800	-0.05575800	2.41452500
H	2.14991200	-0.05707600	4.58599900
H	-0.35992600	-0.03597100	4.67837100
H	-1.64437800	-0.01238400	2.55870700
H	-1.66872400	-0.00912100	-2.53167800
H	-0.40281900	-0.02979400	-4.66006700
H	2.10776300	-0.05102500	-4.58920900
H	3.28319000	-0.05246000	-2.43106900
H	-5.29353000	-1.19880100	-0.03657300
H	-4.83173100	-3.62917000	-0.02179300
H	-0.53369900	-2.89749400	0.02042000

H	-0.39454200	2.88157200	0.02193100
H	-4.65227200	3.81915200	-0.01915900
H	-5.23046200	1.41376700	-0.03534100
H	3.74519900	-2.19274400	-0.01143000
H	6.24298800	-2.21118700	-0.02123800
H	7.50226300	-0.05880600	-0.02478400
H	6.26316700	2.10530100	-0.01852200
H	3.76540500	2.11012700	-0.00873200

CC2TA (9)

S₀ geometry

C	1.164914	2.399193	-0.058501
N	0.579993	3.548382	0.304047
C	-0.761904	3.536327	0.277091
N	-1.509561	2.480460	-0.081982
C	-0.816449	1.390094	-0.436185
N	0.519997	1.288587	-0.443212
C	-1.468905	4.778747	0.673205
C	-0.771865	5.818993	1.313091
C	-1.438851	6.984941	1.688901
C	-2.804929	7.129807	1.423593
C	-3.503763	6.100617	0.783375
C	-2.842677	4.929421	0.413274
N	-1.544773	0.271972	-0.832300
N	2.555318	2.352953	-0.026653
C	3.351445	1.178696	0.048072
C	4.714197	1.560914	0.072646
C	4.763444	3.008707	0.001423
C	3.428978	3.476969	-0.049699
C	-2.900337	0.004442	-0.502744
C	-3.264238	-1.238230	-1.074657
C	-2.110548	-1.743028	-1.794390
C	-1.064082	-0.804596	-1.629386
C	2.988617	-0.169940	0.147120
C	4.005313	-1.121623	0.239771
C	5.363539	-0.751602	0.256977
C	5.721250	0.597224	0.183457
C	5.833556	3.910932	-0.038067
C	5.563052	5.274089	-0.137426
C	4.235651	5.727831	-0.203454
C	3.153286	4.845314	-0.160557
C	-1.914109	-2.894884	-2.565995
C	-0.677611	-3.095110	-3.176440
C	0.347797	-2.147815	-3.023540
C	0.174538	-0.994347	-2.254088
C	-3.810487	0.722648	0.282304
C	-5.081756	0.181155	0.477765
C	-5.460542	-1.042311	-0.106418
C	-4.549903	-1.756484	-0.888794
N	6.371512	-1.752999	0.349394
N	-6.772701	-1.554504	0.109107
C	6.537609	-2.652797	1.407995
C	7.649262	-3.493383	1.130473
C	8.175722	-3.080111	-0.156102
C	7.362387	-2.005124	-0.605873
C	-7.962762	-0.957505	-0.318067
C	-9.058504	-1.765461	0.089889
C	-8.499593	-2.901643	0.797193
C	-7.088091	-2.736059	0.788061
C	5.808338	-2.769508	2.597648
C	6.200747	-3.754060	3.505364
C	7.293461	-4.601952	3.242243
C	8.021616	-4.474954	2.060346
C	9.238906	-3.522775	-0.956290
C	9.472479	-2.900129	-2.181485
C	8.650089	-1.843376	-2.616369
C	7.586102	-1.382486	-1.839910
C	-9.058617	-4.018786	1.434648
C	-8.215309	-4.942012	2.051041

C	-6.819588	-4.756833	2.040325
C	-6.236558	-3.655365	1.412601
C	-8.151290	0.219954	-1.051879
C	-9.460963	0.587459	-1.363347
C	-10.559025	-0.196011	-0.959682
C	-10.364399	-1.371925	-0.236627
H	0.290317	5.692916	1.522416
H	-0.891508	7.784232	2.193184
H	-3.325117	8.044871	1.715928
H	-4.569037	6.212508	0.570349
H	-3.376322	4.125228	-0.093224
H	1.947709	-0.476479	0.133593
H	3.744766	-2.179782	0.291259
H	6.772489	0.886220	0.223814
H	6.862537	3.547641	0.002270
H	6.384648	5.992372	-0.168725
H	4.036571	6.798348	-0.288463
H	2.131520	5.207806	-0.207625
H	-2.721941	-3.618889	-2.690817
H	-0.505790	-3.987948	-3.780725
H	1.309726	-2.310868	-3.514198
H	0.977467	-0.272511	-2.143279
H	-3.534826	1.670630	0.732848
H	-5.803120	0.713030	1.100011
H	-4.845672	-2.703369	-1.342912
H	4.964555	-2.112066	2.811022
H	5.647289	-3.865395	4.440537
H	7.573085	-5.362861	3.973732
H	8.873914	-5.128791	1.861488
H	9.873530	-4.347426	-0.623728
H	10.297899	-3.235347	-2.812826
H	8.845238	-1.373349	-3.582972
H	6.949343	-0.567137	-2.185616
H	-10.141663	-4.160944	1.449990
H	-8.638703	-5.816128	2.549969
H	-6.176788	-5.488586	2.534948
H	-5.154900	-3.514262	1.412550
H	-7.303926	0.827558	-1.372525
H	-9.634885	1.501951	-1.935031
H	-11.571157	0.120894	-1.219401
H	-11.217581	-1.981541	0.069815

CC2TA (9)

T₁ geometry

C	1.18610800	2.40931600	-0.04457400
N	0.60606300	3.56867100	0.29208200
C	-0.73111900	3.57815100	0.23857500
N	-1.48988400	2.52275100	-0.14485600
C	-0.79785900	1.42572800	-0.46794500
N	0.53152300	1.28975200	-0.43106600
C	-1.43265700	4.82399200	0.61797700
C	-0.74251700	5.86879300	1.26173200
C	-1.40913400	7.03947500	1.61993300
C	-2.77236800	7.18935100	1.33768700
C	-3.46534100	6.15683900	0.69683400
C	-2.80419800	4.98065900	0.34201200
N	-1.53849400	0.31121900	-0.88207700
N	2.57592900	2.34173500	0.02353400
C	3.34263100	1.17430100	0.07116700
C	4.76895700	1.57414700	0.17029500
C	4.81648900	2.97641700	0.18573600
C	3.47424400	3.47352300	0.08385100
C	-2.88471600	0.03946900	-0.53824400
C	-3.26113300	-1.19282300	-1.12745900
C	-2.11969900	-1.68275700	-1.87508200
C	-1.07198100	-0.74468000	-1.70559200
C	2.97817300	-0.17007000	0.09038400
C	3.97859700	-1.13725900	0.21505400
C	5.39212900	-0.75275900	0.29834400

C	5.76913900	0.57369300	0.26357600
C	5.89689800	3.89914900	0.25207600
C	5.62765600	5.26328600	0.19023800
C	4.31015000	5.72660200	0.06326500
C	3.21197100	4.82602000	0.01082700
C	-1.93168700	-2.81700100	-2.67531300
C	-0.70474000	-3.00009900	-3.30958000
C	0.32087700	-2.05245100	-3.15258800
C	0.15693900	-0.91742200	-2.35515300
C	-3.78049600	0.74627700	0.27433200
C	-5.04895200	0.20389500	0.48137700
C	-5.43953500	-1.00925400	-0.11784600
C	-4.54526300	-1.71150300	-0.92833200
N	6.34470300	-1.78161400	0.35859500
N	-6.75023400	-1.52377900	0.11155800
C	6.26472600	-2.92186400	1.18118800
C	7.39160700	-3.74768700	0.93844200
C	8.19779800	-3.07846300	-0.06852500
C	7.53202100	-1.86980000	-0.39768300
C	-7.94391400	-0.93831700	-0.31844600
C	-9.03525400	-1.74420800	0.10609200
C	-8.46845900	-2.86775700	0.82696500
C	-7.05743500	-2.69558000	0.80857900
C	5.32168000	-3.24265100	2.16585800
C	5.49423700	-4.44034600	2.86365300
C	6.58945900	-5.28371700	2.61078900
C	7.54895300	-4.93735600	1.65664900
C	9.39051100	-3.41513000	-0.71728900
C	9.90028100	-2.55159500	-1.68872200
C	9.21803100	-1.36917200	-2.02224800
C	8.02639500	-1.01218500	-1.38725400
C	-9.01870200	-3.97898400	1.48224900
C	-8.16777200	-4.89002200	2.10639600
C	-6.77279500	-4.69882300	2.08523200
C	-6.19823600	-3.60321600	1.43987100
C	-8.13967300	0.22924300	-1.06618200
C	-9.45191600	0.58837900	-1.37601700
C	-10.54569900	-0.19349500	-0.95716600
C	-10.34399600	-1.35906700	-0.21945100
H	0.31564000	5.74007400	1.48963400
H	-0.86449100	7.83978100	2.12614200
H	-3.29272900	8.10806900	1.61809100
H	-4.52812800	6.26965400	0.47080500
H	-3.33403700	4.17437400	-0.16503600
H	1.93798700	-0.46294800	-0.00594700
H	3.72467500	-2.19320000	0.14489900
H	6.81743700	0.85417600	0.36292400
H	6.92192200	3.53546300	0.34573200
H	6.45022400	5.98014100	0.23855900
H	4.11203700	6.79822800	0.00554200
H	2.19526000	5.19409300	-0.08003800
H	-2.73972400	-3.54030500	-2.80411900
H	-0.54062100	-3.87855700	-3.93687600
H	1.27426700	-2.20116500	-3.66447400
H	0.95690700	-0.19198800	-2.24086500
H	-3.49322400	1.68815300	0.73157500
H	-5.76007000	0.72653800	1.12315000
H	-4.85195100	-2.64974500	-1.39337000
H	4.48830600	-2.57903300	2.39398700
H	4.76765100	-4.71622800	3.63054800
H	6.69894000	-6.20979500	3.17843400
H	8.41410200	-5.58010500	1.48099600
H	9.90969900	-4.34418000	-0.47283900
H	10.83187800	-2.80003500	-2.20081000
H	9.62308400	-0.71315700	-2.79546000
H	7.49890400	-0.10122100	-1.66663400
H	-10.10100200	-4.12621700	1.50497700
H	-8.58445600	-5.75936700	2.61925800
H	-6.12404300	-5.42148600	2.58559200
H	-5.11730200	-3.45679600	1.42998700

H	-7.29523300	0.83533400	-1.39724200
H	-9.63162400	1.49515800	-1.95817100
H	-11.56008100	0.11689700	-1.21618800
H	-11.19390700	-1.96690900	0.09958500

DTC-DPS (10)

S₀ geometry

C	1.428155	3.179094	0.096485
S	0.000000	4.287659	-0.000001
C	-1.428154	3.179094	-0.096487
O	0.087991	5.003225	-1.303021
O	-0.087989	5.003225	1.303018
C	-2.064634	2.775515	1.079973
C	-3.167329	1.926068	1.003168
C	-3.649590	1.502835	-0.247541
C	-3.015696	1.943903	-1.422290
C	-1.902178	2.779251	-1.348600
C	2.064635	2.775515	-1.079975
C	3.167330	1.926068	-1.003170
C	3.649590	1.502834	0.247540
C	3.015695	1.943902	1.422289
C	1.902178	2.779250	1.348598
N	4.771781	0.645926	0.324428
N	-4.771781	0.645927	-0.324429
C	6.005091	0.838563	-0.321393
C	6.866637	-0.241809	-0.002658
C	6.121887	-1.131903	0.870118
C	4.842712	-0.554865	1.050471
C	-6.005091	0.838564	0.321394
C	-6.866637	-0.241808	0.002659
C	-6.121888	-1.131901	-0.870119
C	-4.842713	-0.554863	-1.050473
C	6.451568	1.891336	-1.122374
C	7.756794	1.834343	-1.619090
C	8.636768	0.765869	-1.338503
C	8.168141	-0.268567	-0.514681
C	6.433038	-2.356058	1.480775
C	5.484126	-3.021458	2.264428
C	4.208436	-2.421831	2.407676
C	3.869340	-1.206862	1.815407
C	-6.451567	1.891337	1.122375
C	-7.756792	1.834343	1.619093
C	-8.636766	0.765869	1.338507
C	-8.168140	-0.268567	0.514684
C	-6.433040	-2.356057	-1.480776
C	-5.484128	-3.021456	-2.264430
C	-4.208439	-2.421829	-2.407679
C	-3.869341	-1.206860	-1.815410
C	10.074238	0.707438	-1.895595
C	5.772236	-4.367686	2.958047
C	-5.772239	-4.367683	-2.958051
C	-10.074235	0.707437	1.895601
C	-4.784405	-5.438643	-2.439477
C	-5.599036	-4.209090	-4.486683
C	-7.203231	-4.866589	-2.687913
C	-11.081451	0.685162	0.722538
C	-10.407354	1.916732	2.788786
C	-10.247171	-0.574876	2.742527
C	10.247179	-0.574883	-2.742508
C	11.081453	0.685179	-0.722531
C	5.599045	-4.209091	4.486681
C	7.203223	-4.866599	2.687900
C	10.407353	1.916726	-2.788791
C	4.784393	-5.438642	2.439481
H	-1.697792	3.129265	2.044151
H	-3.656887	1.579384	1.913905
H	-3.416886	1.648849	-2.392621
H	-1.422198	3.152369	-2.253968
H	1.697794	3.129265	-2.044153

H	3.656889	1.579384	-1.913906
H	3.416884	1.648848	2.392619
H	1.422197	3.152368	2.253966
H	5.814314	2.744909	-1.355275
H	8.091577	2.660154	-2.245440
H	8.818741	-1.107560	-0.259666
H	7.424834	-2.780376	1.326349
H	3.444640	-2.924992	3.003595
H	2.869262	-0.791805	1.944078
H	-5.814312	2.744909	1.355276
H	-8.091574	2.660153	2.245444
H	-8.818741	-1.107559	0.259669
H	-7.424836	-2.780374	-1.326349
H	-3.444644	-2.924989	-3.003599
H	-2.869264	-0.791803	-1.944082
H	-4.972490	-6.407312	-2.932231
H	-4.893090	-5.581198	-1.352200
H	-3.737271	-5.162378	-2.637798
H	-5.795193	-5.166183	-4.998533
H	-4.579058	-3.891848	-4.753436
H	-6.298960	-3.457755	-4.886634
H	-7.365070	-5.828763	-3.199261
H	-7.961959	-4.161449	-3.062686
H	-7.385684	-5.028693	-1.613783
H	-12.115790	0.636727	1.102440
H	-10.926049	-0.184995	0.066062
H	-10.986361	1.592436	0.104475
H	-11.438870	1.826936	3.164799
H	-10.339116	2.867901	2.237457
H	-9.741038	1.978490	3.663888
H	-11.270901	-0.633934	3.148837
H	-9.542228	-0.586527	3.589460
H	-10.071517	-1.485457	2.149014
H	11.270910	-0.633942	-3.148815
H	9.542238	-0.586544	-3.589442
H	10.071526	-1.485459	-2.148986
H	12.115793	0.636745	-1.102432
H	10.926056	-0.184974	-0.066047
H	10.986358	1.592457	-0.104476
H	5.795203	-5.166185	4.998530
H	4.579070	-3.891847	4.753441
H	6.298974	-3.457758	4.886627
H	7.365064	-5.828770	3.199251
H	7.961958	-4.161459	3.062662
H	7.385667	-5.028709	1.613769
H	11.438873	1.826934	-3.164795
H	10.339101	2.867901	-2.237474
H	9.741044	1.978466	-3.663900
H	4.972476	-6.407311	2.932236
H	4.893071	-5.581198	1.352204
H	3.737262	-5.162371	2.637808

DTC-DPS (10)

T₁ geometry

C	1.38034200	3.48597200	0.09771400
S	0.00531300	4.65141700	-0.01631100
C	-1.43990900	3.64641600	-0.12804600
O	0.16045000	5.36243800	-1.32000300
O	-0.04657800	5.37452900	1.28885900
C	-2.09793400	3.18774200	1.07882600
C	-3.10239100	2.27054000	0.99896300
C	-3.51591800	1.73491700	-0.28978600
C	-2.88555500	2.24381800	-1.49711700
C	-1.90049500	3.18254300	-1.42145400
C	1.98454300	3.00915700	-1.07379800
C	3.00511200	2.06528100	-0.98564000
C	3.44223000	1.60996900	0.27094500
C	2.84478400	2.11384000	1.44019700
C	1.81300300	3.04535400	1.35616000

N	4.48731500	0.65652400	0.36018500
N	-4.52453600	0.77629800	-0.37179200
C	5.75280100	0.76136900	-0.23613200
C	6.51797900	-0.38708800	0.09383300
C	5.67609000	-1.22622300	0.92809100
C	4.43932100	-0.55152600	1.06986700
C	-5.74496300	0.78648000	0.32814500
C	-6.49968200	-0.36324500	-0.02081200
C	-5.70589600	-1.10436200	-0.99426800
C	-4.50407900	-0.37800600	-1.17472200
C	6.30573500	1.78825800	-1.00399200
C	7.61980400	1.63917900	-1.45506200
C	8.40624000	0.50276100	-1.16197000
C	7.83105100	-0.50583200	-0.37368700
C	5.86953500	-2.47360700	1.54010700
C	4.84511800	-3.06517500	2.28774200
C	3.61494300	-2.36920700	2.39073700
C	3.39158100	-1.12926600	1.79598600
C	-6.27011100	1.75411700	1.18840700
C	-7.53438800	1.52382700	1.74028400
C	-8.29982500	0.37776500	1.44058400
C	-7.76030400	-0.56004800	0.53363400
C	-5.90762100	-2.30484800	-1.67686700
C	-4.91771000	-2.80444400	-2.54206300
C	-3.71605400	-2.06706800	-2.67305400
C	-3.48368100	-0.87067600	-1.99780800
C	9.85494100	0.34623800	-1.66869200
C	5.00574200	-4.42674000	2.99242000
C	-5.08901100	-4.11834100	-3.32682900
C	-9.69603100	0.13497800	2.04405400
C	-3.98274700	-5.11604000	-2.90921700
C	-4.97374100	-3.82886000	-4.84223000
C	-6.45499700	-4.77979100	-3.06817600
C	-10.74326000	0.08379600	0.90650100
C	-10.10924100	1.24380400	3.02918900
C	-9.69949200	-1.21158400	2.80527900
C	9.96017800	-0.92236800	-2.54658800
C	10.81254400	0.21312300	-0.46150900
C	4.79792700	-4.24673000	4.51436200
C	6.40164100	-5.03703500	2.77054800
C	10.31477100	1.54958100	-2.51214800
C	3.95495000	-5.42155900	2.44656500
H	-1.77316800	3.58923000	2.03874000
H	-3.56829100	1.88659500	1.90766800
H	-3.27896500	1.93667100	-2.46789200
H	-1.47566100	3.63000600	-2.32007700
H	1.65468600	3.38893300	-2.04136400
H	3.46928100	1.67112700	-1.89096700
H	3.21521700	1.78971400	2.41399800
H	1.36311600	3.46686100	2.25567700
H	5.74133000	2.68984700	-1.24387300
H	8.03890200	2.44697900	-2.05363700
H	8.40633400	-1.39590000	-0.11016700
H	6.83096900	-2.97236700	1.41914700
H	2.79570500	-2.81369000	2.95908100
H	2.42493200	-0.63420300	1.89437100
H	-5.72825400	2.67159800	1.41493700
H	-7.93278900	2.27919100	2.41573300
H	-8.33464400	-1.44373800	0.24963800
H	-6.83664000	-2.85202700	-1.52116000
H	-2.92366900	-2.44769600	-3.31910900
H	-2.53282400	-0.34900700	-2.10119500
H	-4.09220300	-6.06149600	-3.46580300
H	-4.04206000	-5.34447700	-1.83297400
H	-2.97471900	-4.72416300	-3.11419200
H	-5.08643400	-4.76223400	-5.41819900
H	-3.99861500	-3.39128600	-5.10558800
H	-5.75717100	-3.12756400	-5.17157400
H	-6.53362500	-5.70729600	-3.65636500
H	-7.29108300	-4.12771400	-3.36679700

H	-6.58909900	-5.04962600	-2.00866700
H	-11.74931500	-0.09522700	1.32061200
H	-10.53056100	-0.72264100	0.18770200
H	-10.76770700	1.03367100	0.34878700
H	-11.10623300	1.02044100	3.44015500
H	-10.16821100	2.22912300	2.54066000
H	-9.41146000	1.32175900	3.87789300
H	-10.69454000	-1.40084800	3.24064000
H	-8.96358000	-1.20455300	3.62521700
H	-9.45928400	-2.05931000	2.14517700
H	10.99260800	-1.05523000	-2.91153000
H	9.29464400	-0.85129200	-3.42202600
H	9.68368200	-1.83085900	-1.98935900
H	11.85419900	0.09619300	-0.80517100
H	10.56742300	-0.66080200	0.16163000
H	10.76302400	1.10665000	0.18147700
H	4.90247700	-5.21320100	5.03571800
H	3.79834600	-3.84866600	4.74804600
H	5.54184900	-3.54998700	4.93316200
H	6.47247100	-6.00348800	3.29431300
H	7.20029100	-4.38831300	3.16370300
H	6.60445300	-5.22326900	1.70398300
H	11.35086300	1.39086700	-2.85106200
H	10.29584500	2.48792200	-1.93560500
H	9.69028400	1.68529400	-3.40931400
H	4.05483000	-6.40035500	2.94532600
H	4.08402600	-5.57501600	1.36297100
H	2.92637200	-5.06622600	2.61404200

2CzPN (11)

S₀ geometry

C	1.325635	2.433168	0.414329
C	0.675818	1.205469	0.217735
C	-0.676097	1.205352	-0.217791
C	-1.326131	2.432940	-0.414373
C	-0.678152	3.654462	-0.206426
C	0.677438	3.654579	0.206411
C	1.387409	4.879899	0.434497
C	-1.388339	4.879660	-0.434495
N	1.983426	5.861529	0.622802
N	-1.984531	5.861187	-0.622785
N	1.394080	0.017135	0.468124
N	-1.394149	0.016902	-0.468218
C	-2.651941	-0.296308	0.082789
C	-3.115653	-1.505491	-0.493825
C	-2.113762	-1.929573	-1.454271
C	-1.072296	-0.968088	-1.423496
C	2.651942	-0.295816	-0.082865
C	3.115947	-1.504846	0.493832
C	2.114174	-1.929086	1.454332
C	1.072480	-0.967850	1.423499
C	3.384373	0.374846	-1.068720
C	4.605425	-0.178651	-1.461588
C	5.083217	-1.372907	-0.893982
C	4.342317	-2.041629	0.080057
C	2.033838	-3.008869	2.344068
C	0.931920	-3.106964	3.192140
C	-0.079675	-2.130606	3.165583
C	-0.023293	-1.047298	2.286841
C	-3.384547	0.374256	1.068581
C	-4.605475	-0.179497	1.461471
C	-5.082979	-1.373906	0.893945
C	-4.341906	-2.042528	-0.080032
C	-2.033158	-3.009404	-2.343924
C	-0.931204	-3.107305	-3.191970
C	0.080162	-2.130706	-3.165473
C	0.023509	-1.047343	-2.286818
H	2.357216	2.430019	0.765295
H	-2.357705	2.429613	-0.765355

H	3.023990	1.298679	-1.523472
H	5.196724	0.329896	-2.225885
H	6.041786	-1.779574	-1.221868
H	4.710930	-2.973156	0.514865
H	2.828869	-3.756893	2.376907
H	0.855736	-3.943248	3.889730
H	-0.930005	-2.216255	3.845166
H	-0.811196	-0.295513	2.287734
H	-3.024387	1.298206	1.523271
H	-5.196905	0.328969	2.225720
H	-6.041459	-1.780773	1.221843
H	-4.710293	-2.974174	-0.514773
H	-2.828013	-3.757617	-2.376722
H	-0.854811	-3.943624	-3.889495
H	0.930523	-2.216208	-3.845036
H	0.811235	-0.295371	-2.287750

2CzPN (11)

T₁ geometry

C	2.47250400	-1.37695900	0.33503200
C	1.25730300	-0.71675600	0.19912000
C	1.25730900	0.71674000	-0.19911500
C	2.47252100	1.37693500	-0.33504300
C	3.70568200	0.73027400	-0.16350100
C	3.70567700	-0.73030700	0.16348900
C	4.90938900	-1.43825500	0.35241100
C	4.90940200	1.43821300	-0.35242700
N	5.90433200	-2.03783000	0.51206000
N	5.90435100	2.03777700	-0.51207100
N	0.05354800	-1.37368600	0.52328500
N	0.05354500	1.37366900	-0.52326700
C	-0.36194300	2.61180600	-0.00978700
C	-1.59652300	2.97388700	-0.61119300
C	-1.92865600	1.92205300	-1.55836400
C	-0.88536500	0.96453800	-1.49173100
C	-0.36196100	-2.61182200	0.00980600
C	-1.59656900	-2.97385500	0.61117800
C	-1.92869100	-1.92201500	1.55834400
C	-0.88536900	-0.96453300	1.49173400
C	0.23758000	-3.40933100	-0.97428100
C	-0.41157800	-4.59111400	-1.33583300
C	-1.62926100	-4.96668100	-0.74139900
C	-2.22998900	-4.15944200	0.22887200
C	-2.97122400	-1.74644200	2.47320000
C	-2.95216700	-0.63123700	3.31537400
C	-1.89169300	0.28882100	3.26257500
C	-0.83740800	0.12985300	2.36024900
C	0.23758500	3.40928200	0.97433800
C	-0.41153600	4.59108900	1.33587200
C	-1.62918400	4.96670300	0.74139700
C	-2.22991200	4.15949100	-0.22889700
C	-2.97117600	1.74650800	-2.47323800
C	-2.95214200	0.63128900	-3.31539600
C	-1.89170000	-0.28880400	-3.26257200
C	-0.83742700	-0.12986300	-2.36022600
H	2.47248300	-2.42159600	0.64893500
H	2.47250400	2.42157000	-0.64894700
H	1.18031600	-3.12452300	-1.44187100
H	0.03864900	-5.23392200	-2.09476400
H	-2.11135200	-5.89799300	-1.04462800
H	-3.18178700	-4.44943100	0.67862500
H	-3.77971600	-2.47740000	2.53962900
H	-3.75971900	-0.48214700	4.03462000
H	-1.88166800	1.14081900	3.94498600
H	-0.00299400	0.82960800	2.35032500
H	1.18029800	3.12443600	1.44195000
H	0.03868900	5.23387600	2.09482200

H	-2.11125500	5.89802600	1.04462200
H	-3.18168100	4.44952200	-0.67868300
H	-3.77964400	2.47749200	-2.53969300
H	-3.75968700	0.48221700	-4.03465400
H	-1.88169000	-1.14081000	-3.94497200
H	-0.00303400	-0.82964300	-2.35027900

4CzPN (12)

S₀ geometry

C	-1.419157	-1.383053	0.093947
C	-0.712278	-0.151012	0.042822
C	0.712279	-0.151019	-0.042814
C	1.419144	-1.383065	-0.093986
C	0.703349	-2.597049	-0.065447
C	-0.703375	-2.597043	0.065371
C	-1.391379	-3.846307	0.217519
C	1.391338	-3.846315	-0.217648
N	-1.922410	-4.870819	0.365364
N	1.922355	-4.870828	-0.365540
N	-1.424225	1.067988	0.108189
N	1.424240	1.067975	-0.108132
C	2.386196	1.522401	0.820122
C	2.891235	2.770750	0.380902
C	2.226338	3.085288	-0.868688
C	1.329673	2.023712	-1.142962
C	-2.386176	1.522462	-0.820047
C	-2.891216	2.770788	-0.380766
C	-2.226324	3.085264	0.868842
C	-1.329655	2.023677	1.143064
C	-2.801709	0.953413	-2.026211
C	-3.753652	1.641685	-2.780874
C	-4.274570	2.874759	-2.351767
C	-3.843703	3.445859	-1.155445
C	-2.337164	4.150328	1.772396
C	-1.564513	4.139703	2.932673
C	-0.692879	3.069765	3.198943
C	-0.567164	1.997999	2.312757
C	2.801741	0.953285	2.026251
C	3.753695	1.641512	2.780940
C	4.274610	2.874608	2.351894
C	3.843732	3.445777	1.155609
C	2.337176	4.150396	-1.772191
C	1.564527	4.139824	-2.932469
C	0.692903	3.069891	-3.198796
C	0.567191	1.998083	-2.312661
N	-2.826877	-1.432829	0.194352
C	-3.691528	-1.997009	-0.766813
C	-5.021853	-1.909159	-0.289332
C	-4.963862	-1.298772	1.025961
C	-3.600277	-1.026885	1.300484
C	-5.934792	-0.997287	1.990380
C	-5.534123	-0.446074	3.206702
C	-4.174118	-0.205029	3.469684
C	-3.188795	-0.495691	2.524260
C	-3.394704	-2.548422	-2.016492
C	-4.458723	-3.014649	-2.791062
C	-5.785942	-2.932414	-2.334266
C	-6.073451	-2.381071	-1.086507
N	2.826862	-1.432847	-0.194415
C	3.691530	-1.997064	0.766713
C	5.021849	-1.909178	0.289219
C	4.963836	-1.298725	-1.026043
C	3.600244	-1.026839	-1.300536
C	5.934750	-0.997174	-1.990456
C	5.534061	-0.445896	-3.206742
C	4.174050	-0.204855	-3.469696
C	3.188742	-0.495584	-2.524279
C	3.394729	-2.548542	2.016369
C	4.458763	-3.014800	2.790899

C	5.785975	-2.932532	2.334088
C	6.073462	-2.381122	1.086353
H	-2.410463	-0.000263	-2.377126
H	-4.099160	1.205652	-3.720375
H	-5.018942	3.388540	-2.963140
H	-4.238413	4.409396	-0.826191
H	-3.026150	4.973446	1.571419
H	-1.639588	4.964609	3.643861
H	-0.096680	3.072293	4.113651
H	0.110273	1.176109	2.538196
H	2.410501	-0.000413	2.377112
H	4.099217	1.205424	3.720410
H	5.018992	3.388353	2.963286
H	4.238440	4.409330	0.826403
H	3.026159	4.973507	-1.571173
H	1.639600	4.964764	-3.643616
H	0.096709	3.072460	-4.113507
H	-0.110237	1.176197	-2.538144
H	-6.989357	-1.201822	1.793723
H	-6.280429	-0.207345	3.966927
H	-3.876719	0.216919	4.431804
H	-2.138304	-0.311571	2.745369
H	-2.369154	-2.628476	-2.380354
H	-4.250402	-3.457012	-3.767421
H	-6.596097	-3.307668	-2.962407
H	-7.104535	-2.317808	-0.732265
H	6.989321	-1.201706	-1.793823
H	6.280356	-0.207113	-3.966962
H	3.876636	0.217144	-4.431789
H	2.138245	-0.311466	-2.745364
H	2.369185	-2.628623	2.380241
H	4.250459	-3.457218	3.767237
H	6.596142	-3.307813	2.962197
H	7.104540	-2.317834	0.732100

4CzPN (12)

T₁ geometry

C	-1.47158000	-1.38559900	0.15940000
C	-0.76241000	-0.19048400	0.08736400
C	0.70624300	-0.22072600	-0.00383500
C	1.37324100	-1.46854100	-0.07312400
C	0.67099100	-2.67486000	-0.01417600
C	-0.79047000	-2.64983500	0.18050900
C	-1.48281500	-3.84116100	0.46492800
C	1.33908600	-3.91064800	-0.20343200
N	-2.03685900	-4.84691900	0.70591200
N	1.88134300	-4.93551200	-0.35526500
N	-1.41652400	1.07123700	0.10501100
N	1.44303100	0.99313500	-0.07242000
C	2.36948000	1.45346100	0.87774000
C	2.90266600	2.69638300	0.44775000
C	2.27482800	3.00391800	-0.82580200
C	1.38712900	1.93484100	-1.11313200
C	-2.28797000	1.56694900	-0.87043100
C	-2.70871000	2.87398700	-0.50050500
C	-2.07419600	3.17640600	0.76865100
C	-1.29519400	2.04523200	1.11697200
C	-2.71439000	0.97385500	-2.06605700
C	-3.57757300	1.70242800	-2.88337300
C	-4.00685000	2.99435800	-2.52615700
C	-3.57366200	3.58591600	-1.33765600
C	-2.12939100	4.27440400	1.63499600
C	-1.41514100	4.22916600	2.83416400
C	-0.66173400	3.09312500	3.17387200
C	-0.59696600	1.98461500	2.32551200
C	2.73144000	0.88869300	2.10593700
C	3.66467200	1.57185900	2.88859400
C	4.21335500	2.79433900	2.46672600
C	3.83043000	3.36609000	1.24914700

C	2.41118700	4.05403300	-1.73685100
C	1.66862100	4.02542200	-2.92195200
C	0.80955000	2.95075100	-3.20363900
C	0.66293000	1.88781700	-2.30948600
N	-2.88879400	-1.41376500	0.24310100
C	-3.73344800	-1.99805500	-0.71846000
C	-5.07768900	-1.86678600	-0.28968200
C	-5.04561300	-1.20432500	1.00165800
C	-3.68074400	-0.95010400	1.30211000
C	-6.03394800	-0.83950800	1.92236300
C	-5.65345000	-0.24131500	3.12547400
C	-4.29597800	-0.01904000	3.41758600
C	-3.29261300	-0.37292300	2.51479800
C	-3.40536000	-2.60151100	-1.93683100
C	-4.45306300	-3.07796300	-2.72738000
C	-5.79250900	-2.95222600	-2.31933700
C	-6.11140100	-2.34732700	-1.10224300
N	2.79034800	-1.50718400	-0.21072100
C	3.68324700	-2.00788100	0.74437100
C	5.00910700	-1.86257600	0.25626300
C	4.90722100	-1.28874200	-1.07432000
C	3.52596900	-1.09941800	-1.33540400
C	5.84506700	-0.97144900	-2.06224700
C	5.39604000	-0.48591000	-3.29364100
C	4.02282700	-0.33363800	-3.54583300
C	3.06778400	-0.64574400	-2.57465500
C	3.41902000	-2.55921900	2.00494200
C	4.50862000	-2.95522600	2.78015700
C	5.82819700	-2.80991100	2.31433900
C	6.08484400	-2.26576200	1.05367300
H	-2.39830200	-0.02962600	-2.34650600
H	-3.93119800	1.25464000	-3.81419400
H	-4.68632500	3.53760800	-3.18583600
H	-3.90380300	4.59085300	-1.06636200
H	-2.72987800	5.15025700	1.37997900
H	-1.44852100	5.07916200	3.51840100
H	-0.11626400	3.06947500	4.11940500
H	-0.02497000	1.10178300	2.60729500
H	2.30463500	-0.05389400	2.44436500
H	3.97068000	1.14297700	3.84467600
H	4.94031800	3.30625200	3.10018700
H	4.24543600	4.32557200	0.93352000
H	3.09442300	4.88081200	-1.53179500
H	1.76505900	4.84143700	-3.64073800
H	0.24441600	2.94016000	-4.13750700
H	0.00725100	1.05102400	-2.54320800
H	-7.08748000	-1.03000400	1.70686600
H	-6.41540200	0.04759400	3.85210500
H	-4.01673700	0.43692200	4.36959000
H	-2.24340200	-0.20997100	2.75447300
H	-2.36821000	-2.71689700	-2.25301700
H	-4.22244700	-3.56451200	-3.67736000
H	-6.58918700	-3.33653700	-2.95926400
H	-7.15262200	-2.25162800	-0.78688500
H	6.91207600	-1.11447200	-1.87901100
H	6.11825700	-0.23715800	-4.07359300
H	3.68976400	0.02756000	-4.52078700
H	2.00367300	-0.55341800	-2.78620800
H	2.39769600	-2.69775800	2.36046100
H	4.32953700	-3.39837500	3.76174000
H	6.65949100	-3.13452000	2.94317100
H	7.11065700	-2.16007700	0.69456400

PXZ-TRZ (13)

S₀ geometry

C	-0.338159	-0.000006	-0.000001
C	0.374488	-1.211352	-0.000328
C	1.768641	-1.211465	-0.000295
C	2.472660	-0.000012	-0.000001

C	1.768647	1.211444	0.000293
C	0.374494	1.211337	0.000323
N	3.904822	-0.000017	0.000001
C	-1.825755	-0.000002	0.000005
N	-2.449863	1.187625	-0.000112
C	-3.793020	1.137802	-0.000095
N	-4.506023	0.000003	-0.000068
C	-3.793024	-1.137801	-0.000050
N	-2.449868	-1.187627	0.000057
C	-4.535764	2.423840	-0.000063
C	-4.535773	-2.423835	0.000011
C	-3.842099	3.646833	-0.000783
C	-4.541540	4.853516	-0.000736
C	-5.940583	4.855188	0.000065
C	-6.637812	3.642202	0.000800
C	-5.941730	2.433604	0.000725
C	-5.941740	-2.433594	-0.000781
C	-6.637826	-3.642189	-0.000779
C	-5.940602	-4.855178	0.000048
C	-4.541559	-4.853512	0.000861
C	-3.842114	-3.646832	0.000827
C	4.616993	0.000028	1.216804
C	6.026818	0.000029	1.185914
O	6.735240	-0.000036	0.000005
C	6.026822	-0.000055	-1.185906
C	4.616997	-0.000039	-1.216799
C	6.769130	-0.000120	-2.360430
C	6.125260	-0.000158	-3.604432
C	4.733309	-0.000129	-3.651236
C	3.984502	-0.000063	-2.467350
C	3.984495	0.000087	2.467352
C	4.733298	0.000172	3.651240
C	6.125249	0.000188	3.604440
C	6.769123	0.000116	2.360439
H	-0.180802	-2.148440	-0.000583
H	2.324425	-2.150760	-0.000503
H	2.324434	2.150738	0.000503
H	-0.180792	2.148428	0.000580
H	-2.752864	3.633052	-0.001375
H	-3.993339	5.798235	-0.001322
H	-6.487187	5.801154	0.000123
H	-7.730060	3.639101	0.001441
H	-6.473497	1.482864	0.001313
H	-6.473504	-1.482852	-0.001440
H	-7.730075	-3.639085	-0.001430
H	-6.487210	-5.801142	0.000052
H	-3.993362	-5.798233	0.001518
H	-2.752878	-3.633054	0.001425
H	7.857296	-0.000142	-2.276991
H	6.715753	-0.000218	-4.522203
H	4.211444	-0.000159	-4.610185
H	2.895709	-0.000036	-2.514288
H	2.895702	0.000071	2.514287
H	4.211431	0.000227	4.610188
H	6.715740	0.000263	4.522212
H	7.857290	0.000126	2.277003

PXZ-TRZ (13)

T₁ geometry

C	-0.32837500	0.00000000	0.00000500
C	0.37974200	-1.21269100	0.00002600
C	1.77732300	-1.21677000	0.00002900
C	2.46328400	0.00000000	0.00000100
C	1.77732300	1.21677000	-0.00002400
C	0.37974200	1.21269100	-0.00001800
N	3.90834800	-0.00000100	0.00000000
C	-1.82004600	0.00000000	0.00000800
N	-2.43266900	1.18996900	0.00011400
C	-3.78572400	1.14027100	0.00005100

N	-4.49284800	0.00000000	0.00000000
C	-3.78572300	-1.14027100	-0.00005000
N	-2.43266900	-1.18996900	-0.00010500
C	-4.52657400	2.42134800	0.00003400
C	-4.52657300	-2.42134900	-0.00003400
C	-3.83500400	3.64789200	0.00081000
C	-4.53494400	4.85414100	0.00078900
C	-5.93419900	4.85789400	-0.00004700
C	-6.62999000	3.64273500	-0.00084700
C	-5.93469800	2.43474000	-0.00079300
C	-5.93469700	-2.43474100	0.00078800
C	-6.62998900	-3.64273600	0.00084000
C	-5.93419800	-4.85789400	0.00004300
C	-4.53494400	-4.85414200	-0.00078700
C	-3.83500300	-3.64789200	-0.00080700
C	4.58882500	0.00006400	1.20572200
C	6.03518900	-0.00015700	1.17672000
O	6.71179700	0.00000000	-0.00000300
C	6.03518600	0.00015700	-1.17672500
C	4.58882200	-0.00006600	-1.20572400
C	6.77780000	0.00038000	-2.36403300
C	6.12911800	0.00034900	-3.58667900
C	4.69439900	0.00005900	-3.63357100
C	3.95049800	-0.00011400	-2.47165300
C	3.95050300	0.00011300	2.47165200
C	4.69440700	-0.00005800	3.63356900
C	6.12912500	-0.00034700	3.58667400
C	6.77780500	-0.00037900	2.36402700
H	-0.18041200	-2.14645600	0.00006000
H	2.33586100	-2.15405300	0.00006100
H	2.33586200	2.15405300	-0.00005700
H	-0.18041100	2.14645700	-0.00005000
H	-2.74575700	3.63505200	0.00143600
H	-3.98605500	5.79884900	0.00142300
H	-6.48100000	5.80375100	-0.00008700
H	-7.72250200	3.63874100	-0.00152400
H	-6.46703900	1.48419800	-0.00142600
H	-6.46703900	-1.48419900	0.00141700
H	-7.72250100	-3.63874200	0.00151200
H	-6.48099900	-5.80375200	0.00008200
H	-3.98605400	-5.79884900	-0.00141800
H	-2.74575700	-3.63505200	-0.00142900
H	7.86661900	0.00054600	-2.28792100
H	6.70683600	0.00053100	-4.51169200
H	4.18370400	-0.00002400	-4.59740400
H	2.86175200	-0.00031300	-2.51568100
H	2.86175700	0.00031200	2.51568300
H	4.18371300	0.00002500	4.59740300
H	6.70684500	-0.00052800	4.51168600
H	7.86662400	-0.00054400	2.28791200

Spiro-CN (14)

S₀ geometry

C	2.542600	0.179606	-0.068193
C	1.189744	0.486737	-0.036966
C	0.733838	1.821369	-0.028188
C	1.669562	2.862047	-0.056526
C	3.031432	2.563299	-0.102033
C	3.487908	1.227690	-0.104876
H	2.883735	-0.856717	-0.063013
H	1.345558	3.905223	-0.058933
H	3.762412	3.371919	-0.138204
C	-0.731508	1.822172	0.011393
C	-1.666527	2.863673	0.025406
C	-1.188378	0.488013	0.036578
C	-3.028779	2.566379	0.071823
H	-1.341866	3.906600	0.015476
C	-2.541402	0.182202	0.068777
C	-3.486177	1.231271	0.089581

H	-3.759206	3.375928	0.096373
H	-2.883139	-0.853891	0.076062
C	0.080382	-3.539903	3.047691
C	0.045816	-3.838787	1.687112
C	0.020998	-2.788737	0.761110
C	0.032821	-1.446880	1.197159
C	0.066550	-1.141060	2.550755
C	0.090022	-2.198002	3.483086
H	0.099502	-4.340112	3.788579
H	0.037570	-4.879369	1.357108
H	0.074143	-0.106404	2.896313
C	-0.019730	-2.801378	-0.706135
C	-0.032302	-1.467193	-1.165200
C	-0.044407	-3.867146	-1.613998
C	-0.066864	-1.184550	-2.523812
C	-0.079795	-3.591548	-2.979471
H	-0.035568	-4.901925	-1.266247
C	-0.090348	-2.257330	-3.437885
H	-0.075189	-0.155910	-2.886854
H	-0.098992	-4.404339	-3.706546
C	0.000390	-0.484916	0.007553
N	4.873721	0.941303	-0.144888
N	-4.872248	0.945565	0.127653
C	5.795191	1.740170	0.591256
C	7.001056	2.161495	0.010250
C	5.522742	2.114656	1.919273
C	7.909337	2.927779	0.743857
H	7.227765	1.881564	-1.019861
C	6.430384	2.894722	2.632939
H	4.593265	1.789407	2.389777
C	7.644934	3.314935	2.064952
H	8.842927	3.241474	0.268957
H	6.194742	3.171265	3.664567
C	5.356801	-0.156404	-0.914036
C	6.311117	-1.038646	-0.384761
C	6.790320	-2.103724	-1.150605
C	6.327661	-2.338755	-2.452867
C	5.366014	-1.453815	-2.969092
C	4.893186	-0.375640	-2.223613
H	6.680850	-0.885047	0.630435
H	7.535501	-2.775540	-0.715944
H	4.988169	-1.601529	-3.984772
H	4.157375	0.305678	-2.654397
C	-5.792156	1.737360	-0.617479
C	-5.514628	2.104800	-1.946588
C	-7.002500	2.157865	-0.045159
C	-6.421498	2.877161	-2.669368
H	-4.581798	1.780067	-2.410745
C	-7.909913	2.916365	-0.788015
H	-7.233375	1.883739	0.985586
C	-7.640420	3.296533	-2.110006
H	-6.181695	3.148204	-3.701504
H	-8.846975	3.229473	-0.319604
C	-6.784909	-2.092775	1.154219
C	-6.331324	-2.310172	2.466222
C	-5.381587	-1.415816	2.979466
C	-4.906607	-0.341524	2.223907
C	-5.358346	-0.141454	0.910339
C	-6.305704	-1.036284	0.382203
H	-7.521940	-2.774470	0.720041
H	-5.012213	-1.550285	3.999677
H	-4.177798	0.347914	2.653613
H	-6.665773	-0.895653	-0.638396
C	8.623731	4.147194	2.857897
H	8.972913	3.609844	3.756195
H	9.509247	4.407639	2.259261
H	8.164432	5.088043	3.205502
C	6.842213	-3.491910	-3.280429
H	6.021371	-4.153486	-3.605064
H	7.347436	-3.136460	-4.194787

H	7.563071	-4.102755	-2.716845
C	-8.618205	4.120436	-2.912840
H	-8.160019	5.059997	-3.265353
H	-8.962415	3.575757	-3.808659
H	-9.506799	4.382789	-2.319613
C	-6.855036	-3.465181	3.285472
H	-7.947152	-3.396490	3.426384
H	-6.655818	-4.431808	2.792177
H	-6.390400	-3.495760	4.282131
C	0.121695	-1.908611	4.889593
C	-0.122894	-1.992207	-4.849145
N	0.145436	-1.675926	6.030445
N	-0.147315	-1.779236	-5.993832

Spiro-CN (14)

T₁ geometry

C	-2.53029800	-0.16651400	-0.04570200
C	-1.18133600	-0.46518500	-0.02424100
C	-0.72277000	-1.81023800	-0.01515500
C	-1.65781600	-2.86186800	-0.03507400
C	-3.01200500	-2.56848900	-0.06257600
C	-3.47316200	-1.22161800	-0.06663900
H	-2.86729400	0.86981900	-0.03691900
H	-1.32922700	-3.90316800	-0.04634500
H	-3.74133600	-3.37728900	-0.10185500
C	0.72276800	-1.81021800	0.01336000
C	1.65786200	-2.86181400	0.03258800
C	1.18128200	-0.46515200	0.02337400
C	3.01204100	-2.56840500	0.06034200
H	1.32932200	-3.90313800	0.04313900
C	2.53022500	-0.16644300	0.04508100
C	3.47315300	-1.22151700	0.06534400
H	3.74138300	-3.37721600	0.09913100
H	2.86717500	0.86991100	0.03702400
C	-0.03162200	3.60267900	3.00996800
C	-0.01975300	3.89868100	1.66585700
C	-0.00920300	2.83623700	0.70635700
C	-0.01572900	1.47404300	1.19032000
C	-0.02690000	1.18023200	2.53003900
C	-0.03373200	2.24855400	3.48201300
H	-0.03909400	4.40806600	3.74716600
H	-0.01729400	4.93922200	1.33476100
H	-0.03012300	0.14750500	2.88498600
C	0.00885600	2.83676400	-0.70477400
C	0.01555800	1.47492900	-1.18974800
C	0.01928800	3.89991400	-1.66349100
C	0.02680300	1.18209900	-2.52968200
C	0.03122600	3.60489600	-3.00781900
H	0.01668800	4.94021300	-1.33163900
C	0.03352400	2.25112000	-3.48086500
H	0.03017300	0.14962700	-2.88537100
H	0.03861000	4.41082600	-3.74442400
C	-0.00004500	0.50436100	-0.00007200
N	-4.84641000	-0.95149400	-0.10579100
N	4.84634900	-0.95128900	0.10483300
C	-5.78488400	-1.85426900	0.47950900
C	-6.92695200	-2.24891300	-0.23240200
C	-5.59030700	-2.34360900	1.78281000
C	-7.84976800	-3.11889900	0.34999600
H	-7.08840000	-1.87240500	-1.24377600
C	-6.51503200	-3.21995800	2.34653100
H	-4.71590100	-2.02517200	2.35301700
C	-7.66313200	-3.62599000	1.64470800
H	-8.73246700	-3.41676100	-0.22164100
H	-6.34828000	-3.58464300	3.36366200
C	-5.34130600	0.24284100	-0.71458700
C	-6.30104000	1.02653800	-0.05813100
C	-6.79123600	2.18510600	-0.66261000
C	-6.33784400	2.60219400	-1.92266100

C	-5.37706000	1.80501500	-2.56902700
C	-4.88772700	0.63987600	-1.98450400
H	-6.65874300	0.72893600	0.92879000
H	-7.53538900	2.78541400	-0.13309100
H	-5.00844900	2.09684400	-3.55580600
H	-4.14961700	0.03273400	-2.51088200
C	5.78513500	-1.85376000	-0.48044500
C	5.59110800	-2.34264100	-1.78401600
C	6.92692100	-2.24860500	0.23177500
C	6.51610600	-3.21871200	-2.34769300
H	4.71684200	-2.02414000	-2.35440400
C	7.85003800	-3.11831400	-0.35059200
H	7.08788300	-1.87257300	1.24340200
C	7.66400600	-3.62486100	-1.64558300
H	6.34971900	-3.58312500	-3.36498300
H	8.73246900	-3.41642800	0.22132700
C	6.79068300	2.18522700	0.66383600
C	6.33727100	2.60134300	1.92420400
C	5.37662300	1.80357000	2.57003500
C	4.88743300	0.63877900	1.98468500
C	5.34104000	0.24272600	0.71448600
C	6.30063100	1.02702200	0.05854600
H	7.53474200	2.78601700	0.13473200
H	5.00800900	2.09464400	3.55703500
H	4.14942100	0.03115200	2.51064300
H	6.65835100	0.73014600	-0.92858700
C	-8.65338400	-4.57777400	2.26959800
H	-8.98770500	-4.21762300	3.25654600
H	-9.54362500	-4.70741200	1.63701100
H	-8.20520000	-5.57395700	2.42625200
C	-6.85014100	3.86617400	-2.56763500
H	-6.04265500	4.60943400	-2.68038800
H	-7.24738400	3.66877900	-3.57711000
H	-7.65089600	4.32822800	-1.97196300
C	8.65504200	-4.57560700	-2.27081600
H	8.20436300	-5.56883900	-2.43832700
H	8.99761400	-4.20908800	-3.25263800
H	9.54044400	-4.71318900	-1.63315000
C	6.84938400	3.86496400	2.57002700
H	7.65043700	4.32725400	1.97493400
H	6.04190300	4.60823400	2.68276700
H	7.24616000	3.66705200	3.57958000
C	-0.03745400	1.97126000	4.87264500
C	0.03732500	1.97485900	-4.87170400
N	-0.03687300	1.73775600	6.02066200
N	0.03682200	1.74221400	-6.01989500

4CzIPN (15)

S₀ geometry

C	0.081941	1.194701	0.274158
C	-0.637590	0.000032	-0.000023
C	0.081694	-1.194781	-0.274215
C	1.498321	-1.173831	-0.306340
C	2.211761	-0.000251	-0.000061
C	1.498563	1.173471	0.306244
C	2.226145	2.331318	0.742048
N	3.623366	-0.000397	-0.000088
N	-0.576550	-2.410230	-0.552742
N	-2.050775	0.000168	-0.000006
N	2.826030	3.253152	1.120717
C	-0.460598	-3.589541	0.214084
C	-1.250183	-4.600831	-0.384858
C	-1.845999	-4.027650	-1.577381
C	-1.408207	-2.682593	-1.658734
C	-2.672620	-4.546409	-2.582777
C	-3.037483	-3.726938	-3.650108
C	-2.572382	-2.402533	-3.726655
C	-1.747480	-1.864063	-2.737404
C	0.251587	-3.817475	1.394812

C	0.166500	-5.086238	1.971621
C	-0.611999	-6.102096	1.390079
C	-1.322454	-5.865521	0.213997
C	-2.878733	0.734099	-0.875357
C	-4.232577	0.464380	-0.557120
C	-4.232647	-0.463648	0.557163
C	-2.878844	-0.733623	0.875357
C	-2.532195	1.567998	-1.941330
C	-3.565838	2.152373	-2.676097
C	-4.914351	1.907102	-2.363819
C	-5.253368	1.061170	-1.308880
C	-5.253525	-1.060250	1.308953
C	-4.914634	-1.906252	2.363876
C	-3.566157	-2.151783	2.676108
C	-2.532428	-1.567599	1.941308
C	2.225663	-2.331824	-0.742157
N	2.825352	-3.253783	-1.120834
N	-0.576056	2.410281	0.552708
C	-0.459849	3.589583	-0.214090
C	-1.249139	4.601059	0.384928
C	-1.845019	4.028001	1.577476
C	-1.407562	2.682831	1.658769
C	4.443452	0.571750	-0.988287
C	5.798581	0.361540	-0.629387
C	5.798531	-0.362403	0.629344
C	4.443373	-0.572555	0.988170
C	0.252319	3.817366	-1.394857
C	0.167510	5.086162	-1.971634
C	-0.610698	6.102202	-1.390021
C	-1.321133	5.865780	-0.213896
C	-2.671448	4.546944	2.582935
C	-3.036452	3.727539	3.650269
C	-2.571679	2.403015	3.726755
C	-1.746974	1.864361	2.737440
C	6.811595	-0.833888	1.475307
C	6.460885	-1.496072	2.651304
C	5.109933	-1.686526	2.992989
C	4.081757	-1.225545	2.168752
C	4.081926	1.224757	-2.168887
C	5.110165	1.685697	-2.993068
C	6.461091	1.495183	-2.651311
C	6.811711	0.832980	-1.475297
H	-3.016803	-5.581658	-2.534128
H	-3.681372	-4.118448	-4.440047
H	-2.857553	-1.778078	-4.575643
H	-1.386070	-0.839888	-2.815909
H	0.867036	-3.041959	1.852757
H	0.721931	-5.290360	2.889290
H	-0.656867	-7.084525	1.863932
H	-1.928897	-6.654338	-0.236053
H	-1.493652	1.769317	-2.200534
H	-3.314972	2.814881	-3.506984
H	-5.700147	2.380352	-2.955790
H	-6.300543	0.860167	-1.072869
H	-6.300671	-0.859051	1.072976
H	-5.700500	-2.379359	2.955869
H	-3.315388	-2.814343	3.506981
H	-1.493914	-1.769118	2.200472
H	0.867550	3.041709	-1.852856
H	0.722933	5.290166	-2.889335
H	-0.655351	7.084652	-1.863850
H	-1.927347	6.654740	0.236212
H	-3.015375	5.582280	2.534331
H	-3.680193	4.119193	4.440258
H	-2.856955	1.778612	4.575747
H	-1.385819	0.840093	2.815899
H	7.861700	-0.680901	1.217452
H	7.241506	-1.868356	3.317483
H	4.856982	-2.202546	3.921533
H	3.035792	-1.366200	2.445892

H	3.035981	1.365452	-2.446083
H	4.857287	2.201731	-3.921623
H	7.241764	1.867435	-3.317447
H	7.861795	0.679946	-1.217389

4CzIPN (15)

T₁ geometry

C	0.06611300	1.20382300	0.23424800
C	-0.62319000	-0.00001200	0.00000300
C	0.06616100	-1.20382300	-0.23424200
C	1.52817600	-1.20127300	-0.27068600
C	2.21273700	0.00004200	0.00000500
C	1.52812700	1.20133100	0.27069600
C	2.23367200	2.36187800	0.67974100
N	3.63187300	0.00007100	0.00000700
N	-0.62323500	-2.41606200	-0.50853600
N	-2.05480100	-0.00003500	0.00000200
N	2.79779800	3.33084400	1.01341700
C	-0.65798300	-3.53198000	0.33126200
C	-1.38007400	-4.57740500	-0.30485300
C	-1.76801900	-4.07813900	-1.61355700
C	-1.26159400	-2.75591800	-1.71144400
C	-2.45143100	-4.63632900	-2.69761700
C	-2.60956200	-3.87869900	-3.86298400
C	-2.08045200	-2.58067800	-3.95195700
C	-1.39565900	-2.00203900	-2.88026200
C	-0.09659400	-3.69418400	1.60444600
C	-0.28343000	-4.91870600	2.24594300
C	-1.01073500	-5.95670300	1.63589300
C	-1.55974000	-5.79315000	0.36013000
C	-2.87513100	0.60169600	-0.96373300
C	-4.23440300	0.38102100	-0.61770600
C	-4.23439400	-0.38115000	0.61770700
C	-2.87511700	-0.60177600	0.96374300
C	-2.51991500	1.28071600	-2.13446800
C	-3.54844500	1.76154000	-2.94724600
C	-4.89784900	1.56158300	-2.61115100
C	-5.24736700	0.86750300	-1.44954800
C	-5.24734700	-0.86765900	1.44954500
C	-4.89781400	-1.56171400	2.61115900
C	-3.54840600	-1.76161800	2.94726700
C	-2.51988600	-1.28076700	2.13449000
C	2.23376600	-2.36179500	-0.67972900
N	2.79792800	-3.33074000	-1.01340100
N	-0.62333500	2.41603300	0.50853700
C	-0.65814700	3.53194100	-0.33127200
C	-1.38028100	4.57733600	0.30484000
C	-1.76819800	4.07806000	1.61354900
C	-1.26171300	2.75586300	1.71144000
C	4.44854900	0.65555200	-0.92960800
C	5.80719100	0.41575200	-0.59665500
C	5.80720600	-0.41554900	0.59665700
C	4.44857300	-0.65539000	0.92961600
C	-0.09677900	3.69416000	-1.60446300
C	-0.28367700	4.91866900	-2.24596800
C	-1.01102300	5.95663700	-1.63591800
C	-1.56000900	5.79306800	-0.36015000
C	-2.45163300	4.63622400	2.69760700
C	-2.60972900	3.87859200	3.86297700
C	-2.08056300	2.58059400	3.95195300
C	-1.39574600	2.00198100	2.88026100
C	6.81584900	-0.95208400	1.40098900
C	6.45889600	-1.71262000	2.51916000
C	5.10793800	-1.93288300	2.83860700
C	4.08292200	-1.40581500	2.05171700
C	4.08287100	1.40596800	-2.05170600
C	5.10786800	1.93306600	-2.83860000
C	6.45883400	1.71284400	-2.51916000
C	6.81581500	0.95231800	-1.40099000

H	-2.84669500	-5.65286000	-2.64097300
H	-3.13964200	-4.30447000	-4.71716300
H	-2.20034500	-2.01169000	-4.87604800
H	-0.96887800	-1.00314100	-2.95721700
H	0.48499200	-2.89613300	2.06685700
H	0.15025800	-5.07548100	3.23569800
H	-1.13931400	-6.90452600	2.16224000
H	-2.11481600	-6.60699600	-0.11115700
H	-1.47676500	1.43540800	-2.40362800
H	-3.29398000	2.30404800	-3.85984100
H	-5.68002600	1.94826200	-3.26726700
H	-6.29712700	0.70266000	-1.19777300
H	-6.29711100	-0.70285000	1.19776400
H	-5.67998300	-1.94841200	3.26727400
H	-3.29392800	-2.30410500	3.85987100
H	-1.47673200	-1.43541700	2.40366200
H	0.48483900	2.89613300	-2.06687300
H	0.14999500	5.07545600	-3.23572800
H	-1.13965000	6.90445000	-2.16227100
H	-2.11511900	6.60689000	0.11113500
H	-2.84694300	5.65273600	2.64095800
H	-3.13982700	4.30434200	4.71715400
H	-2.20043000	2.01160400	4.87604600
H	-0.96892200	1.00310200	2.95721800
H	7.86724000	-0.77696000	1.16376600
H	7.23825400	-2.13833400	3.15413000
H	4.85286100	-2.52731000	3.71812300
H	3.03536300	-1.57404900	2.30061000
H	3.03530700	1.57417300	-2.30059400
H	4.85277000	2.52748700	-3.71811400
H	7.23817800	2.13858100	-3.15413200
H	7.86721200	0.77722300	-1.16377200

4CzTPN (16)

S₀ geometry

C	1.239271	-0.654999	-0.263424
C	1.239272	0.654991	0.263419
C	0.000005	1.282654	0.538610
C	-1.239264	0.654992	0.263425
C	-1.239266	-0.654997	-0.263427
C	0.000002	-1.282662	-0.538611
C	0.000002	-2.543771	-1.224733
C	0.000008	2.543767	1.224724
N	0.000001	-3.549106	-1.809972
N	0.000012	3.549107	1.809956
N	2.438164	-1.346414	-0.538591
N	2.438167	1.346405	0.538583
N	-2.438158	-1.346407	-0.538606
N	-2.438154	1.346407	0.538605
C	2.864870	-2.525754	0.104310
C	4.098161	-2.931983	-0.461861
C	4.422411	-1.978403	-1.506652
C	3.380160	-1.018499	-1.533693
C	-2.864869	-2.525756	0.104275
C	-4.098170	-2.931963	-0.461894
C	-4.422417	-1.978361	-1.506667
C	-3.380156	-1.018468	-1.533699
C	-2.864854	2.525766	-0.104263
C	-4.098157	2.931972	0.461902
C	-4.422416	1.978359	1.506661
C	-3.380159	1.018460	1.533689
C	3.380165	1.018487	1.533681
C	4.422410	1.978398	1.506648
C	4.098150	2.931989	0.461868
C	2.864860	2.525756	-0.104304
C	2.266444	-3.236901	1.147886
C	2.923321	-4.374433	1.621108
C	4.147937	-4.792281	1.071043
C	4.739931	-4.075726	0.031905

C	5.476020	-1.877698	-2.425223
C	5.469076	-0.837197	-3.353175
C	4.415986	0.094303	-3.376755
C	3.355492	0.014692	-2.472441
C	-5.476028	-1.877633	-2.425232
C	-5.469078	-0.837119	-3.353169
C	-4.415978	0.094369	-3.376743
C	-3.355481	0.014735	-2.472435
C	-2.266443	-3.236929	1.147832
C	-2.923328	-4.374464	1.621037
C	-4.147953	-4.792288	1.070975
C	-4.739947	-4.075708	0.031854
C	-5.476034	1.877625	2.425218
C	-5.469095	0.837100	3.353142
C	-4.416000	-0.094394	3.376711
C	-3.355496	-0.014754	2.472412
C	-2.266415	3.236951	-1.147805
C	-2.923290	4.374495	-1.621000
C	-4.147918	4.792318	-1.070943
C	-4.739924	4.075727	-0.031837
C	4.739909	4.075743	-0.031885
C	4.147905	4.792306	-1.071012
C	2.923290	4.374456	-1.621077
C	2.266424	3.236912	-1.147868
C	3.355508	-0.014716	2.472417
C	4.416005	-0.094329	3.376727
C	5.469088	0.837179	3.353155
C	5.476022	1.877691	2.425215
H	1.314661	-2.926473	1.581435
H	2.471949	-4.950048	2.431868
H	4.636532	-5.686951	1.461593
H	5.691977	-4.399941	-0.393641
H	6.285921	-2.610241	-2.417794
H	6.283907	-0.747307	-4.074177
H	4.422618	0.897683	-4.116115
H	2.541510	0.737797	-2.507575
H	-6.285936	-2.610169	-2.417810
H	-6.283911	-0.747211	-4.074167
H	-4.422605	0.897759	-4.116091
H	-2.541491	0.737831	-2.507563
H	-1.314653	-2.926522	1.581379
H	-2.471956	-4.950100	2.431783
H	-4.636553	-5.686961	1.461511
H	-5.692000	-4.399906	-0.393691
H	-6.285938	2.610165	2.417799
H	-6.283933	0.747187	4.074134
H	-4.422636	-0.897794	4.116050
H	-2.541509	-0.737855	2.507536
H	-1.314622	2.926545	-1.581348
H	-2.471908	4.950140	-2.431734
H	-4.636511	5.686998	-1.461471
H	-5.691979	4.399923	0.393705
H	5.691954	4.399961	0.393662
H	4.636492	5.686985	-1.461552
H	2.471911	4.950079	-2.431828
H	1.314642	2.926483	-1.581417
H	2.541531	-0.737828	2.507543
H	4.422645	-0.897718	4.116077
H	6.283921	0.747286	4.074154
H	6.285917	2.610240	2.417793

4CzTPN (16)

T₁ geometry

C	1.23626100	-0.65380000	-0.23424300
C	1.23626000	0.65380500	0.23423600
C	0.00001400	1.36254600	0.47647200
C	-1.23623000	0.65380200	0.23423600
C	-1.23622900	-0.65380400	-0.23423300
C	0.00001600	-1.36254400	-0.47647300

C	0.00001800	-2.60651700	-1.14465500
C	0.00001500	2.60651700	1.14465600
N	0.00000500	-3.64518900	-1.68755300
N	0.00003800	3.64518900	1.68755500
N	2.45835400	-1.31570200	-0.52816400
N	2.45835200	1.31570900	0.52815800
N	-2.45833100	-1.31569200	-0.52814200
N	-2.45833300	1.31568800	0.52814700
C	2.91708500	-2.47856300	0.09994600
C	4.14532200	-2.87354900	-0.49345200
C	4.42042800	-1.92466900	-1.55884200
C	3.35391200	-0.98956400	-1.56127800
C	-2.91708100	-2.47854300	0.09997400
C	-4.14532000	-2.87351600	-0.49342900
C	-4.42042300	-1.92462000	-1.55880800
C	-3.35390400	-0.98952000	-1.56123200
C	-2.91709100	2.47853100	-0.09997700
C	-4.14533000	2.87350300	0.49342900
C	-4.42042300	1.92461500	1.55881700
C	-3.35389900	0.98952000	1.56124400
C	3.35391500	0.98956400	1.56126500
C	4.42042800	1.92467300	1.55883500
C	4.14531500	2.87356200	0.49345400
C	2.91707700	2.47857600	-0.09994500
C	2.35264600	-3.19120200	1.16559500
C	3.03816400	-4.31260500	1.63212700
C	4.25780400	-4.71323800	1.05757000
C	4.81734500	-3.99716400	-0.00422100
C	5.43659600	-1.81456200	-2.51287700
C	5.37033000	-0.78743600	-3.45905600
C	4.29349000	0.11411200	-3.46331400
C	3.26712900	0.02302600	-2.51960600
C	-5.43659600	-1.81449100	-2.51283400
C	-5.37033500	-0.78734200	-3.45898900
C	-4.29349600	0.11420600	-3.46323100
C	-3.26712800	0.02309700	-2.51953200
C	-2.35265400	-3.19118800	1.16562500
C	-3.03818300	-4.31258600	1.63215100
C	-4.25782200	-4.71321000	1.05758500
C	-4.81735300	-3.99712700	-0.00420600
C	-5.43659100	1.81448900	2.51284900
C	-5.37032000	0.78735000	3.45901400
C	-4.29347600	-0.11419300	3.46325800
C	-3.26711300	-0.02308700	2.51955400
C	-2.35267500	3.19116900	-1.16563800
C	-3.03821200	4.31255900	-1.63217000
C	-4.25784900	4.71318200	-1.05760100
C	-4.81737200	3.99710600	0.00419900
C	4.81733200	3.99718300	0.00423100
C	4.25778500	4.71326400	-1.05755200
C	3.03814500	4.31263200	-1.63211000
C	2.35263300	3.19122300	-1.16558500
C	3.26713900	-0.02303500	2.51958400
C	4.29350400	-0.11412600	3.46328700
C	5.37034000	0.78742600	3.45903500
C	5.43659800	1.81456200	2.51286500
H	1.40107500	-2.89101200	1.60412200
H	2.61518800	-4.89170600	2.45540400
H	4.77068900	-5.59574700	1.44485000
H	5.76527400	-4.31186200	-0.44558900
H	6.26355100	-2.52768200	-2.52605700
H	6.15703000	-0.69162300	-4.20991900
H	4.25075500	0.90034900	-4.21957400
H	2.42428100	0.71195300	-2.54100100
H	-6.26355600	-2.52760600	-2.52602200
H	-6.15704100	-0.69151000	-4.20984400
H	-4.25076500	0.90046200	-4.21947200
H	-2.42427900	0.71202500	-2.54091500
H	-1.40108200	-2.89100800	1.60415700
H	-2.61521600	-4.89169400	2.45542800

H	-4.77071600	-5.59571600	1.44486100
H	-5.76528500	-4.31181400	-0.44557600
H	-6.26355400	2.52760000	2.52603400
H	-6.15702100	0.69152000	4.20987300
H	-4.25073700	-0.90044200	4.21950600
H	-2.42426000	-0.71201000	2.54093800
H	-1.40110300	2.89098900	-1.60417200
H	-2.61525200	4.89166200	-2.45545500
H	-4.77075000	5.59568200	-1.44488300
H	-5.76530300	4.31179200	0.44557000
H	5.76526100	4.31188000	0.44559900
H	4.77066600	5.59577800	-1.44482700
H	2.61516500	4.89173900	-2.45538100
H	1.40106100	2.89103300	-1.60411200
H	2.42429400	-0.71196700	2.54097500
H	4.25077400	-0.90037000	4.21954000
H	6.15704300	0.69161000	4.20989500
H	6.26355100	2.52768500	2.52604900

4CzTPN-Me (17)

S₀ geometry

C	-1.238674	0.705908	0.015645
C	-1.238677	-0.705934	-0.015936
C	0.000033	-1.391904	-0.000133
C	1.238744	-0.705935	0.015647
C	1.238746	0.705915	-0.015940
C	0.000030	1.391880	-0.000151
N	-2.438855	1.445703	0.070743
N	2.438927	1.445729	-0.070908
N	2.438912	-1.445760	0.070722
N	-2.438875	-1.445712	-0.070903
C	0.000009	2.827462	-0.000006
C	0.000042	-2.827486	-0.000055
C	3.398987	1.559193	0.952911
C	4.445722	2.400014	0.506082
C	4.108841	2.820851	-0.841204
C	2.864853	2.229743	-1.161924
C	-3.399000	-1.559014	0.952870
C	-4.445747	-2.399838	0.506076
C	-4.108839	-2.820787	-0.841170
C	-2.864825	-2.229739	-1.161901
C	2.864731	-2.229753	1.161793
C	4.108745	-2.820877	0.841202
C	4.445750	-2.400077	-0.506065
C	3.399058	-1.559265	-0.953013
C	-2.864677	2.229695	1.161813
C	-4.108711	2.820781	0.841234
C	-4.445748	2.399921	-0.506007
C	-3.399052	1.559113	-0.952952
C	-2.260092	2.439694	2.404366
C	-2.922467	3.254399	3.321212
C	-4.166065	3.860836	3.033445
C	-4.751455	3.634705	1.785315
C	-5.518179	2.684658	-1.363708
C	-5.547584	2.146706	-2.652761
C	-4.476741	1.325575	-3.072216
C	-3.397279	1.025191	-2.243370
C	-3.397111	-1.024990	2.243246
C	-4.476506	-1.325296	3.072207
C	-5.547396	-2.146443	2.652905
C	-5.518108	-2.684497	1.363890
C	-4.751691	-3.634749	-1.785145
C	-4.166431	-3.860953	-3.033322
C	-2.922855	-3.254546	-3.321247
C	-2.260374	-2.439807	-2.404507
C	2.260175	-2.439703	2.404368
C	2.922557	-3.254394	3.321223
C	4.166133	-3.860867	3.033442
C	4.751495	-3.634785	1.785291

C	5.518148	-2.684876	-1.363788
C	5.547518	-2.146992	-2.652869
C	4.476674	-1.325867	-3.072331
C	3.397248	-1.025418	-2.243463
C	3.397072	1.025285	2.243336
C	4.476430	1.325697	3.072306
C	5.547308	2.146844	2.652970
C	5.518049	2.684775	1.363906
C	4.751685	3.634778	-1.785214
C	4.166442	3.860891	-3.033416
C	2.922891	3.254429	-3.321329
C	2.260419	2.439722	-2.404554
N	-0.000057	3.990724	0.000120
N	0.000069	-3.990747	0.000017
C	-4.834108	4.739581	4.065125
C	-6.694617	2.430127	-3.594418
C	-6.694376	-2.429742	3.594664
C	-4.834588	-4.739746	-4.064887
C	4.834177	-4.739608	4.065125
C	6.694502	-2.430500	-3.594560
C	6.694180	2.430365	3.594793
C	4.834589	4.739650	-4.065016
H	-1.295351	1.996373	2.656621
H	-2.458678	3.433753	4.294689
H	-5.713691	4.093172	1.543648
H	-6.328993	3.334744	-1.025423
H	-4.492811	0.909162	-4.082710
H	-2.587136	0.390429	-2.601165
H	-2.586922	-0.390219	2.600924
H	-4.492482	-0.908811	4.082673
H	-6.328961	-3.334594	1.025724
H	-5.713912	-4.093183	-1.543359
H	-2.459165	-3.433957	-4.294760
H	-1.295650	-1.996517	-2.656884
H	1.295453	-1.996349	2.656639
H	2.458790	-3.433703	4.294719
H	5.713713	-4.093282	1.543611
H	6.328958	-3.334965	-1.025501
H	4.492717	-0.909506	-4.082848
H	2.587106	-0.390659	-2.601264
H	2.586905	0.390503	2.601038
H	4.492394	0.909286	4.082803
H	6.328895	3.334866	1.025709
H	5.713883	4.093263	-1.543434
H	2.459218	3.433761	-4.294865
H	1.295719	1.996379	-2.656929
H	-4.207997	5.612819	4.315778
H	-5.014369	4.192257	5.005909
H	-5.803448	5.116080	3.706094
H	-6.340480	2.877752	-4.538353
H	-7.421501	3.124003	-3.146677
H	-7.234594	1.505085	-3.859817
H	-7.421132	-3.123911	3.147171
H	-7.234528	-1.504703	3.859726
H	-6.340157	-2.876957	4.538761
H	-5.014886	-4.192488	-5.005702
H	-5.803923	-5.116169	-3.705758
H	-4.208538	-5.613035	-4.315514
H	4.208117	-5.612907	4.315694
H	5.014334	-4.192317	5.005947
H	5.803569	-5.116018	3.706137
H	6.340326	-2.878311	-4.538392
H	7.421462	-3.124254	-3.146752
H	7.234400	-1.505469	-3.860157
H	7.233689	1.505265	3.860930
H	6.339945	2.878724	4.538346
H	7.421479	3.123671	3.146845
H	5.014858	4.192370	-5.005823
H	5.803936	5.116069	-3.705917
H	4.208545	5.612943	-4.315647

4CzTPN-Me (17)

T₁ geometry

C	1.23637000	-0.69367800	0.00030400
C	1.23637000	0.69368100	-0.00039700
C	-0.00000500	1.44006700	-0.00004500
C	-1.23637100	0.69367600	0.00030900
C	-1.23637000	-0.69367900	-0.00040600
C	0.00000100	-1.44006700	-0.00006000
N	2.46602400	-1.41504700	0.00808300
N	-2.46603000	-1.41503700	-0.00817100
N	-2.46603200	1.41503300	0.00811400
N	2.46602200	1.41505100	-0.00812800
C	0.00000100	-2.85086000	-0.00009800
C	-0.00001400	2.85086000	-0.00002200
C	-3.38651200	-1.49929200	1.04706900
C	-4.46618100	-2.32860100	0.65480200
C	-4.17513600	-2.78464400	-0.69311500
C	-2.92682600	-2.21549800	-1.05556800
C	3.38650600	1.49926200	1.04711700
C	4.46618400	2.32857100	0.65487700
C	4.17514400	2.78466400	-0.69302300
C	2.92682900	2.21554100	-1.05549800
C	-2.92681100	2.21546300	1.05554100
C	-4.17512700	2.78462000	0.69312500
C	-4.46619300	2.32861600	-0.65480000
C	-3.38653100	1.49931800	-1.04710900
C	2.92680700	-2.21550300	1.05548800
C	4.17513300	-2.78463200	0.69306200
C	4.46620100	-2.32858500	-0.65484700
C	3.38652800	-1.49929500	-1.04714100
C	2.34874100	-2.46909500	2.30717900
C	3.04036700	-3.29685800	3.18581400
C	4.28828800	-3.87592100	2.85555200
C	4.84843100	-3.60952600	1.59944200
C	5.50908800	-2.57873500	-1.55316800
C	5.48001200	-2.01812400	-2.83741900
C	4.37812700	-1.21608900	-3.20494100
C	3.32434600	-0.95018000	-2.33088900
C	3.32430100	0.95009300	2.33084100
C	4.37806300	1.21597200	3.20492500
C	5.47995000	2.01803000	2.83745800
C	5.50905000	2.57869200	1.55323000
C	4.84845900	3.60959100	-1.59935900
C	4.28834600	3.87602400	-2.85547400
C	3.04043500	3.29696600	-3.18578600
C	2.34879100	2.46917100	-2.30719400
C	-2.34874500	2.46901100	2.30724000
C	-3.04036600	3.29675700	3.18589800
C	-4.28827800	3.87584500	2.85564800
C	-4.84841900	3.60949300	1.59952700
C	-5.50907500	2.57879600	-1.55311900
C	-5.48000700	2.01820200	-2.83737800
C	-4.37813700	1.21615000	-3.20491000
C	-3.32436100	0.95021200	-2.33086100
C	-3.32432300	-0.95014300	2.33080300
C	-4.37808600	-1.21605400	3.20487500
C	-5.47996000	-2.01812000	2.83738500
C	-5.50904800	-2.57875400	1.55314400
C	-4.84844300	-3.60954300	-1.59948200
C	-4.28832300	-3.87593100	-2.85560400
C	-3.04041600	-3.29685300	-3.18589100
C	-2.34878100	-2.46908300	-2.30726900
N	-0.00003300	-4.02344400	-0.00007800
N	-0.00006100	4.02344500	-0.00004500
C	4.98713800	-4.77369900	3.84704700
C	6.59938900	-2.26273400	-3.82104100
C	6.59930700	2.26260400	3.82111100
C	4.98721800	4.77383400	-3.84692600

C	-4.98711100	4.77362400	3.84715500
C	-6.59938100	2.26284100	-3.82099600
C	-6.59931800	-2.26273200	3.82102900
C	-4.98717300	-4.77373700	-3.84707400
H	1.37832900	-2.05187900	2.57707900
H	2.59979600	-3.51435700	4.16206700
H	5.81177500	-4.04938100	1.32957000
H	6.34310700	-3.22079200	-1.25885200
H	4.34566500	-0.78955700	-4.21071300
H	2.47926400	-0.33983000	-2.64604400
H	2.47921700	0.33972200	2.64595300
H	4.34558300	0.78940000	4.21067800
H	6.34307200	3.22076400	1.25895600
H	5.81179500	4.04944100	-1.32945000
H	2.59988600	3.51449600	-4.16204100
H	1.37838700	2.05196100	-2.57713000
H	-1.37833900	2.05177700	2.57713100
H	-2.59979600	3.51422000	4.16215900
H	-5.81175800	4.04936600	1.32966500
H	-6.34308700	3.22085700	-1.25879200
H	-4.34568400	0.78963000	-4.21068700
H	-2.47929000	0.33984700	-2.64601900
H	-2.47925000	-0.33976300	2.64592700
H	-4.34562000	-0.78950000	4.21063700
H	-6.34306400	-3.22082400	1.25885000
H	-5.81177800	-4.04940700	-1.32959200
H	-2.59986200	-3.51434600	-4.16215300
H	-1.37837800	-2.05185700	-2.57718700
H	4.38814900	-5.67579400	4.06036500
H	5.14776600	-4.26103900	4.81065000
H	5.96758300	-5.10367700	3.47326400
H	6.21645700	-2.65691100	-4.77724000
H	7.33137200	-2.98426400	-3.42887700
H	7.14102800	-1.32919100	-4.05240000
H	7.33128200	2.98417100	3.42900000
H	7.14096100	1.32905900	4.05242400
H	6.21635300	2.65671800	4.77732800
H	5.14791300	4.26118700	-4.81052500
H	5.96763200	5.10384000	-3.47308900
H	4.38820900	5.67591000	-4.06026800
H	-4.38823200	5.67584300	4.06026500
H	-5.14749500	4.26105300	4.81084400
H	-5.96766900	5.10340300	3.47349200
H	-6.21644400	2.65702600	-4.77719000
H	-7.33135400	2.98437700	-3.42882100
H	-7.14103400	1.32931000	-4.05236700
H	-7.14094600	-1.32918900	4.05240900
H	-6.21636700	-2.65692000	4.77721600
H	-7.33131400	-2.98425400	3.42887400
H	-5.14757500	-4.26119300	-4.81077400
H	-5.96772400	-5.10350600	-3.47338500
H	-4.38829800	-5.67596100	-4.06017100