Ru–NO and Ru–NO_2 Bonding Linkage Isomerism in *cis*-$[Ru(NO)(NO_2)(bpy)_2]^{2+/+}$ Complexes – A Theoretical Insight

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Table S1. Calculated and experimental (in italic) vibrational frequencies (cm^{-1}), bond lengths (Å), angles (°) for complexes prior (**1a-3a**) and after (**1b-3b**) the monoeletronic reduction at BP86/TZVPP level of theory.

Geometric Parameters	**1a**	**2a**	**3a**	**1b**	**2b**	**3b**
Simmetry	C_1	C_1	C_1	C_1	C_1	C_1
ν(NO)	1946*(1943)*	1825*(1892)*	1924*(1897)*	1706	1584	1701
$\nu_a(NO_2)$	1508*(1430)*	1673*(1815)*	1692*(1495)*	1297	1584	1557
R(N(1)–O(1))	1.149		1.152	1.184		1.185
R(O(1)–N(1))		1.152			1,190	
R(Ru–N(1))	1.732*(1.769)*		1.737*(1.682)*	1.809		1.799
R(Ru–O(1))		1.848*(1.592)*			2.059	
R(Ru–N(3))	2.096*(2.079)*	2.068*(2.023)*	2.070*(2.071)*	2.061	2.045	2.033
R(Ru–N(4))	2.127*(2.079)*	2.089*(2.056)*	2.102*(2.091)*	2.093	2.028	2.053
R(Ru–N(5))	2.114*(2.077)*	2.040*(2.089)*	2.116*(2.021)*	2.154	1.983	2.161
R(Ru–N(6))	2.069*(2.072)*	2.058*(2.050)*	2.068*(2.011)*	2.069	2.024	2.071
R(Ru–N(2))	2.116*(2.088)*			2.076		
R(Ru–O(2))		1.977*(2,022)*	1.981*(2.082)*		2.010	2.024
R(N(2)–O(2))	1.226*(1.236)*			1.241		
R(O(2)–N(2))		1.452*(1.443)*	1.450*(1.103)*		1.395	1.394
R(N(2)–O(3))	1.232*(1.232)*	1.174*(1.094)*	1.172*(1.414)*	1.242	1.195	1.195
∠Ru–N(1)–O(1)	177.73		175.62	145.34		146.65
∠Ru–O(1)–N(1)		178.86			133.34	
∠Ru–N(2)–O(2)	177.96			118.07		
∠Ru–O(2)–N(2)		116.04	113.86		118.46	115.39
∠O(2)–N(2)–O(3)	124.60	112.08	112.44	122.04	112.44	112.41

Table S2. Natural Population Analysis (NPA) of the charge distribution at M06/Def2-SVP level, respectively.

Group	**1a**	**2a**	**3a**
N(1)O(1)	0.308	0.266	0.281
N(1)	0.378	0.360	0.366
O(1)	-0.070	-0.094	-0.085
(Ru)	0.695	0.867	0.816
(NO_2)	-0.338		
N(2)	0.401		
O(2)	-0.361		
O(3)	-0.378		
(ONO)		-0.465	-0.442
O(2)		-0.579	-0.192
N(2)		0.313	0.318
O(3)		-0.200	-0.568
	1b	**2b**	**3b**
N(1)O(1)	-0.022	-0.066	-0.043
N(1)	0.197	0.206	0.187
O(1)	-0.219	-0.272	-0.230
(Ru)	0.555	0.707	0.677
(NO_2)	-0.479		
N(2)	0.382		
O(2)	-0.433		
O(3)	-0.428		
(ONO)		-0.574	-0.566
O(2)		-0.297	-0.296
N(2)		0.301	0.306
O(3)		-0.578	-0.576

Table S3. Atomic polarization, coefficients, and hybridizations of Ru–NO and Ru–NO_2 at M06/Def2-SVP level.

Polarization Coefficients/Hybridization									
Compound	Bond(Ru−L)	Ru%	L%	s%(Ru)	p%(Ru)	d%(Ru)	s%(L)	p%(L)	d%(L)
1a	Ru−NO	26.21	73.79	18.33	1.00	79.64	64.24	35.74	0.02
1b	Ru−NO	69.51	30.49	0.23	1.44	97.46	0.07	99.85	0.07
2a	Ru−ON	54.10	45.90	0.03	0.07	99.98	0.02	98.03	1.96
2b	Ru−ON	39.57	60.43	1.01	0.12	98.81	0.50	98.29	1.20
3a	Ru−NO	77.87	22.13	0.47	0.13	99.35	0.62	73.14	26.24
3b	Ru−NO	69.63	30.37	0.01	0.10	99.85	0.26	99.54	0.21
Compound	Bond(Ru−L)	Ru%	L%	s%(Ru)	p%(Ru)	d%(Ru)	s%(L)	p%(L)	d%(L)
1a	Ru−NO_2	36.62	63.38	16.88	0.50	82.38	29.96	70.03	0.01
1b	Ru−NO_2	25.21	74.79	26.35	5.19	65.09	37.45	61.98	0.58
2a	Ru−ONO	25.99	74.01	24.92	1.43	72.48	18.90	81.06	0.04
2b	Ru−ONO	17.93	82.07	30.18	4.32	61.42	21.99	77.99	0.02
3a	Ru−ONO	26.46	73.58	27.59	0.99	70.62	18.68	81.28	0.04
3b	Ru−ONO	29.79	71.21	15.43	1.23	82.45	20.15	79.83	0.03

Table S4. Bond critical points properties (a.u): electron densities (p_b), Laplacian ($\nabla^2 p_b$), bond ellipticity (ε) for Ru−NO and Ru−NO_2 bonds at M06/Def2-SVP level.

Compound	BCPs	ρ_b	$\nabla^2\rho_b$	ε
1a	Ru−NO	0.194	1.148	0.061
1b	Ru−NO	0.172	0.798	0.078
2a	Ru−ON	0.127	1.010	0.059
2b	Ru−ON	0.081	0.517	0.201
3a	Ru−NO	0.191	1.134	0.029
3b	Ru−NO	0.176	0.817	0.082
1a	Ru−NO_2	0.101	0.298	0.003
1b	Ru−NO_2	0.106	0.366	0.252
2a	Ru−ONO	0.118	0.508	0.179
2b	Ru−ONO	0.105	0.495	0.063
3a	Ru−ONO	0.118	0.486	0.245
3b	Ru−ONO	0.104	0.465	0.239

Coordinates in .xyz

1a				2a				3a			
N	-2.865154	1.356467	-5.408528	O	0.770090	-1.202013	4.994763	N	-0.643113	0.835682	-2.536740
O	-3.582069	1.321404	-6.305111	N	1.562559	-2.037107	5.041504	O	-0.705110	0.898959	-3.685584
Ru	-1.759772	1.347645	-4.074686	Ru	-0.494039	0.141369	4.883832	Ru	-0.496902	0.619295	-0.819322
N	-3.282246	1.471457	-2.639227	N	-1.989708	-1.132418	5.529081	N	1.212249	1.778377	-0.673656
C	-4.040829	0.431575	-2.235575	C	-2.292249	-1.343275	6.827042	C	1.197986	3.114690	-0.496587
C	-5.024203	0.575112	-1.258619	C	-3.308806	-2.217300	7.205284	C	2.378324	3.848236	-0.404282
C	-5.230832	1.831485	-0.687458	C	-4.028902	-2.886538	6.212645	C	3.599344	3.175676	-0.495599
C	-4.454374	2.909124	-1.116756	C	-3.715779	-2.661741	4.870622	C	3.607709	1.790409	-0.669828
C	-3.482440	2.716028	-2.101727	C	-2.686326	-1.776277	4.542370	C	2.396573	1.099506	-0.758894
N	-1.758026	3.423434	-3.612031	N	-1.236040	-0.564091	3.062944	N	1.003691	-0.843109	-0.986424
C	-2.634788	3.794047	-2.635688	C	-2.268997	-1.455815	3.167847	C	2.280043	-0.357397	-0.935926
C	-2.703548	5.126479	-2.214862	C	-2.855544	-2.002931	2.023463	C	3.372255	-1.221708	-1.051772
C	-1.873698	6.078662	-2.805924	C	-2.382936	-1.635784	0.763321	C	3.153798	-2.588916	-1.223757
C	-0.986780	5.682987	-3.810265	C	-1.329149	-0.723367	0.670403	C	1.843180	-3.069580	-1.272740
C	-0.956215	4.341659	-4.182498	C	-0.784759	-0.208412	1.843295	C	0.793774	-2.162877	-1.148527
N	-0.293456	1.182443	-2.560944	N	-1.753724	1.737240	4.711352	N	-0.467611	0.225776	1.259947
C	-0.534059	1.082956	-1.238320	C	-3.070410	1.718566	5.012957	C	0.433088	0.708972	2.138530
C	0.484693	0.881876	-0.313724	C	-3.856612	2.862774	4.960136	C	0.342261	0.462491	3.504078
C	1.799187	0.780304	-0.775107	C	-3.266060	4.073159	4.587124	C	-0.720527	-0.310294	3.977986
C	2.049254	0.885001	-2.142576	C	-1.909190	4.094085	4.273125	C	-1.653044	-0.810034	3.071242
C	0.986786	1.080334	-3.028112	C	-1.161331	2.915521	4.340034	C	-1.513606	-0.530219	1.708510
N	-0.015933	1.374823	-5.188031	N	0.800022	1.574550	4.170869	N	-2.137299	-0.621736	-0.605473
C	1.141449	1.191749	-4.482215	C	0.265189	2.825480	4.032898	C	-2.443036	-0.996681	0.675064
C	2.372779	1.131443	-5.140110	C	1.055134	3.904870	3.625100	C	-3.577627	-1.769933	0.940137
C	2.426956	1.247305	-6.527622	C	2.406141	3.706614	3.350679	C	-4.414206	-2.159174	-0.103541
C	1.238495	1.435488	-7.235684	C	2.941428	2.423229	3.490793	C	-4.095680	-1.764321	-1.404326
C	0.039991	1.494177	-6.533020	C	2.111636	1.388390	3.907758	C	-2.955906	-0.995958	-1.614617
H	-3.840143	-0.518462	-2.731320	H	-1.694908	-0.776934	7.543412	H	0.208790	3.567204	-0.420729
H	-5.613896	-0.292223	-0.963315	H	-3.524704	-2.365108	8.263075	H	2.330878	4.927975	-0.264438
H	-5.992522	1.976878	0.079596	H	-4.829216	-3.578084	6.478974	H	4.540130	3.723241	-0.430072
H	-4.611723	3.898602	-0.692323	H	-4.267404	-3.175546	4.085314	H	4.551872	1.252509	-0.738206
H	-3.402199	5.421503	-1.434035	H	-3.675634	-2.713747	2.114910	H	4.387145	-0.830029	-1.014329
H	-1.922189	7.120229	-2.486720	H	-2.832863	-2.058416	-0.135184	H	3.999438	-3.270327	-1.321231
H	-0.327013	6.397136	-4.301805	H	-0.930010	-0.411200	-0.293848	H	1.629541	-4.129336	-1.409096
H	0.242970	0.797806	0.745244	H	0.037426	0.507489	1.832156	H	-0.248776	-2.478375	-1.180432
H	-1.573638	1.156351	-0.926786	H	-3.484138	0.760233	5.314566	H	1.236825	1.315085	1.725952
H	-0.281089	3.973912	-4.955244	H	-4.912812	2.799537	5.218807	H	1.090096	0.878325	4.178140
H	2.622170	0.616507	-0.078759	H	-3.854277	4.990247	4.544543	H	-0.824906	-0.519780	5.043062
H	3.066965	0.804467	-2.518480	H	-1.426728	5.025454	3.982662	H	-2.489437	-1.410440	3.423596
H	3.287764	0.984418	-4.569581	H	0.614661	4.895236	3.526394	H	-3.810789	-2.059626	1.962676
H	3.383278	1.189232	-7.047954	H	3.032943	4.541064	3.036012	H	-5.304090	-2.755970	0.097261
H	1.226765	1.528300	-8.321477	H	3.992959	2.218263	3.292626	H	-4.721299	-2.035102	-2.254190
H	-0.906511	1.630064	-7.052436	H	2.503542	0.382938	4.050023	H	-2.688218	-0.657311	-2.613078
N	-1.627198	-0.763558	-4.142969	O	-0.192534	0.798524	6.723904	O	-1.674735	2.125536	-0.302149
O	-0.512709	-1.271965	-4.082750	N	1.193560	0.987004	7.114624	N	-2.514032	2.610863	-1.380578
O	-2.679464	-1.395273	-4.251165	O	1.292800	1.359603	8.223634	O	-3.180646	3.518563	-1.054949

1b				2b				3b			
N	-4.549867	3.995113	-5.759392	O	0.964411	-2.413738	7.924112	N	-1.772062	3.560980	-3.507090
O	-4.952282	4.769869	-4.960304	N	1.018991	-2.152115	9.083959	O	-2.528715	4.345954	-3.042048
Ru	-5.007917	2.843429	-7.077709	Ru	2.240620	-3.385334	6.633182	Ru	-1.313453	2.588381	-4.949350
N	-6.500479	4.101503	-7.738408	N	2.838142	-4.545664	8.208095	N	-1.896237	4.053312	-6.232590
N	-6.670182	2.114691	-6.034589	N	3.725609	-2.239292	7.403587	N	-3.269073	2.059290	-5.280504
N	-5.436049	1.326782	-8.546293	N	3.444514	-4.140517	5.250389	N	-0.796179	1.195644	-6.517993
N	-3.698820	1.333649	-6.541055	N	1.746824	-2.211832	5.060132	N	-0.689585	0.919813	-3.893927
C	-6.314438	5.150493	-8.571516	C	2.315844	-5.752254	8.522253	C	-1.086571	5.041998	-6.676377
C	-7.367210	5.952452	-8.999499	C	2.720687	-6.458604	9.649614	C	-1.537961	6.021808	-7.552251
C	-8.661285	5.680648	-8.545696	C	3.692087	-5.904568	10.489409	C	-2.870411	5.992812	-7.982619
C	-8.854307	4.617215	-7.668083	C	4.230195	-4.660569	10.169822	C	-3.705551	4.977239	-7.526169
C	-7.763138	3.838424	-7.268460	C	3.791064	-3.993905	9.022047	C	-3.202808	4.010595	-6.648722
C	-7.859064	2.719806	-6.329408	C	4.290066	-2.694488	8.569724	C	-3.972410	2.890394	-6.113573
C	-9.052396	2.279219	-5.743720	C	5.275230	-1.953540	9.231633	C	-5.319442	2.642817	-6.403470
C	-9.027613	1.216891	-4.845377	C	5.702048	-0.740396	8.700650	C	-5.953821	1.537324	-5.845928
C	-7.802997	0.608806	-4.546999	C	5.132342	-0.289847	7.504545	C	-5.224268	0.691389	-5.001525
C	-6.652370	1.085110	-5.163615	C	4.154703	-1.062142	6.891157	C	-3.891776	0.987297	-4.744227

C	-6.348375	1.416805	-9.527041
C	-6.564179	0.388247	-10.439588
C	-5.810190	-0.781345	-10.315544
C	-4.867257	-0.878032	-9.294550
C	-4.685705	0.198445	-8.419107
C	-3.701941	0.213541	-7.326321
C	-2.807277	-0.833554	-7.081656
C	-1.889503	-0.735152	-6.039433
C	-1.885462	0.419938	-5.254324
C	-2.798798	1.428876	-5.539476
H	-5.277917	5.325147	-8.865136
H	-7.162494	6.783508	-9.673610
H	-9.505360	6.293899	-8.861248
H	-9.848128	4.396277	-7.282893
H	-9.993895	2.766958	-5.989933
H	-9.949889	0.867602	-4.381597
H	-7.736500	-0.222400	-3.845771
H	-5.672482	0.648387	-4.973071
H	-6.904992	2.353211	-9.573372
H	-7.304001	0.508321	-11.230273
H	-5.952942	-1.610427	-11.009425
H	-4.272044	-1.782968	-9.186379
H	-2.817299	-1.717463	-7.717023
H	-1.182711	-1.543119	-5.849085
H	-1.179942	0.551044	-4.434553
H	-2.825796	2.359795	-4.974028
N	-3.520648	3.494354	-8.372350
O	-2.865707	2.638419	-8.986564
O	-3.318353	4.710976	-8.521055

C	4.293770	-5.175426	5.450907
C	5.085445	-5.696292	4.436510
C	5.010046	-5.133895	3.157441
C	4.140434	-4.069594	2.943490
C	3.359999	-3.583574	3.997446
C	2.402521	-2.490657	3.888599
C	2.132931	-1.779394	2.714571
C	1.184983	-0.762254	2.728364
C	0.523229	-0.479228	3.929718
C	0.823799	-1.222392	5.062553
H	1.550840	-6.113475	7.831750
H	2.269876	-7.426274	9.865556
H	4.022567	-6.433270	11.383418
H	4.984858	-4.204780	10.808899
H	5.702108	-2.330551	10.158956
H	6.466437	-0.153626	9.209773
H	5.436106	0.652749	7.051087
H	3.673218	-0.753848	5.964222
H	4.308471	-5.581593	6.459798
H	5.744730	-6.536458	4.651234
H	5.615869	-5.523521	2.339687
H	4.054659	-3.615635	1.957463
H	2.661703	-2.029897	1.796408
H	0.960265	-0.202663	1.820822
H	-0.233356	0.302476	3.990593
H	0.312648	-1.056088	6.009300
O	0.854683	-4.762675	6.160977
N	-0.165098	-4.404470	5.279355
O	-0.941801	-5.293388	5.095168

C	-0.884975	1.436942	-7.836839
C	-0.625115	0.458835	-8.791006
C	-0.271262	-0.822637	-8.356264
C	-0.176077	-1.074617	-6.990119
C	-0.434096	-0.041701	-6.079469
C	-0.318525	-0.178748	-4.621314
C	0.175601	-1.326375	-3.989714
C	0.301401	-1.354948	-2.603948
C	-0.060785	-0.219765	-1.873042
C	-0.538246	0.895349	-2.551113
H	-0.062910	4.998717	-6.301327
H	-0.851033	6.798831	-7.885559
H	-3.251268	6.753486	-8.664426
H	-4.745464	4.931808	-7.845696
H	-5.864805	3.318007	-7.061318
H	-7.002720	1.336566	-6.063690
H	-5.680564	-0.184368	-4.541988
H	-3.276991	0.370622	-4.088972
H	-1.169257	2.451846	-8.114918
H	-0.698492	0.699490	-9.851116
H	-0.068985	-1.616900	-9.075214
H	0.099726	-2.065101	-6.633003
H	0.478460	-2.185003	-4.586047
H	0.690482	-2.241695	-2.103454
H	0.036602	-0.185021	-0.788356
H	-0.804653	1.817335	-2.036262
O	0.613657	3.196188	-5.057830
N	1.279762	3.292575	-3.836973
O	2.396636	3.699271	-3.958415

2aU				**3aU**			
O	-1.669240	2.176180	-0.228998	N	-0.599184	0.881104	-2.566685
N	-2.562375	2.714698	-1.073512	O	-0.534753	0.853122	-3.715952
O	-2.639904	2.240886	-2.175661	Ru	-0.470608	0.649265	-0.813644
Ru	-0.466323	0.619034	-0.750096	N	1.256824	1.791529	-0.679082
N	-0.500180	0.238263	1.251783	C	1.266100	3.132660	-0.540547
C	-1.533711	-0.547395	1.688150	C	2.456584	3.849518	-0.477496
C	-1.671150	-0.839066	3.047070	C	3.665546	3.156978	-0.560359
C	-0.760332	-0.323687	3.964619	C	3.650660	1.769527	-0.700000
C	0.283121	0.480471	3.503135	C	2.429870	1.094195	-0.759702
C	0.382728	0.738483	2.142828	N	1.006984	-0.827767	-0.961197
C	-2.446335	-1.018064	0.646244	C	2.290405	-0.362237	-0.909202
N	-2.127737	-0.611973	-0.619208	C	3.366253	-1.248442	-1.002419
C	-2.918869	-0.977950	-1.650097	C	3.125676	-2.612845	-1.154409
C	-4.047971	-1.768172	-1.472026	C	1.808438	-3.070008	-1.209631
C	-4.382230	-2.192744	-0.185083	C	0.774470	-2.145486	-1.108195
C	-3.572038	-1.811956	0.880893	N	-0.481090	0.258999	1.248397
O	-0.519134	0.847416	-2.614640	C	0.398742	0.757923	2.140135
N	-0.380657	0.848018	-3.755637	C	0.311398	0.485233	3.499331
N	1.015805	-0.842291	-0.932840	C	-0.719574	-0.336882	3.956000
C	2.298043	-0.366635	-0.924114	C	-1.630407	-0.851313	3.037367
C	3.377989	-1.244695	-1.043256	C	-1.501473	-0.539286	1.681514
C	3.145016	-2.612785	-1.172613	N	-2.129234	-0.590463	-0.628548
C	1.830551	-3.082049	-1.179517	C	-2.423501	-1.003115	0.641257
C	0.792388	-2.165465	-1.055319	C	-3.545020	-1.799208	0.889316
C	2.428839	1.091851	-0.784565	C	-4.377330	-2.173048	-0.161828
N	1.249590	1.774961	-0.662873	C	-4.069754	-1.738145	-1.451314
C	1.251201	3.117134	-0.522217	C	-2.943620	-0.948495	-1.646210
C	2.435596	3.846438	-0.500059	H	0.292169	3.613902	-0.473171
C	3.648704	3.167378	-0.626148	H	2.426044	4.932263	-0.368755
C	3.643674	1.779910	-0.767746	H	4.613949	3.691222	-0.518541
H	-0.249821	-2.478833	-1.053987	H	4.585762	1.218237	-0.767006
H	1.604907	-4.142071	-1.281042	H	4.387870	-0.877587	-0.961842
H	3.981932	-3.303269	-1.267974	H	3.959290	-3.309538	-1.232071
H	4.397110	-0.864729	-1.037497	H	1.576787	-4.126402	-1.332612
H	4.581823	1.238877	-0.868345	H	-0.269603	-2.449397	-1.147198
H	4.592231	3.711630	-0.615316	H	1.182020	1.399961	1.746389
H	2.397761	4.928557	-0.387203	H	1.039321	0.918442	4.182343
H	0.273375	3.584649	-0.417178	H	-0.817434	-0.570872	5.015276
H	1.173492	1.367123	1.744563	H	-2.444567	-1.487458	3.376006
H	1.013222	0.912737	4.184422	H	-3.771576	-2.119106	1.903242
H	-0.866532	-0.543097	5.026167	H	-5.256419	-2.788125	0.024577
H	-2.495078	-1.462326	3.386493	H	-4.694298	-1.994908	-2.304860
H	-3.817784	-2.125213	1.892612	H	-2.688161	-0.578617	-2.635243
H	-5.265331	-2.806148	-0.012907	O	-1.698028	2.188149	-0.271636
H	-4.655538	-2.032240	-2.335448	N	-2.485780	2.799965	-1.151057
H	-2.646993	-0.610288	-2.635941	O	-2.447957	2.432869	-2.297309

2bU				**3bU**			
O	-0.526325	0.795805	-2.664974	O	0.631366	3.077016	-5.173044
N	0.270423	1.064834	-3.506637	N	1.364549	3.614416	-4.187761
Ru	-0.435454	0.612957	-0.649154	O	0.814120	3.822342	-3.131653
N	1.008774	-0.830056	-0.896877	Ru	-1.334173	2.543882	-4.988112
C	2.292663	-0.365426	-1.011971	N	-1.933095	4.042029	-6.237837
C	3.355193	-1.248998	-1.228649	N	-3.324933	2.047988	-5.292847
C	3.111775	-2.614972	-1.321706	N	-0.832134	1.145045	-6.519514
C	1.799003	-3.077719	-1.192509	N	-0.724403	0.894134	-3.896874
C	0.780577	-2.158699	-0.982552	C	-1.127103	5.036091	-6.676417
C	2.437370	1.084683	-0.871479	C	-1.586577	6.039740	-7.517785
N	1.263485	1.753705	-0.643762	C	-2.924682	6.032562	-7.923679
C	1.287040	3.096297	-0.486553	C	-3.757943	5.014665	-7.471621
C	2.468785	3.824006	-0.548313	C	-3.248409	4.024618	-6.626373
C	3.672051	3.153823	-0.783258	C	-4.025885	2.905939	-6.095372
C	3.651658	1.771670	-0.944149	C	-5.381806	2.683882	-6.362387
O	-1.547596	2.272694	-0.215704	C	-6.022181	1.579555	-5.811924
N	-2.592837	2.697698	-0.943680	C	-5.292532	0.709168	-4.996947
O	-2.879174	2.039677	-1.917961	C	-3.951220	0.978528	-4.761261
N	-2.083431	-0.593583	-0.574661	C	-0.921510	1.369432	-7.841950
C	-2.812444	-0.995934	-1.640590	C	-0.553966	0.417976	-8.785527
C	-3.927320	-1.810512	-1.512121	C	-0.074542	-0.815864	-8.339750
C	-4.327230	-2.227351	-0.238272	C	0.020152	-1.051075	-6.972062
C	-3.585353	-1.816231	0.862179	C	-0.363864	-0.052280	-6.069640
C	-2.463102	-1.001466	0.676705	C	-0.295302	-0.191408	-4.609923
C	-1.601841	-0.520063	1.753488	C	0.177279	-1.335900	-3.958604
N	-0.544280	0.248231	1.343602	C	0.218441	-1.375651	-2.569427
C	0.308774	0.745385	2.264761	C	-0.214492	-0.257028	-1.852957
C	0.155933	0.506416	3.622818	C	-0.671955	0.854286	-2.547325
C	-0.917268	-0.277583	4.055598	H	-0.095928	4.985161	-6.332763
C	-1.797769	-0.792489	3.111198	H	-0.899214	6.817558	-7.844639
H	-0.257991	-2.467816	-0.883131	H	-3.311793	6.809861	-8.580662
H	1.561258	-4.137851	-1.258282	H	-4.803215	4.989118	-7.771574
H	3.932994	-3.309161	-1.492132	H	-5.931470	3.375047	-6.997776
H	4.368847	-0.866158	-1.323741	H	-7.076993	1.399525	-6.013242
H	4.574962	1.227609	-1.130614	H	-5.754046	-0.166088	-4.544336
H	4.611931	3.700298	-0.842829	H	-3.340115	0.337919	-4.128062
H	2.437677	4.904300	-0.418641	H	-1.293533	2.349583	-8.135038
H	0.316470	3.557026	-0.308166	H	-0.639085	0.645208	-9.846535
H	1.122507	1.354758	1.879191	H	0.225376	-1.584771	-9.050166
H	0.866730	0.934881	4.326382	H	0.395826	-2.004227	-6.607570
H	-1.066582	-0.480916	5.114873	H	0.519660	-2.189727	-4.538703
H	-2.643531	-1.400299	3.424250	H	0.589501	-2.260105	-2.054143
H	-3.873775	-2.123726	1.864600	H	-0.190520	-0.234321	-0.764897
H	-5.204676	-2.858275	-0.107360	H	-0.997632	1.761808	-2.042323
H	-4.480165	-2.100517	-2.403236	N	-1.731096	3.567748	-3.492623
H	-2.484888	-0.619398	-2.606078	O	-2.339305	4.517883	-3.128644