Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information for

The use of 1,2-dipiperidinoacetylene for the preparation of monometallic diaminoacetylene and homo- or heterobimetallic diaminodicarbene ruthenium(II) complexes

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Computational Details

For the cationic ruthenium complex **4** all computations were performed using the DFT functional methods M06-L, BP86 and B3LYP as implemented in the Gaussian09 program.[1] The all-electron double-ζ basis set (6-31+G**)[2] was applied for all main-group elements (C, H, N, P and Cl), together with the effective core potential double-ζ basis set (Stuttgart RSC 1997 ECP) for the transition metal (Ru).[3] For the optimization of the diaminoacetylene (**1**) the Møller–Plesset perturbation method (MP2)[4] has been used in combination with the correlation-consistent polarized triple-ζ basis set (cc-pVTZ).[5]

[1] Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

[2] X. Cao and M. Dolg, *J. Chem. Phys.* 2001, **115**, 7348.

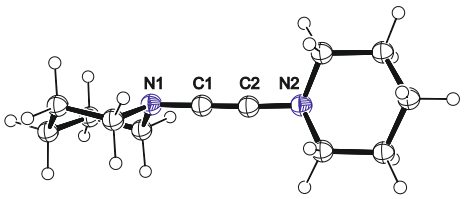
[3] (a) A. Bergner, M. Dolg, W. Kuechle, H. Stoll, H. Preuss, *Mol. Phys.* **1993**, *80*, 1431; (b) M. Kaupp, P. v. R. Schleyer, H. Stoll, H. Preuss, *J. Chem. Phys.* **1991**, *94*, 1360; (c) M. Dolg, H. Stoll, H. Preuss, R. M. Pitzer, *J. Phys. Chem.* **1993**, *97*, 5852.

[4] (a) M. Head-Gordon, J. A. Pople, M. J. Frisch, *Chem. Phys. Lett.* 1988, *153*, 503; (b) S. Saebø, J. Almlöf, *Chem. Phys. Lett.* 1989, *154*, 83; (c) M. J. Frisch, M. Head-Gordon, J. A. Pople, *Chem. Phys. Lett.* **1990**, *166*, 275; (d) M. J. Frisch, M. Head-Gordon, J. A. Pople, *Chem. Phys. Lett.* **1990**, *166*, 281; (e) M. Head-Gordon, T. Head-Gordon, *Chem. Phys. Lett.* **1994**, *220*, 122.

[5] T. H. Dunning, Jr., *J. Chem. Phys.* **1989**, *90*, 1007.

Table 1. Selected bond lengths and angles in diaminoacetylene **1**.

			MP2
Basis set			cc-pVTZ
Geometry	Bond length [Å]	C1-C2	1.221
		C1-N1	1.351
		C2-N2	1.352
	Bond angles [°]	C1-C2-N2	177.4
		C2-C1-N1	177.8



Structure of 1 (atom, x-, y-, z-positions in Å):

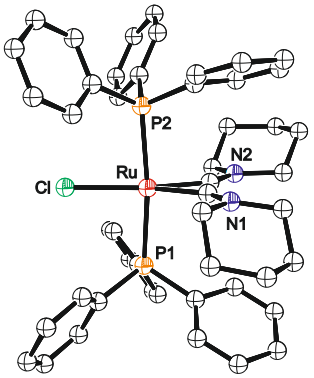
MP2/cc-pVTZ			
N	-1.953700	-0.215000	-0.172700
N	1.953200	-0.212300	0.171700
C	-0.607400	-0.168400	-0.064500
C	0.607000	-0.164000	0.061500
C	-2.564200	1.009300	-0.698700
C	-4.018100	0.754700	-1.060400
C	-4.784300	0.224200	0.146200
C	-4.095500	-1.019300	0.697300
C	-2.639800	-0.724300	1.018700
C	2.640300	-0.725400	-1.017500
C	4.095100	-1.021700	-0.693200
C	4.784900	0.222000	-0.144000
C	4.017500	0.756800	1.059900
C	2.564600	1.012700	0.695000
H	-1.986900	1.314700	-1.569200
H	-2.500400	1.815200	0.048200
H	-4.054900	0.023000	-1.869700
H	-4.465300	1.679400	-1.427600
H	-4.811200	0.994400	0.922300
H	-5.818000	0.004000	-0.121600
H	-4.598400	-1.374000	1.597900
H	-4.135500	-1.820200	-0.043400
H	-2.578100	0.012300	1.834100
H	-2.115000	-1.621900	1.339700
H	2.581000	0.009300	-1.834800
H	2.114700	-1.623000	-1.337200
H	4.598900	-1.379400	-1.592100
H	4.132700	-1.820900	0.049500
H	5.817800	0.000900	0.126100
H	4.814300	0.990300	-0.922100
H	4.465500	1.681700	1.425500
H	4.051700	0.027100	1.871200
H	1.986300	1.321700	1.563600
H	2.503500	1.816600	-0.054400

Table 2. Comparison of theoretical with experimental results of complex **4**.

			X-ray[a]	DFT					
	Functional			M06-L		BP86		B3LYP	
	Spin state			singlet	triplet	singlet	triplet	singlet	triplet
	Basis set			6-31+G** (MGE)[b], Stuttgart RSC 1997 ECP (Ru)					
Geometry	Bond length [Å]	C1-C2	1.399(2) / 1.404(2)	1.388	1.322	1.405	1.337	1.405	1.327
		C1-N1	1.301(2) / 1.298(2)	1.316	1.338	1.328	1.353	1.318	1.342
		C2-N2	1.303(2) / 1.303(2)	1.312	1.332	1.322	1.342	1.313	1.334
		Ru-C1	1.9188(15) / 1.9265(16)	1.910	2.025	1.923	2.036	1.914	2.032
		Ru-C2	1.9215(15) / 1.9174(16)	1.910	2.018	1.936	2.043	1.929	2.043
		Ru-Cl	2.3840(4) / 2.3856(4)	2.408	2.382	2.388	2.371	2.412	2.385
		Ru-P1	2.3836(4) / 2.3839(4)	2.418	2.432	2.429	2.445	2.455	2.476
		Ru-P2	2.3890(4) / 2.3959(4)	2.423	2.419	2.433	2.439	2.459	2.478
	Bond angles [°]	C1-C2-N2	146.27(15) / 148.11(15)	148.4	151.5	148.8	151.1	146.3	149.5
		C2-C1-N1	147.23(15) / 146.56(16)	148.4	151.0	148.1	151.2	147.5	149.7
		P1-Ru-P2	175.422(13) / 174.475(14)	170.6	173.1	169.7	173.9	169.4	172.7
		P1-Ru-Cl	87.995(12) / 86.253(14)	86.5	88.6	84.8	87.0	84.7	86.6
		P2-Ru-Cl	87.429(12) / 89.294(14)	86.4	88.7	85.0	86.8	84.8	86.1
Energies	$\Delta E_{S\text{-}T}$ [kcal/mol]			-22.6		-27.4		-22.1	
	$\Delta E_{LUMO\text{-}HOMO}$ [eV]			1.52	---	1.38	---	3.08	---
	$\Delta E_{SOMO\text{-}SOMO\text{-}1}$ [eV]			---	1.74	---	1.79	---	1.68

[a] [**4**]Cl / [**4**](BPh_4)

[b] MGE = **m**ain **g**roup **e**lements

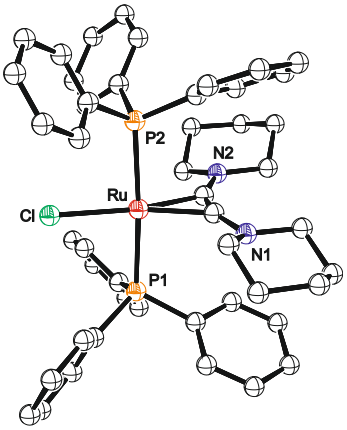


(M06-L)

Structure of the cation 4 (S = 0) (atom, x-, y-, z-positions in Å):

singlet

M06-L				BP86				B3LYP			
Ru	-0.029200	-0.230600	-0.487200	Ru	-0.005700	-0.448600	0.052700	Ru	-0.006000	-0.443500	0.043000
Cl	-0.065300	-0.631900	-2.861000	Cl	-0.003500	-2.818000	0.352700	Cl	-0.002400	-2.836800	0.344500
N	-0.165100	1.948200	1.663000	N	0.049600	2.144500	1.725700	N	0.025900	2.124700	1.731800
N	0.089900	-1.622900	2.235300	N	0.018500	1.967500	-1.909200	N	0.034600	1.994000	-1.875600
P	2.351600	0.140100	-0.741500	P	2.404200	-0.689700	-0.133000	P	-2.450300	-0.649800	0.208600
P	-2.440100	-0.397800	-0.570300	P	-2.424900	-0.642200	0.231200	P	2.429900	-0.691800	-0.130400
C	-0.071400	0.735700	1.159900	C	0.031400	1.382700	0.638500	C	0.026200	1.371000	0.650300
C	0.034300	-0.630400	1.379600	C	-0.008000	1.306300	-0.766300	C	-0.002800	1.313300	-0.753500
C	-0.171000	2.283800	3.092100	C	-0.031900	3.622600	1.759800	C	-0.087900	3.596200	1.776500
C	-1.309100	3.239500	3.427900	C	1.097000	4.222500	2.617200	C	1.026600	4.214300	2.630700
C	-1.310100	4.456900	2.512000	C	1.118700	3.599900	4.025800	C	1.063400	3.590200	4.033400
C	-1.343200	4.021300	1.052900	C	1.191700	2.063800	3.937300	C	1.155000	2.059900	3.943800
C	-0.177000	3.100200	0.744900	C	0.057000	1.502400	3.066200	C	0.036400	1.484200	3.068900
C	0.289900	-1.506800	3.683400	C	0.136400	3.434700	-2.073500	C	0.189300	3.456700	-2.015300
C	1.639400	-2.103300	4.063500	C	-0.975700	3.978400	-2.987100	C	-0.903600	4.044000	-2.916800
C	1.775500	-3.537100	3.562100	C	-0.991300	3.239600	-4.338700	C	-0.936700	3.335600	-4.279000
C	1.508600	-3.617400	2.064100	C	-1.104200	1.719500	-4.118200	C	-1.073800	1.817700	-4.092200
C	0.160000	-3.002400	1.727700	C	0.007900	1.211700	-3.186800	C	0.019800	1.271300	-3.168100
C	2.685900	1.827600	-1.364200	C	-3.083300	-0.935400	1.941600	C	-3.109500	-0.973100	1.906500
C	1.784400	2.385900	-2.282200	C	-2.343600	-1.748400	2.830200	C	-2.362100	-1.765100	2.795000
C	1.983700	3.673400	-2.770600	C	-2.836700	-2.020400	4.116900	C	-2.856000	-2.055700	4.069000
C	3.082100	4.420900	-2.348600	C	-4.066200	-1.481900	4.535100	C	-4.097100	-1.558200	4.475800
C	3.990300	3.869100	-1.447000	C	-4.808300	-0.675100	3.655700	C	-4.848800	-0.772900	3.597600
C	3.797500	2.578300	-0.958100	C	-4.323700	-0.404200	2.364200	C	-4.361300	-0.483300	2.320300
C	3.309900	0.053000	0.819400	C	-3.361800	0.861500	-0.330600	C	-3.387600	0.857900	-0.328300
C	3.124500	1.041800	1.798100	C	-3.278100	2.058000	0.419100	C	-3.322400	2.030000	0.446600
C	3.822200	0.994200	3.001000	C	-3.958100	3.214100	0.003300	C	-3.999700	3.186100	0.054900
C	4.715100	-0.048700	3.250800	C	-4.729600	3.196400	-1.173300	C	-4.752300	3.194600	-1.124800
C	4.898400	-1.041500	2.291800	C	-4.819700	2.012800	-1.923700	C	-4.824800	2.036800	-1.901200
C	4.202300	-0.992900	1.083500	C	-4.142700	0.851900	-1.506000	C	-4.149300	0.876000	-1.506500
C	3.221300	-1.006200	-1.852300	C	-3.147100	-2.000200	-0.793800	C	-3.151400	-1.988700	-0.846000
C	4.339400	-0.607600	-2.591700	C	-4.284100	-2.722100	-0.373900	C	-4.282800	-2.720500	-0.455400
C	5.017600	-1.533400	-3.380800	C	-4.835500	-3.713500	-1.203700	C	-4.814900	-3.699400	-1.299500
C	4.587500	-2.857800	-3.431500	C	-4.261500	-3.989800	-2.456100	C	-4.226300	-3.955600	-2.540100
C	3.471500	-3.258800	-2.698000	C	-3.125500	-3.276300	-2.877000	C	-3.095900	-3.233400	-2.933800
C	2.785200	-2.335100	-1.916700	C	-2.566800	-2.292000	-2.047100	C	-2.558200	-2.261700	-2.088700
C	-3.181800	1.202700	-1.041700	C	3.294500	-0.907400	1.479400	C	3.298700	-0.945100	1.482100
C	-2.465900	2.018800	-1.929400	C	2.663000	-1.635400	2.513300	C	2.657300	-1.675800	2.497200
C	-2.979400	3.250200	-2.324200	C	3.326500	-1.853900	3.732100	C	3.304300	-1.915300	3.712100
C	-4.210000	3.684300	-1.833600	C	4.620800	-1.344300	3.936400	C	4.595000	-1.426500	3.932600
C	-4.931300	2.877700	-0.954400	C	5.255000	-0.620600	2.912100	C	5.241200	-0.701400	2.927900
C	-4.423400	1.641600	-0.559900	C	4.599000	-0.404100	1.687700	C	4.600000	-0.463200	1.709000
C	-3.124400	-0.779500	1.082100	C	3.261200	0.770000	-0.901700	C	3.297200	0.777700	-0.857100
C	-3.138400	0.211100	2.075800	C	3.320000	1.993800	-0.159500	C	3.353300	1.980000	-0.129300
C	-3.489400	-0.101900	3.385400	C	3.939600	3.118900	-0.765300	C	3.977100	3.109600	-0.661600
C	-3.830400	-1.411400	3.724800	C	4.495900	3.042700	-2.055900	C	4.547200	3.061600	-1.938800
C	-3.824600	-2.400500	2.744100	C	4.433700	1.833200	-2.767100	C	4.491400	1.875200	-2.672700
C	-3.473300	-2.089000	1.431000	C	3.823100	0.702000	-2.194400	C	3.873300	0.739700	-2.136000
C	-3.169800	-1.659900	-1.657500	C	2.962000	-2.108300	-1.179100	C	2.979500	-2.087400	-1.200900
C	-2.457300	-2.840700	-1.898400	C	2.199900	-2.469400	-2.310900	C	2.224200	-2.422000	-2.335800
C	-3.025200	-3.856800	-2.660600	C	2.633100	-3.502000	-3.157100	C	2.647100	-3.438400	-3.193700
C	-4.300700	-3.694500	-3.199400	C	3.823800	-4.193500	-2.872300	C	3.823000	-4.142900	-2.919300
C	-5.008400	-2.515700	-2.974200	C	4.579500	-3.846800	-1.739700	C	4.573200	-3.824500	-1.784800
C	-4.447500	-1.500000	-2.204400	C	4.153700	-2.807100	-0.895400	C	4.156000	-2.801100	-0.929300
H	0.797600	2.748800	3.334200	H	-1.016300	3.893400	2.193000	H	-1.067400	3.839400	2.212400
H	-0.247900	1.352600	3.657100	H	-0.004600	3.997300	0.727700	H	-0.075400	3.980500	0.759300
H	-2.265000	2.709100	3.331600	H	2.066100	4.049200	2.112300	H	1.990600	4.064800	2.127900
H	-1.218200	3.533500	4.478500	H	0.952500	5.316300	2.670300	H	0.860500	5.295900	2.689300
H	-0.406500	5.055200	2.694900	H	0.201700	3.896000	4.575600	H	0.153200	3.871900	4.581200
H	-2.161200	5.103000	2.745000	H	1.971600	3.995100	4.603900	H	1.908100	3.991000	4.603200
H	-1.305200	4.882400	0.378000	H	1.121600	1.607700	4.940400	H	1.085100	1.607400	4.939000
H	-2.282400	3.492300	0.831100	H	2.163200	1.750100	3.510900	H	2.125600	1.761900	3.527600
H	-0.209700	2.694300	-0.271200	H	0.149200	0.417600	2.900600	H	0.146600	0.410500	2.915100
H	0.781600	3.632500	0.862000	H	-0.926400	1.699900	3.538700	H	-0.942900	1.665500	3.533800
H	-0.533400	-2.044100	4.174400	H	1.133500	3.639100	-2.511300	H	1.182000	3.640400	-2.447700
H	0.217900	-0.452700	3.958000	H	0.105100	3.898400	-1.078300	H	0.173000	3.905800	-1.025900
H	1.757800	-2.053700	5.150800	H	-0.811900	5.061400	-3.130800	H	-0.712800	5.116200	-3.040000
H	2.429800	-1.480400	3.625000	H	-1.950300	3.856900	-2.478500	H	-1.874600	3.940300	-2.417100
H	1.062300	-4.182200	4.094400	H	-0.060200	3.465800	-4.895000	H	-0.011700	3.556700	-4.829800
H	2.773200	-3.922800	3.794600	H	-1.827500	3.601000	-4.961800	H	-1.763000	3.720500	-4.885600
H	2.289600	-3.074800	1.513200	H	-2.086500	1.475600	-3.672400	H	-2.055300	1.581900	-3.663300
H	1.531100	-4.654300	1.713600	H	-1.035200	1.176200	-5.077400	H	-1.006900	1.299800	-5.055600
H	-0.027300	-2.959500	0.649700	H	-0.113600	0.150000	-2.919200	H	-0.122500	0.214200	-2.940700
H	-0.656800	-3.564600	2.201800	H	1.001400	1.342500	-3.659400	H	1.009300	1.295300	-3.628600
H	0.931700	1.799500	-2.619300	H	-1.394600	-2.183700	2.501800	H	-1.408000	-2.173200	2.480800
H	1.280900	4.091200	-3.486100	H	-2.258400	-2.659600	4.792300	H	-2.270700	-2.676900	4.740800
H	3.234900	5.427700	-2.726800	H	-4.447400	-1.694600	5.539200	H	-4.478800	-1.785400	5.466800
H	4.855500	4.441700	-1.125400	H	-5.771400	-0.258800	3.969100	H	-5.818500	-0.388900	3.900700
H	4.513900	2.157900	-0.256200	H	-4.917000	0.220400	1.689200	H	-4.963100	0.122900	1.651700
H	2.466600	1.884000	1.591900	H	-2.708800	2.077000	1.354600	H	-2.769600	2.031900	1.381000
H	3.683900	1.782100	3.737100	H	-2.900900	3.925300	0.609300	H	-3.954900	4.074800	0.678300
H	5.268700	-0.081400	4.184700	H	-5.268100	4.094700	-1.492300	H	-5.287400	4.090400	-1.425400
H	5.597400	-1.853100	2.473900	H	-5.431600	1.982300	-2.831400	H	-5.419400	2.025900	-2.810300
H	4.373000	-1.764800	0.336800	H	-4.240900	-0.068300	-2.089900	H	-4.235600	-0.018600	-2.113500
H	4.675000	0.426600	-2.558400	H	-4.736900	-2.521700	0.602000	H	-4.748400	-2.540000	0.507400
H	5.880400	-1.218200	-3.960000	H	-5.713500	-4.273400	-0.865500	H	-5.686800	-4.263600	-0.982200
H	5.116300	-3.576200	-4.051200	H	-4.691600	-4.765300	-3.098100	H	-4.639500	-4.719300	-3.192200
H	3.126400	-4.287300	-2.748800	H	-2.645200	-3.496000	-3.848800	H	-2.624600	-3.467000	-3.891000
H	1.893100	-2.633600	-1.365900	H	-1.663600	-1.757800	-2.360900	H	-1.663000	-1.725900	-2.388500
H	-1.507600	1.674600	-2.316400	H	1.661100	-2.045900	2.350400	H	1.663400	-2.075600	2.327500
H	-2.417100	3.871500	-3.016200	H	2.830400	-2.427900	4.522000	H	2.799500	-2.489800	4.483500
H	-4.609800	4.647100	-2.139100	H	5.135400	-1.514700	4.887700	H	5.096000	-1.613700	4.877900
H	-5.894200	3.208800	-0.576100	H	6.266300	-0.227500	3.060100	H	6.247500	-0.324600	3.086700
H	-4.992800	1.018900	0.127200	H	5.107900	0.156100	0.897200	H	5.120600	0.097000	0.939600
H	-2.882700	1.237100	1.814300	H	2.910200	2.058600	0.817400	H	2.932700	2.027700	0.875500
H	-3.510100	0.679700	4.141800	H	4.000300	4.052300	-0.196100	H	4.030700	4.023200	-0.075700
H	-4.110700	-1.655300	4.745500	H	4.985600	3.917200	-2.496500	H	5.040400	3.937300	-2.350300
H	-4.103300	-3.419800	2.996800	H	4.876200	1.759200	-3.766100	H	4.942100	1.822400	-3.659500
H	-3.475200	-2.870300	0.673800	H	3.801300	-0.239900	-2.751000	H	3.857700	-0.178500	-2.713000
H	-1.445400	-2.945900	-1.508600	H	1.254300	-1.955000	-2.512700	H	1.292800	-1.902500	-2.537700
H	-2.464900	-4.767800	-2.849700	H	2.032300	-3.778000	-4.029800	H	2.051000	-3.690800	-4.065800
H	-4.738800	-4.483400	-3.803900	H	4.155700	-5.006700	-3.525800	H	4.146700	-4.941200	-3.580400
H	-5.997800	-2.383200	-3.401700	H	5.501700	-4.388800	-1.506200	H	5.482000	-4.374500	-1.559000
H	-5.002800	-0.579400	-2.037900	H	4.746200	-2.550700	-0.011900	H	4.745800	-2.571800	-0.048400



(M06-L)

Structure of the cation 4 (S = 1) (atom, x-, y-, z-positions in Å):

triplet

M06-L				BP86				B3LYP			
Ru	-0.032800	0.019700	0.633300	Ru	0.002300	-0.228000	0.464100	Ru	0.008200	-0.489000	0.059300
Cl	-0.035800	0.635000	2.934800	Cl	-0.003300	-1.388200	2.531800	Cl	0.020300	-2.837400	0.477000
N	0.420400	1.040100	-2.297800	N	-0.317700	-0.690700	-2.645100	N	0.337800	2.289800	1.511900
N	-0.451100	-2.391100	-1.294800	N	0.220200	2.579500	-0.991900	N	-0.315700	1.854600	-2.053600
P	-2.411600	0.456100	0.570100	P	2.429200	-0.472000	0.488300	P	2.469500	-0.663100	-0.145000
P	2.392300	-0.132800	0.740600	P	-2.432600	-0.123500	0.663300	P	-2.453900	-0.627400	0.307900
C	0.071400	0.125700	-1.385900	C	-0.068600	0.062500	-1.549400	C	0.053600	1.502000	0.463300
C	-0.116800	-1.130900	-1.022100	C	0.043400	1.250100	-0.945100	C	-0.062800	1.339400	-0.848900
C	0.479100	0.692000	-3.721600	C	-0.274400	-0.101400	-4.002700	C	0.418200	3.757000	1.373200
C	1.522600	1.529200	-4.445400	C	-1.209800	-0.851800	-4.965800	C	1.436800	4.357100	2.350700
C	1.330600	3.016100	-4.176900	C	-0.932000	-2.365800	-4.953900	C	1.183500	3.892000	3.791100
C	1.345600	3.282600	-2.677100	C	-1.038500	-2.912200	-3.518200	C	1.157100	2.359100	3.858400
C	0.278000	2.464400	-1.947200	C	-0.096800	-2.154900	-2.572000	C	0.126100	1.785600	2.884000
C	-0.379100	-2.899000	-2.670500	C	0.142700	3.343900	-2.257000	C	-0.467900	3.308500	-2.260200
C	-1.381800	-4.018200	-2.890400	C	1.154900	4.501400	-2.265600	C	-1.508300	3.610200	-3.345100
C	-1.245700	-5.101000	-1.828200	C	1.003700	5.387100	-1.015100	C	-1.210500	2.843700	-4.640700
C	-1.398800	-4.493800	-0.439200	C	1.122700	4.531900	0.260400	C	-1.108600	1.339300	-4.352900
C	-0.377900	-3.392100	-0.224000	C	0.104400	3.382300	0.243800	C	-0.062800	1.060300	-3.270200
C	-2.634000	2.244300	0.265700	C	3.010700	-2.183800	0.070000	C	-3.030700	-0.870500	2.048500
C	-1.748900	3.132600	0.895400	C	2.277300	-3.290300	0.557800	C	-2.264300	-1.653000	2.929800
C	-1.839000	4.501400	0.660700	C	2.707700	-4.599900	0.288500	C	-2.697700	-1.872600	4.239800
C	-2.814400	5.000200	-0.201700	C	3.868200	-4.822600	-0.472800	C	-3.897100	-1.313900	4.689400
C	-3.711500	4.126700	-0.814100	C	4.603700	-3.727500	-0.957600	C	-4.668000	-0.539200	3.818500
C	-3.625000	2.755500	-0.582300	C	4.181900	-2.414100	-0.687200	C	-4.240800	-0.319400	2.506300
C	-3.293900	-0.370900	-0.798400	C	3.363800	0.610000	-0.691000	C	-3.423900	0.847200	-0.250200
C	-3.014000	-0.010800	-2.126100	C	3.214500	0.413900	-2.083800	C	-3.252200	2.077200	0.410500
C	-3.606900	-0.690400	-3.185200	C	3.902700	1.227800	-2.997900	C	-3.982800	3.202300	0.025300
C	-4.485700	-1.744900	-2.935400	C	4.740300	2.259100	-2.535000	C	-4.892800	3.120900	-1.034600
C	-4.767400	-2.112100	-1.622000	C	4.887800	2.466600	-1.153500	C	-5.065800	1.906900	-1.701700
C	-4.174900	-1.432100	-0.558500	C	4.205800	1.647500	-0.235500	C	-4.337800	0.776700	-1.312800
C	-3.389400	0.060400	2.048700	C	3.201400	-0.098600	2.124500	C	-3.180600	-2.023300	-0.647400
C	-4.517000	0.812400	2.394800	C	4.344300	-0.791000	2.576500	C	-4.219600	-2.814900	-0.137000
C	-5.285700	0.448300	3.497100	C	4.932000	-0.453700	3.807700	C	-4.758400	-3.851200	-0.905300
C	-4.936000	-0.667700	4.255100	C	4.387600	0.575700	4.594200	C	-4.269200	-4.104700	-2.188700
C	-3.812200	-1.419600	3.915400	C	3.247500	1.268000	4.149900	C	-3.232400	-3.320600	-2.703900
C	-3.037000	-1.053300	2.819600	C	2.654500	0.927800	2.924100	C	-2.687900	-2.291900	-1.934500
C	3.112000	1.512600	0.416300	C	-3.279500	-1.704400	0.197200	C	3.329200	-0.720200	1.488200
C	2.430900	2.633500	0.915100	C	-2.703800	-2.922300	0.629100	C	2.732400	-1.441100	2.537900
C	2.928700	3.915100	0.698500	C	-3.331400	-4.144200	0.337100	C	3.366000	-1.537500	3.779000
C	4.111000	4.093300	-0.018200	C	-4.533500	-4.166900	-0.392000	C	4.599200	-0.913900	3.990500
C	4.800300	2.985000	-0.507700	C	-5.111100	-2.960100	-0.822300	C	5.200900	-0.199000	2.951400
C	4.306800	1.699900	-0.291200	C	-4.491500	-1.732500	-0.528400	C	4.572800	-0.103200	1.706200
C	3.118000	-1.246500	-0.515800	C	-3.259600	1.175300	-0.374800	C	3.300200	0.717800	-1.054500
C	3.123000	-0.868700	-1.867700	C	-3.222200	1.080400	-1.786200	C	3.282700	2.016200	-0.513700
C	3.559200	-1.752900	-2.849500	C	-3.805200	2.079300	-2.583200	C	3.877500	3.080100	-1.194200
C	3.987800	-3.033100	-2.499200	C	-4.423100	3.193100	-1.985900	C	4.488800	2.868500	-2.434800
C	3.985600	-3.417800	-1.160700	C	-4.458400	3.298000	-0.585700	C	4.505400	1.585000	-2.983600
C	3.555100	-2.532000	-0.173700	C	-3.882500	2.296300	0.216500	C	3.918500	0.515300	-2.298600
C	3.103100	-0.705100	2.312200	C	-3.041700	0.251500	2.364600	C	3.038300	-2.169500	-1.037900
C	2.428500	-1.704400	3.024100	C	-2.287900	1.112300	3.190600	C	2.296100	-2.637100	-2.113500
C	2.973600	-2.222900	4.193300	C	-2.762200	1.474600	4.461000	C	2.730300	-3.742300	-2.866200
C	4.189200	-1.733100	4.669400	C	-3.990200	0.969300	4.922600	C	3.907100	-4.403500	-2.502200
C	4.857800	-0.727900	3.973900	C	-4.740700	0.102900	4.109600	C	4.646000	-3.952300	-1.406000
C	4.320600	-0.215300	2.795300	C	-4.271600	-0.255600	2.834300	C	4.216900	-2.839400	-0.677100
H	-0.516600	0.847700	-4.173000	H	0.769600	-0.139300	-4.383600	H	-0.577600	4.190500	1.560000
H	0.712100	-0.375200	-3.790100	H	-0.566800	0.956700	-3.919500	H	0.695600	3.983300	0.342400
H	2.523900	1.226600	-4.109100	H	-2.260400	-2.760100	-4.672200	H	2.448600	4.063100	2.043500
H	1.469700	1.308500	-5.516400	H	-1.077400	-0.431800	-5.979000	H	1.384200	5.449300	2.277400
H	0.371300	3.346600	-4.600200	H	0.084200	-2.560300	-5.351000	H	0.223200	4.293300	4.145100
H	2.108500	3.596600	-4.681300	H	-1.638200	-2.890200	-5.620400	H	1.955100	4.290900	4.457700
H	1.182200	4.342900	-2.457300	H	-0.780600	-3.985400	-3.484600	H	0.908100	2.017900	4.869300
H	2.327300	3.017800	-2.258200	H	-2.078100	-2.816200	-3.153100	H	2.147900	1.954400	3.616700
H	0.343000	2.562800	-0.888800	H	-0.247300	-2.461100	-1.523300	H	0.176700	0.695200	2.851400
H	-0.703700	2.805900	-2.273000	H	0.961500	-2.373200	-2.834500	H	-0.889500	2.060900	3.212200
H	0.648000	-3.252800	-2.862400	H	-0.891400	3.733000	-2.369800	H	0.510100	3.728200	-2.543500
H	-0.575200	-2.056100	-3.339400	H	0.338600	2.647400	-3.085500	H	-0.769700	3.751300	-1.310200
H	-1.234500	-4.429200	-3.894400	H	1.001900	5.091700	-3.186900	H	-1.516600	4.691400	-3.524800
H	-2.395000	-3.598200	-2.860000	H	2.177700	4.083300	-2.308300	H	-2.501000	3.334300	-2.971000
H	-0.260200	-5.581100	-1.912300	H	0.017300	5.891800	-1.032400	H	-0.265800	3.200500	-5.074700
H	-1.988800	-5.887700	-1.987100	H	1.767500	6.183700	-1.015400	H	-1.991300	3.037100	-5.383600
H	-2.408000	-4.075800	-0.326800	H	2.142700	4.111000	0.334600	H	-2.083300	0.959100	-4.022400
H	-1.274600	-5.251800	0.340400	H	0.951500	5.144300	1.163700	H	-0.831800	0.785500	-5.257800
H	-0.540900	-2.864700	0.724800	H	0.253700	2.696100	1.095300	H	-0.057100	0.005200	-2.984400
H	0.642100	-3.813300	-0.197100	H	-0.929800	3.782500	0.312200	H	0.942600	1.306500	-3.645500
H	-0.997000	2.745500	1.582300	H	1.385800	-3.124100	1.171400	H	-1.345600	-2.114800	2.585300
H	-1.147900	5.179000	1.155200	H	2.135600	-5.447200	0.681000	H	-2.098500	-2.486800	4.905600
H	-2.882500	6.068100	-0.388100	H	4.201700	-5.844300	-0.681600	H	-4.232000	-1.485800	5.708100
H	-4.483700	4.512300	-1.473700	H	5.514200	-3.891200	-1.543500	H	-5.606400	-0.108200	4.155200
H	-4.328500	2.082100	-1.066200	H	4.770700	-1.573300	-1.063900	H	-4.856720	0.279900	1.844800
H	-2.349300	0.827000	-2.329700	H	2.584600	-0.401500	-2.455500	H	-2.567500	2.152500	1.249400
H	-3.391200	-0.390000	-4.207600	H	3.795800	1.048200	-4.073100	H	-3.852100	4.139100	0.559900
H	-4.954200	-2.271400	-3.762000	H	5.283300	2.888500	-3.247600	H	-5.467300	3.994100	-1.329200
H	-5.458800	-2.925500	-1.419600	H	5.546900	3.259000	-0.783500	H	-5.777000	1.829400	-2.518900
H	-4.410000	-1.722800	0.462900	H	4.346400	1.807900	0.837800	H	-4.500700	-0.162100	-1.830400
H	-4.790300	1.685500	1.806300	H	4.773000	-1.598500	1.975100	H	-4.607700	-2.634400	0.859700
H	-6.156300	1.039100	3.765700	H	5.814600	-4.001500	1.153200	H	-5.558300	-4.461100	-0.496100
H	-5.534700	-0.947100	5.116900	H	4.844800	0.833000	5.555100	H	-4.687500	-4.912300	-2.782000
H	-3.531400	-2.281700	4.512900	H	2.812100	2.063100	4.763900	H	-2.841100	-3.517700	-3.697700
H	-2.141900	-1.621800	2.569800	H	1.752100	1.454300	2.593600	H	-1.870300	-1.701300	-2.338900
H	1.516000	2.496700	1.492600	H	-1.780900	-2.908500	1.218900	H	1.787700	-1.950900	2.377100
H	2.392700	4.774400	1.093000	H	-2.882300	-5.079600	0.687100	H	2.897700	-2.105800	4.577300
H	4.499000	5.093400	-0.189100	H	-5.021700	-5.120600	-0.617800	H	5.090900	-0.989800	4.955900
H	5.728800	3.118600	-1.055700	H	-6.052300	-2.969500	-1.382000	H	6.163600	0.280100	3.104000
H	4.853800	0.840600	-0.672500	H	-4.957300	-0.799900	-0.860800	H	5.058200	0.449300	0.908900
H	2.798600	0.132100	-2.146700	H	-2.754300	0.212100	-2.262000	H	2.823700	2.192300	0.453400
H	3.571500	-1.439100	-3.890700	H	-3.785700	1.983500	-3.674300	H	3.873000	4.072700	-0.752200
H	4.332900	-3.722200	-3.264600	H	-4.881500	3.968400	-2.608300	H	4.955500	3.695300	-2.962000
H	4.331800	-4.407800	-0.877200	H	-4.946700	4.154800	-0.109800	H	4.986900	1.406800	-3.940700
H	3.570500	-2.843200	0.868100	H	-3.931400	2.384600	1.305800	H	3.958000	-0.476700	-2.734300
H	1.462700	-2.061300	2.667700	H	-1.318600	1.488300	2.845600	H	1.366100	-2.149000	-2.408900
H	2.443800	-2.996400	4.741200	H	-2.167200	2.139900	5.095000	H	2.143800	-4.095600	-3.709000
H	4.610200	-2.128400	5.589100	H	-4.357400	1.243900	5.916600	H	4.241000	-5.270300	-3.064800
H	5.799700	-0.339400	4.349400	H	-5.694100	-0.299200	4.467600	H	5.556400	-4.466400	-1.112500
H	4.845000	0.570500	2.256200	H	-4.862600	-0.933300	2.210200	H	4.800000	-2.504000	0.174100