

Supporting Information:

Computational Studies of the Interaction Between Ruthenium Dyes and X^- and X_2^- , $X = Br, I, At$. Implications for Dye-Sensitized Solar Cells

Ching-Han Hu, Abu Md. Asaduzzaman and Georg Schreckenbach

Full citations of references 18, 36, 37, 39, 55, 67;

Reference 18: Gao, F.; Wang, Y.; Shi, D.; Zhang, J.; Wang, M. K.; Jing, X. Y.; Humphry-Baker, R.; Wang, P.; Zakeeruddin, S. M.; Grätzel, M. *J. Am. Chem. Soc.* **2008**, *130*, 10720-10728.

Reference 36: Wolpher, H.; Sinha, S.; Pan, J. X.; Johansson, A.; Lundqvist, M. J.; Persson, P.; Lomoth, R.; Bergquist, J.; Sun, L. C.; Sundstrom, V.; Akermark, B.; Polivka, T. *Inorg. Chem.* **2007**, *46*, 638-651.

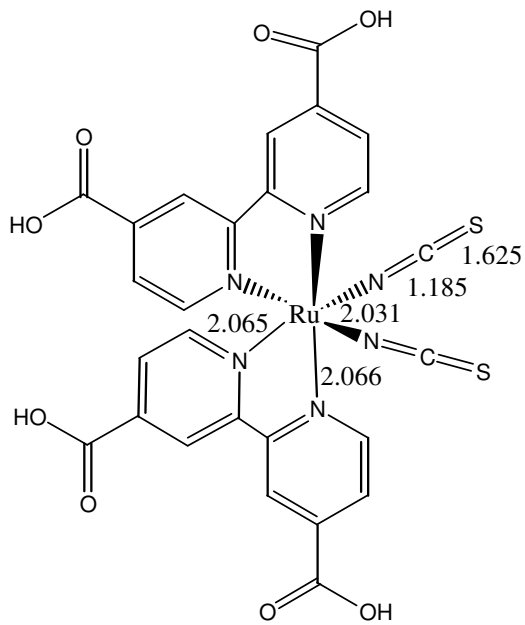
Reference 37: Barolo, C.; Nazeeruddin, M. K.; Fantacci, S.; Di Censo, D.; Comte, P.; Liska, P.; Viscardi, G.; Quagliotto, P.; De Angelis, F.; Ito, S.; Grätzel, M. *Inorg. Chem.* **2006**, *45*, 4642-4653.

Reference 39: Nazeeruddin, M. K.; Wang, Q.; Cevey, L.; Aranyos, V.; Liska, P.; Figgemeier, E.; Klein, C.; Hirata, N.; Koops, S.; Haque, S. A.; Durrant, J. R.; Hagfeldt, A.; Lever, A. B. P.; Grätzel, M. *Inorg. Chem.* **2006**, *45*, 787-797.

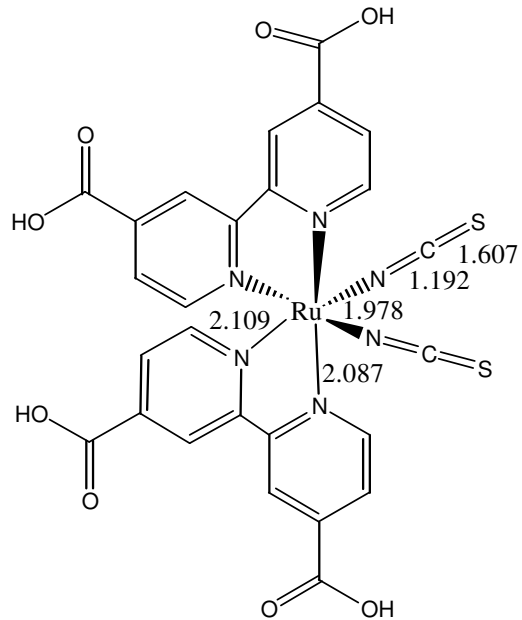
Reference 55: Ogiya, K.; Lv, C.; Suzuki, A.; Sahnoun, R.; Koyama, M.; Tsuboi, H.; Hatakeyama, N.; Endou, A.; Takaba, H.; Kubo, M.; Del Carpio, C. A.; Miyamoto, A. *Jpn. J. Appl. Phys., Part 1* **2008**, *47*, 3010-3014.

Reference 67: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Gaussian, Inc.: Wallingford CT, 2004.

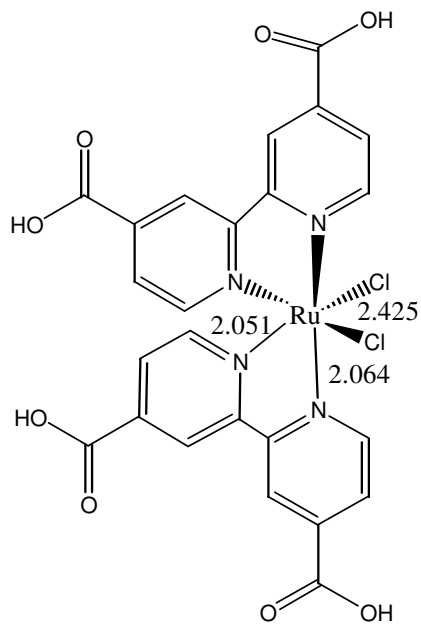
Scheme S1. Schematic structures and key geometry parameters of N3, 4, N3⁺ and 4⁺ (Å).



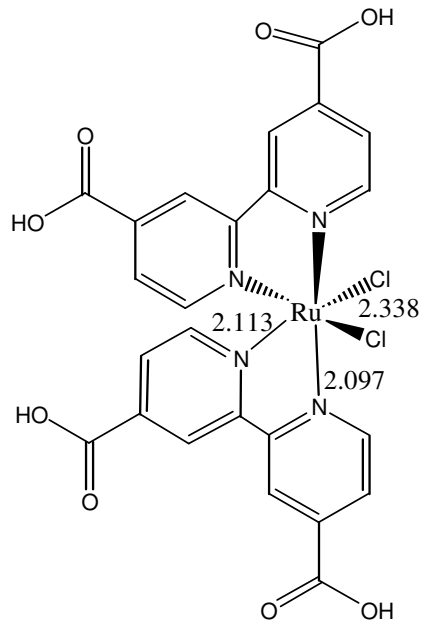
N3



N3⁺

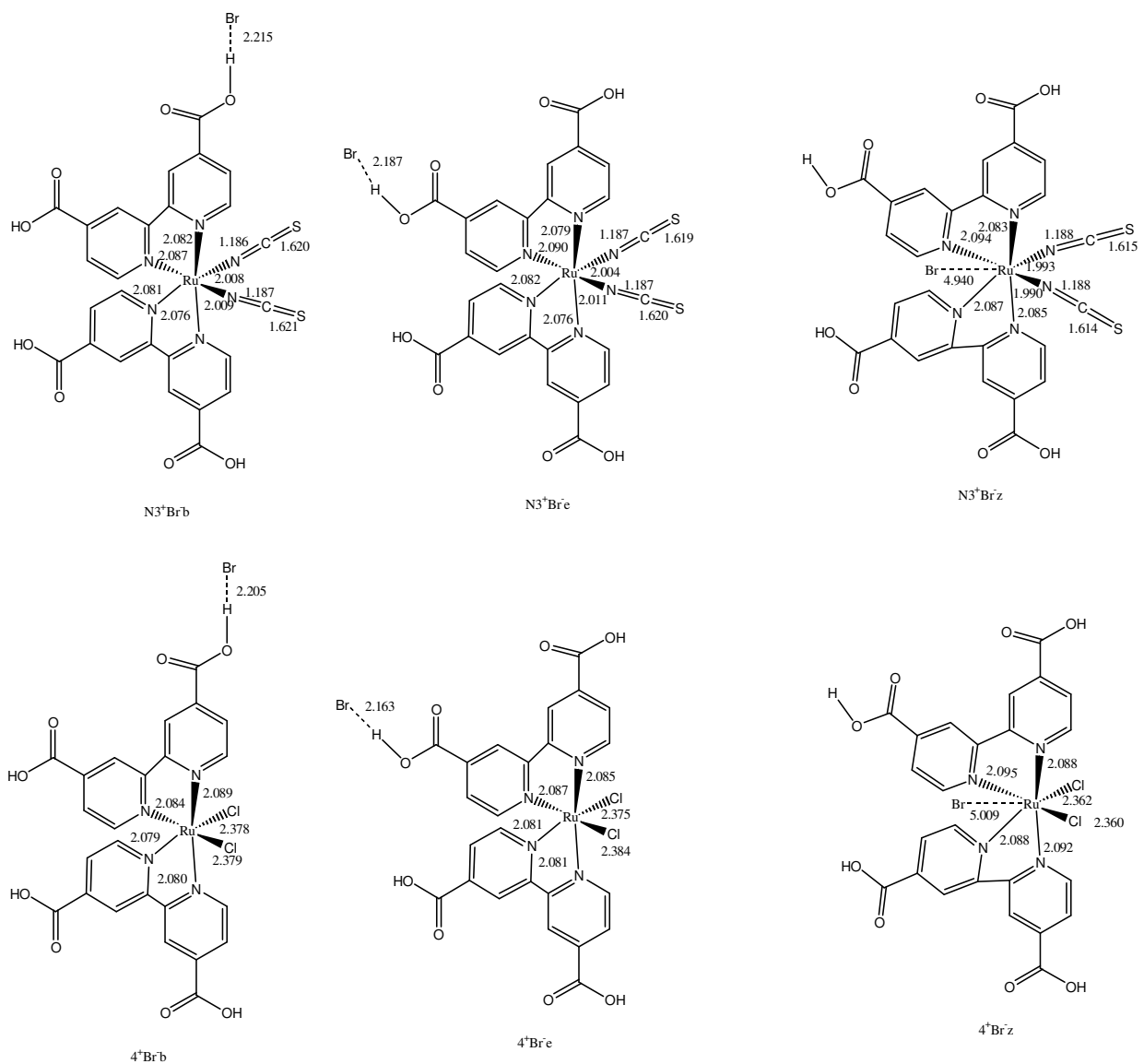


4

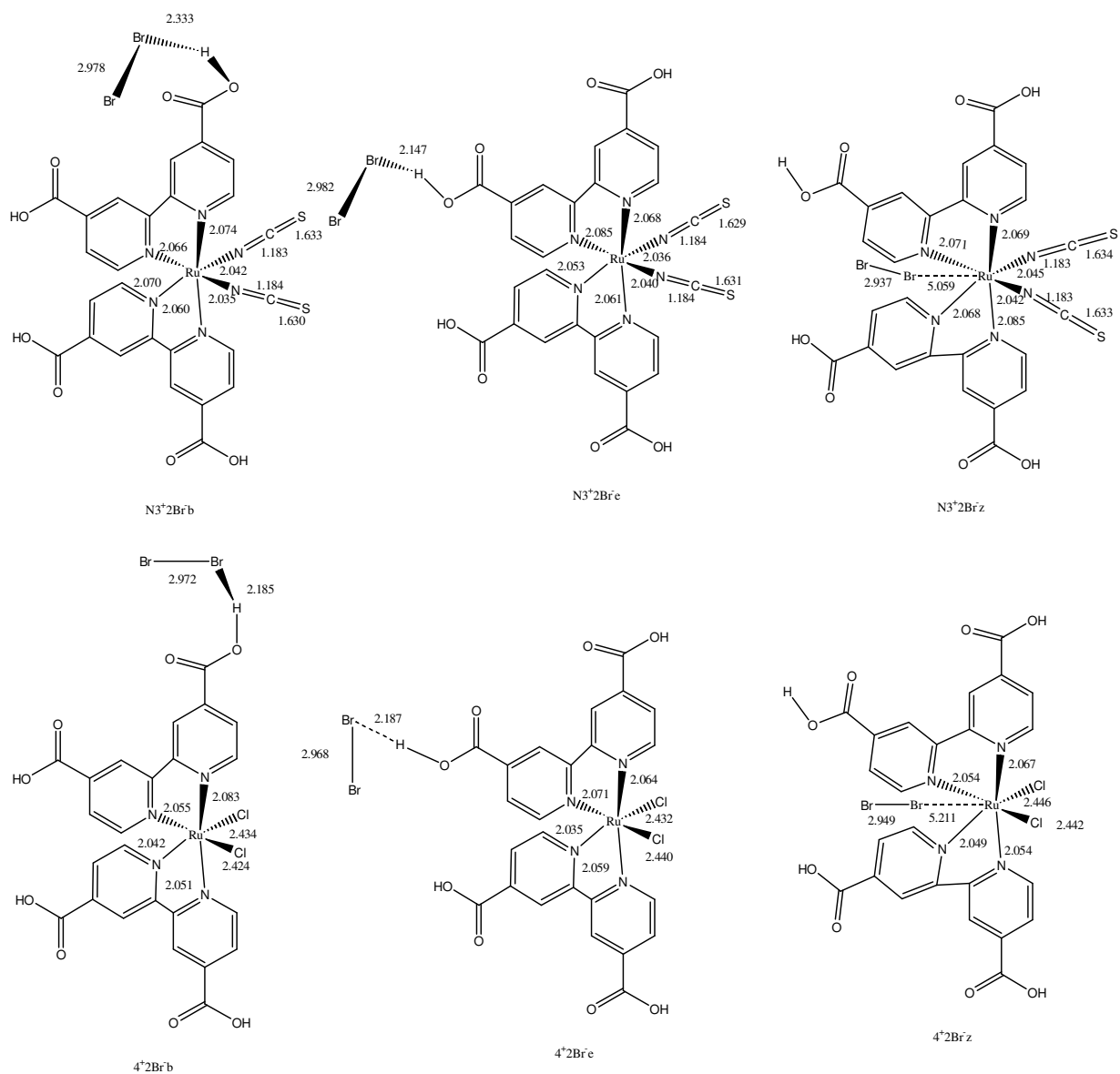


4⁺

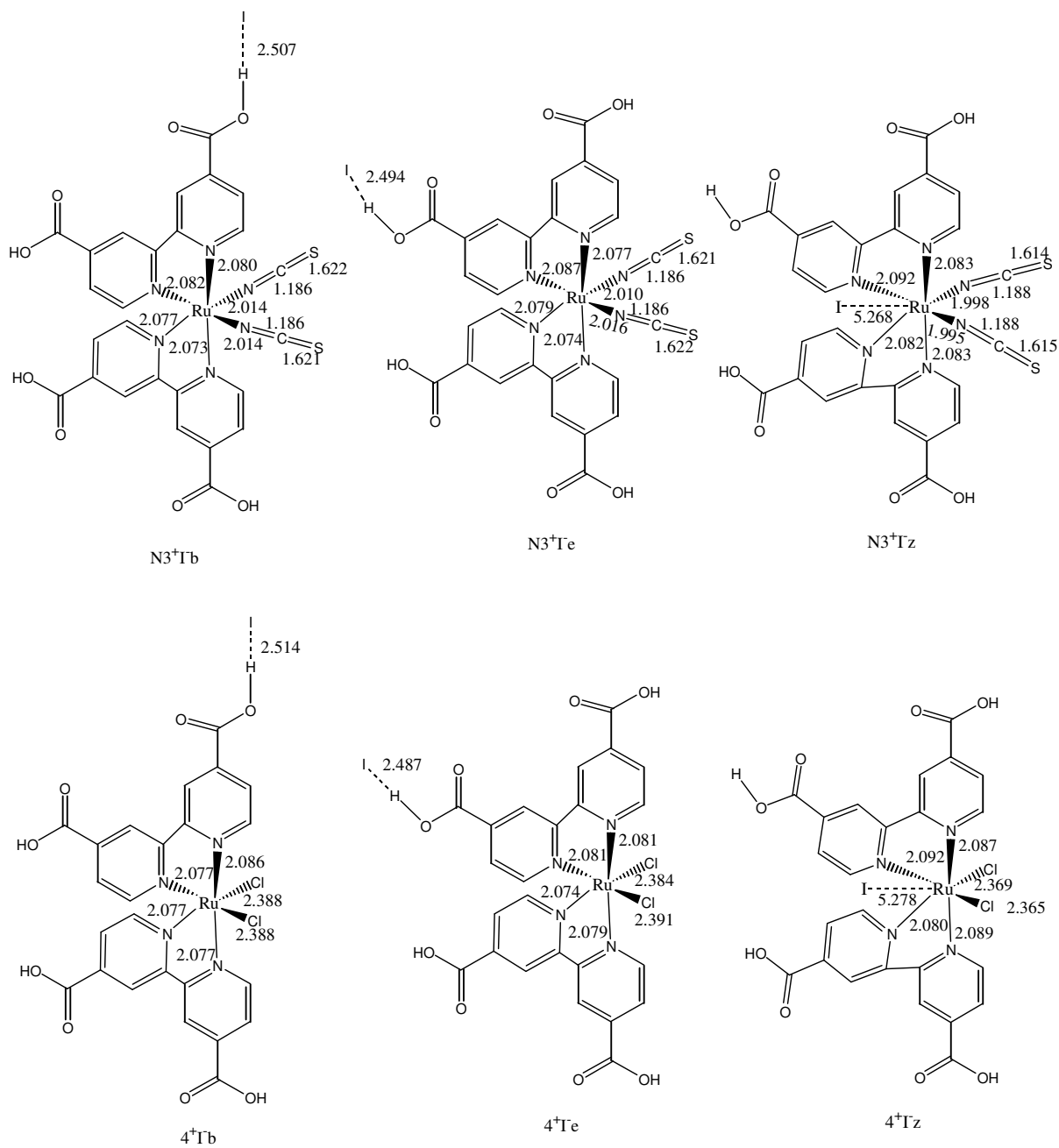
Scheme S2. Schematic structures and key geometry parameters of complexes containing Br⁻ (Å).



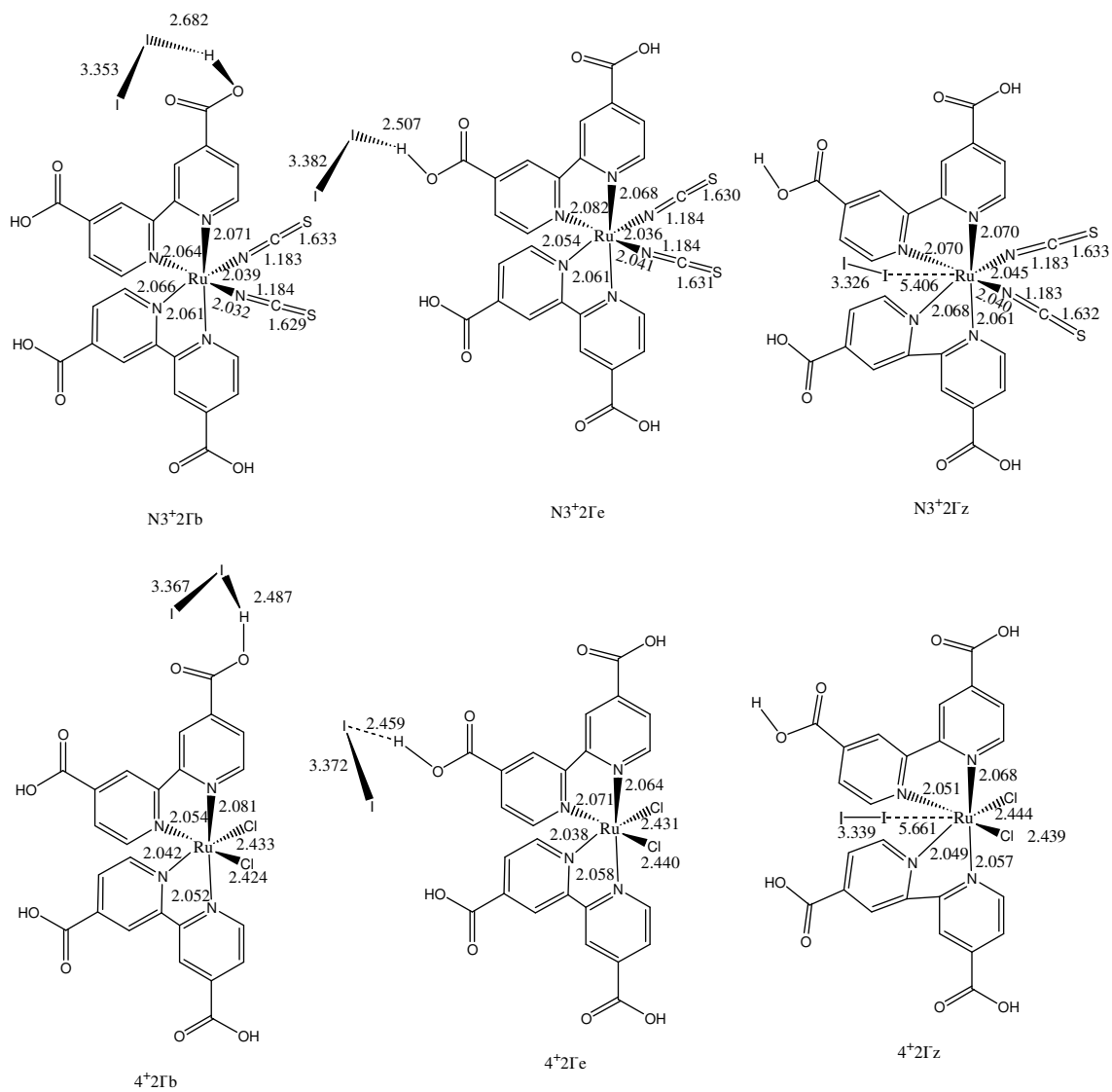
Scheme S3. Schematic structures and key geometry parameters of complexes containing Br_2^- (Å).



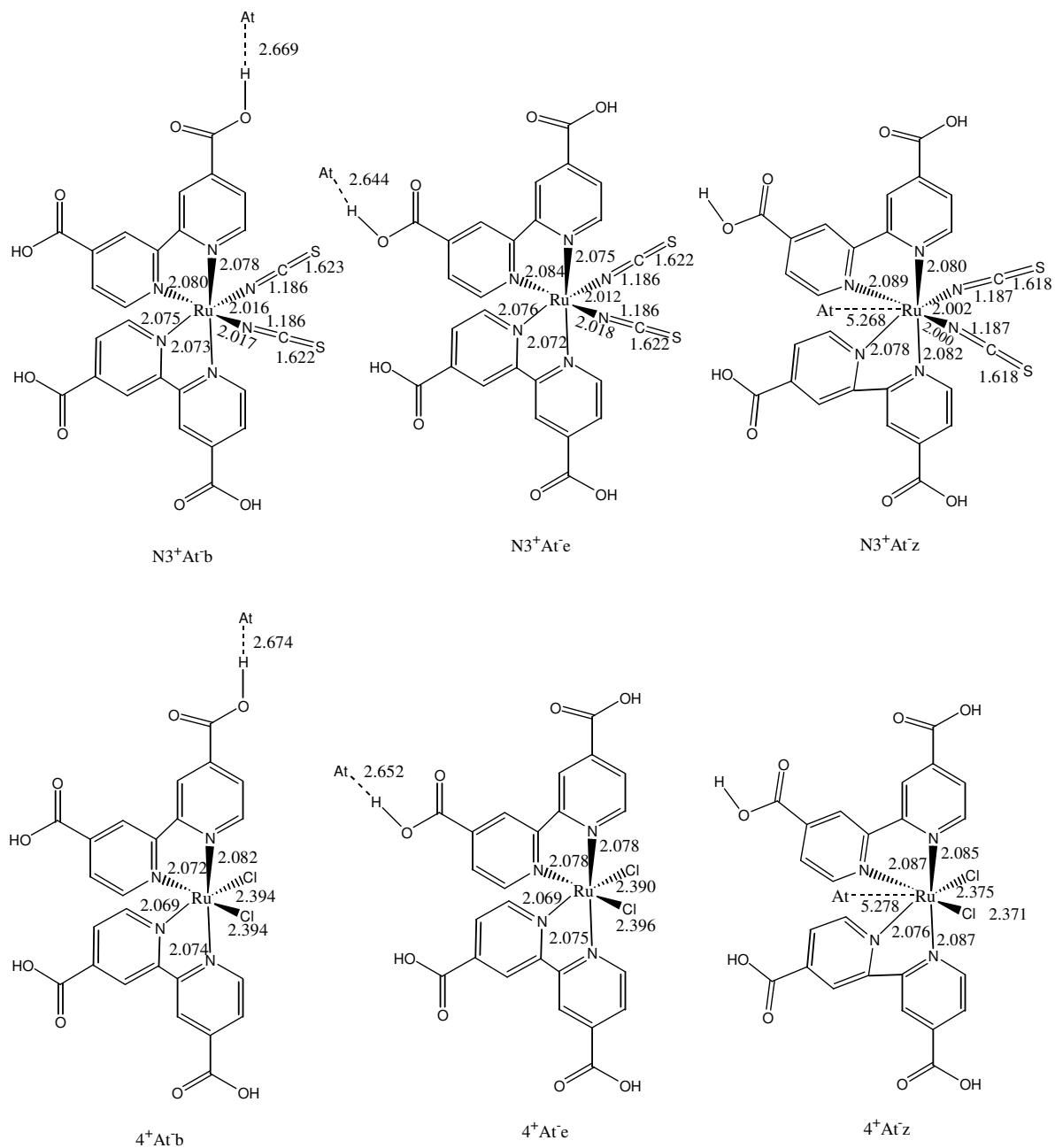
Scheme S4. Schematic structures and key geometry parameters of complexes containing I⁻ (Å).



Scheme S5. Schematic structures and key geometry parameters of complexes containing I_2^- (Å).



Scheme S6. Schematic structures and key geometry parameters of complexes containing At⁻ (Å).



Scheme S7. Schematic structures and key geometry parameters of complexes containing At_2^- (Å).

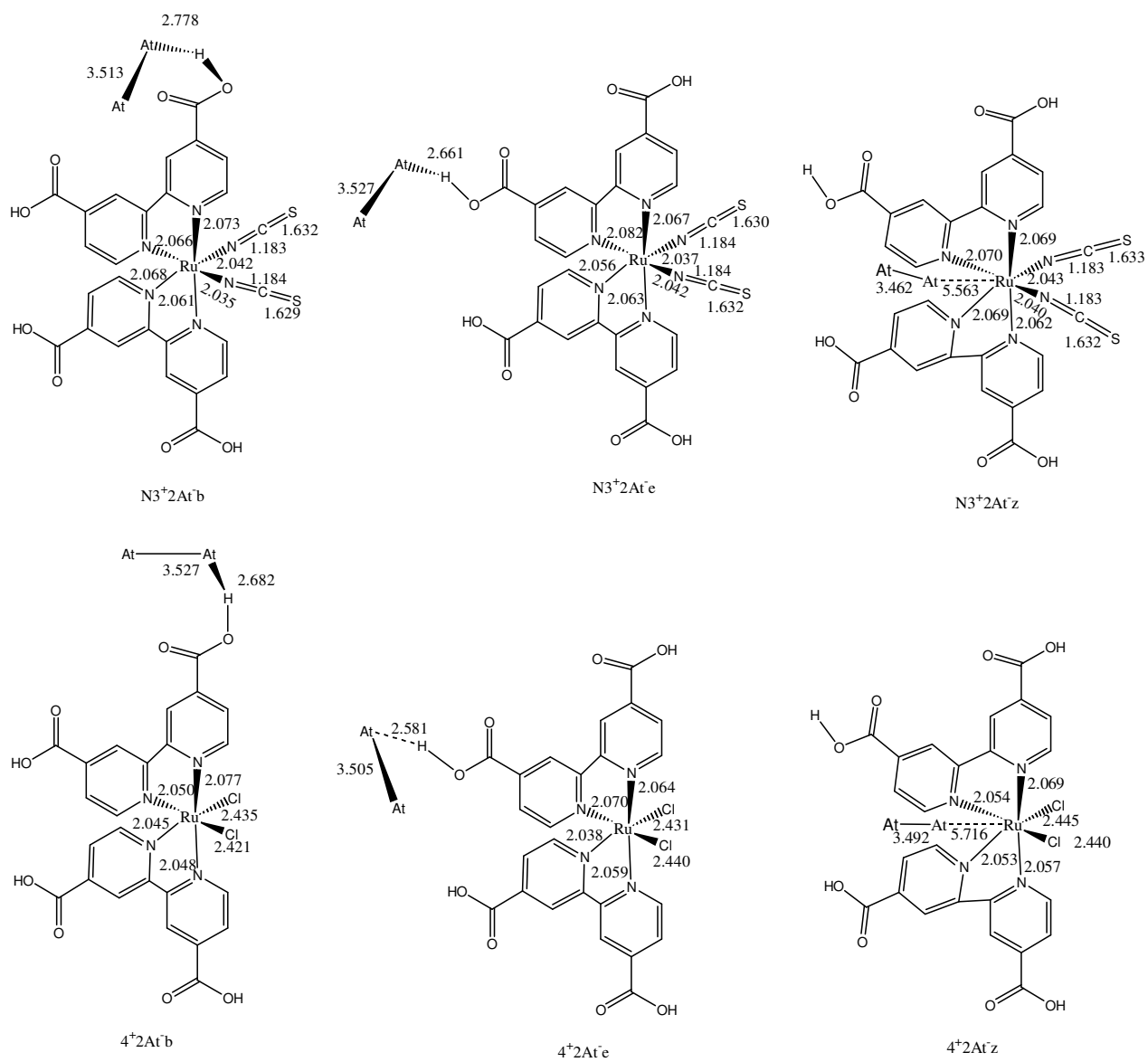


Table S1. Calculated Mulliken charges for N₃, N₃⁺ and their complexes (PCM calculations).

X(close) represents the only X or the X that is closer to Ru (z) or to H (b, e).

	Ru	N ^a	C ^a	S ^a	X(close)	X(far)	X ₂ total
N ₃	0.619	-0.261	0.054	-0.441			
N ₃ ⁺	0.792	-0.282	0.102	-0.262			
N ₃ ⁺ Br ⁻ (b)	0.802	-0.281	0.090	-0.272	-0.888		
N ₃ ⁺ Br ⁻ (e)	0.807	-0.278	0.092	-0.277	-0.884		
N ₃ ⁺ Br ⁻ (z)	0.796	-0.276	0.089	-0.284	-0.869		
N ₃ Br ₂ ⁻ (b)	0.616	-0.254	0.045	-0.445	-0.462	-0.449	-0.911
N ₃ Br ₂ ⁻ (e)	0.629	-0.254	0.047	-0.448	-0.449	-0.449	-0.898
N ₃ Br ₂ ⁻ (z)	0.631	-0.254	0.046	-0.449	-0.454	-0.514	-0.968
N ₃ Br ₂ ⁻ (b)	0.804	-0.278	0.088	-0.268	-0.907		
N ₃ ⁺ I ⁻ (e)	0.807	-0.282	0.089	-0.269	-0.903		
N ₃ ⁺ I ⁻ (z)	0.793	-0.274	0.088	-0.284	-0.883		
N ₃ I ₂ ⁻ (b)	0.602	-0.250	0.044	-0.444	-0.467	-0.462	-0.929
N ₃ I ₂ ⁻ (e)	0.622	-0.258	0.046	-0.444	-0.469	-0.451	-0.920
N ₃ I ₂ ⁻ (z)	0.622	-0.260	0.048	-0.443	-0.463	-0.508	-0.971
N ₃ ⁺ At ⁻ (b)	0.809	-0.280	0.088	-0.270	-0.919		
N ₃ ⁺ At ⁻ (e)	0.810	-0.278	0.087	-0.272	-0.915		
N ₃ ⁺ At ⁻ (z)	0.789	-0.278	0.088	-0.288	-0.858		
N ₃ At ₂ ⁻ (b)	0.611	-0.267	0.054	-0.442	-0.467	-0.468	-0.935
N ₃ At ₂ ⁻ (e)	0.615	-0.265	0.050	-0.442	-0.475	-0.456	-0.931
N ₃ At ₂ ⁻ (z)	0.615	-0.264	0.050	-0.443	-0.467	-0.507	-0.974

a ... Average over the two sides.

Table S2. Calculated Mulliken charges for 4, 4⁺ and their complexes (PCM calculations).

X(close) represents the only X or the X that is closer to Ru (z) or to H (b, e).

	Ru	Cl ^a	X(close)	X(far)	X ₂ total
4	0.381	-0.498			
4 ⁺	0.510	-0.320			
4 ⁺ Br ⁻ (b)	0.530	-0.342	-0.888		
4 ⁺ Br ⁻ (e)	0.524	-0.342	-0.879		
4 ⁺ Br ⁻ (z)	0.510	-0.350	-0.866		
4Br ₂ ⁻ (b)	0.413	-0.509	-0.456	-0.450	-0.906
4Br ₂ ⁻ (e)	0.415	-0.511	-0.455	-0.450	-0.905
4Br ₂ ⁻ (z)	0.418	-0.514	-0.451	-0.523	-0.974
4 ⁺ I ⁻ (b)	0.533	-0.347	-0.907		
4 ⁺ I ⁻ (e)	0.528	-0.346	-0.902		
4 ⁺ I ⁻ (z)	0.508	-0.339	-0.861		
4I ₂ ⁻ (b)	0.415	-0.508	-0.464	-0.459	-0.923
4I ₂ ⁻ (e)	0.428	-0.511	-0.458	-0.459	-0.917
4I ₂ ⁻ (z)	0.432	-0.514	-0.465	-0.511	-0.976
4 ⁺ At ⁻ (b)	0.530	-0.348	-0.919		
4 ⁺ At ⁻ (e)	0.528	-0.348	-0.916		
4 ⁺ At ⁻ (z)	0.515	-0.353	-0.866		
4At ₂ ⁻ (b)	0.419	-0.509	-0.471	-0.462	-0.933
4At ₂ ⁻ (e)	0.427	-0.512	-0.463	-0.462	-0.925
4At ₂ ⁻ (z)	0.423	-0.514	-0.465	-0.511	-0.976

a ... Average over the two sides.

Table S3. Extended version of Table 3: Optimized geometries of the $N3^+X^-$ and $N3X_2^-$ complexes, key geometry parameters ($X = Br, I, At$; bond lengths in Å)^a.

Adsorbed Species	Complex	Bond lengths						
		Ru–N(CS)	N–C	C–S	Ru–N(dcpby ^b)	H–X	Ru–X	X–X
Br ⁻	N3⁺Br⁻(b)	2.008, 2.009	1.186, 1.187	1.620, 1.621	2.082, 2.087, 2.081, 2.076	2.215		
	N3⁺Br⁻(e)	2.004, 2.011	1.187, 1.187	1.619, 1.620	2.079, 2.090, 2.082, 2.076	2.187		
	N3⁺Br⁻(z)	1.993, 1.990	1.188, 1.188	1.615, 1.614	2.083, 2.094, 2.087, 2.085		4.940	
2Br ⁻	N3Br₂⁻(b)	2.042, 2.035	1.183, 1.184	1.633, 1.630	2.074, 2.066, 2.070, 2.060	2.333		2.978
	N3Br₂⁻(e)	2.036, 2.040	1.184, 1.184	1.629, 1.631	2.068, 2.085, 2.053, 2.061	2.147		2.982
	N3Br₂⁻(z)	2.045, 2.042	1.183, 1.183	1.634, 1.633	2.069, 2.071, 2.068, 2.085		5.059	2.937
I ⁻	N3⁺I⁻(b)	2.014, 2.014	1.186, 1.186	1.622, 1.621	2.080, 2.082, 2.077, 2.073	2.507		
	N3⁺I⁻(e)	2.010, 2.016	1.186, 1.186	1.621, 1.622	2.077, 2.087, 2.079, 2.074	2.494		
	N3⁺I⁻(z)	1.198, 1.195	1.188, 1.188	1.614, 1.615	2.083, 2.092, 2.082, 2.083		5.268	
2I ⁻	N3I₂⁻(b)	2.039, 2.032	1.183, 1.184	1.633, 1.629	2.071, 2.064, 2.066, 2.061	2.682		3.353
	N3I₂⁻(e)	2.036, 2.041	1.184, 1.184	1.630, 1.631	2.068, 2.082, 2.054, 2.061	2.607		3.382
	N3I₂⁻(z)	2.045, 2.040	1.183, 1.183	1.633, 1.632	2.070, 2.070, 2.068, 2.061		5.406	3.326
At ⁻	N3⁺At⁻(b)	2.016, 2.017	1.186, 1.186	1.623, 1.622	2.078, 2.080, 2.075, 2.073	2.669		
	N3⁺At⁻(e)	2.012, 2.018	1.186, 1.186	1.622, 1.622	2.075, 2.084, 2.076, 2.072	2.644		
	N3⁺At⁻(z)	2.002, 2.000	1.187, 1.187	1.618, 1.618	2.080, 2.089, 2.078, 2.082		5.268	
2At ⁻	N3At₂⁻(b)	2.042, 2.035	1.183, 1.184	1.632, 1.629	2.073, 2.066, 2.068, 2.061	2.778		3.513
	N3⁺At₂⁻e	2.037, 2.042	1.184, 1.184	1.630, 1.632	2.067, 2.082, 2.056, 2.063	2.661		3.527
	N3At₂⁻z	2.043, 2.040	1.183, 1.183	1.633, 1.632	2.069, 2.070, 2.069, 2.062		5.563	3.462

a ... Essentially the same data is also provided in the context of the structural drawings in Schemes S2 to S7.

b ... dcpby = 4,4'-dicarboxy-2,2'-bipyridyl.

Table S4. Extended version of Table 4: Optimized geometries of the 4^+X^- and $4X_2^-$ complexes, key geometry parameters (X = Br, I, At; bond lengths in Å)^a.

Adsorbed Species	Complex	Bond lengths				
		Ru–Cl	Ru–N(dcpby ^b)	H–X	Ru–X	X–X
Br ⁻	4⁺Br⁻(b)	2.378, 2.379	2.089, 2.084, 2.079, 2.080	2.205		
	4⁺Br⁻(e)	2.375, 2.384	2.085, 2.087, 2.081, 2.081	2.163		
	4⁺Br⁻(z)	2.362, 2.360	2.088, 2.095, 2.088, 2.092		5.009	
2Br ⁻	4Br₂⁻(b)	2.434, 2.424	2.083, 2.055, 2.042, 2.051	2.185		2.972
	4Br₂⁻(e)	2.432, 2.440	2.064, 2.071, 2.035, 2.059	2.187		2.968
	4Br₂⁻(z)	2.446, 2.442	2.067, 2.054, 2.049, 2.054		5.211	2.949
I ⁻	4⁺I⁻(b)	2.388, 2.388	2.086, 2.077, 2.077, 2.077	2.514		
	4⁺I⁻(e)	2.384, 2.391	2.081, 2.081, 2.074, 2.079	2.487		
	4⁺I⁻(z)	2.369, 2.365	2.087, 2.092, 2.080, 2.089		5.278	
2I ⁻	4I₂⁻(b)	2.433, 2.424	2.081, 2.054, 2.042, 2.052	2.487		3.367
	4I₂⁻(e)	2.431, 2.440	2.064, 2.071, 2.038, 2.058	2.459		3.372
	4I₂⁻(z)	2.444, 2.439	2.068, 2.051, 2.049, 2.057		5.661	3.339
At ⁻	4⁺At⁻(b)	2.394, 2.394	2.082, 2.072, 2.069, 2.074	2.674		
	4⁺At⁻(e)	2.390, 2.396	2.078, 2.078, 2.069, 2.075	2.652		
	4⁺At⁻(z)	2.375, 2.371	2.085, 2.087, 2.076, 2.087		5.278	
2At ⁻	4At₂⁻(b)	2.435, 2.421	2.077, 2.050, 2.045, 2.048	2.682		3.527
	4At₂⁻(e)	2.431, 2.440	2.064, 2.070, 2.038, 2.059	2.581		3.505
	4At₂⁻(z)	2.445, 2.440	2.069, 2.054, 2.053, 2.057		5.716	3.492

a ... Essentially the same data is also provided in the context of the structural drawings in Schemes S2 to S7.

b ... dcpby = 4,4'-dicarboxy-2,2'-bipyridyl.

Table S5. Energies in solution ($\Delta E + \Delta\Delta G_{\text{solv}}$) for reactions of involved in the dye regeneration process (kcal/mol).

Dye reaction	Br			I			At		
	b	e	z	b	e	z	b	e	z
$\text{N3}^+ + \text{X}^- \rightarrow \text{N3}^+\text{X}^-$	-7.09	-7.02	3.29	-4.82	-5.45	3.08	-5.17	-5.59	0.52
$\text{N3}^+\text{X}^- + \text{X}^- \rightarrow \text{N3X}_2^-$	14.05	9.89	4.64	6.82	3.96	-2.05	-3.95	-4.37	-10.27
$\text{N3X}_2^- \rightarrow \text{N3} + \text{X}_2^-$	-4.62	-0.53	-5.59	-5.87	-2.39	-4.90	-2.05	-1.20	-1.40
$\text{N3}^+ + 2\text{X}^- \rightarrow \text{N3} + 1/2(\text{X}^- + \text{X}_3^-)$	-6.86	-6.86	-6.86	-12.73	-12.73	-12.73	-20.02	-20.02	-20.02
$4^+ + \text{X}^- \rightarrow 4^+\text{X}^-$	-7.28	-6.82	3.13	-5.21	-5.12	6.12	-5.14	-5.53	0.21
$4^+\text{X}^- + \text{X}^- \rightarrow 4\text{X}_2^-$	12.79	11.89	8.09	6.24	5.45	-0.56	0.29	-2.72	-3.70
$4\text{X}_2^- \rightarrow 4 + \text{X}_2^-$	2.51	2.95	-3.21	0.77	1.47	-3.76	-0.63	2.78	-1.99
$4^+ + 2\text{X}^- \rightarrow 4 + 1/2(\text{X}^- + \text{X}_3^-)$	-1.18	-1.18	-1.18	-7.05	-7.05	-7.05	-14.34	-14.34	-14.34
$2 \text{X}^- \rightarrow \text{X}_2^-$	117.22	117.22	117.22	111.01	111.01	111.01	103.72	103.72	103.72
$\text{X}_2^- \rightarrow 1/2(\text{X}^- + \text{X}_3^-)$	-9.20	-9.20	-9.20	-8.86	-8.86	-8.86	-8.86	-8.86	-8.86
$2 \text{X}^- \rightarrow 1/2(\text{X}^- + \text{X}_3^-)$	108.02	108.02	108.02	102.15	102.15	102.15	94.86	94.86	94.86

Cartesian coordinates (Å):**N3**

Charge = 0 Multiplicity = 1

Ru -0.0000181613,-0.0001353449,-0.7233018751
N 1.8726256356,-0.8709612259,-0.6755330704
C 2.7958036631,-0.2469474842,0.1135154306
C 4.1195606601,-0.684426366,0.154114774
C 4.5114113025,-1.7690901663,-0.6287273001
C 3.5595747694,-2.3923854534,-1.44492317
C 2.2569766825,-1.912640589,-1.4412980282
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C 2.4596067187,2.6681628624,2.5091882423
C 3.0399510897,1.6204831221,1.7967990513
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C -4.1197464802,0.6859366581,0.152765836
C -2.7962000761,0.2478085399,0.1126884853
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N -0.718033623,-1.2714750849,-2.1351613841
C -1.2313468949,-2.0635878008,-2.8523303837
S -1.9132318404,-3.1524277787,-3.8477412581
H 4.8617372318,-0.1967351879,0.7745809281
H 3.8265818484,-3.2286942357,-2.079290763
H 1.4804256899,-2.3394431299,-2.0647197614
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H -3.2843717399,-4.8660535895,4.6690958133
H -1.4802408176,2.3359817923,-2.0693121239
H -3.8260747092,3.2259700779,-2.0853480261
H -4.8619738936,0.1996947147,0.774313226
H -7.1491958533,3.4503619556,-1.2720856269

N3+

Charge = 1 Multiplicity = 2

Ru -0.0001581431,-0.003093952,-0.8071797394
N 1.9108733733,-0.8418127405,-0.7592887478
C 2.8001257933,-0.2488839653,0.0870591982
C 4.1277126541,-0.6694794093,0.1419042444
C 4.5574117897,-1.7033248699,-0.690181986
C 3.6420281572,-2.2927418499,-1.5647416668
C 2.3294602746,-1.8315424737,-1.5695270009
C 5.9963751054,-2.1195960441,-0.5982267075
O 6.7823416781,-1.6178567337,0.1735459431
O 6.2963644485,-3.1036920046,-1.4628859748
N 0.9402877778,1.1459444945,0.6900687368
C 0.369528869,2.1463284445,1.3852649392
C 1.0612722772,2.8971529117,2.3279261121

C	2.4058841976,2.5967172944,2.5601815995	S	2.0158548984,3.1732292635,-3.7276618728	C	4.1702681824,-0.3612297405,-0.1769762274
C	3.0028477081,1.5631823257,1.8402819793	N	-0.6959391913,-1.306763331,-2.1222830414	C	4.6310696806,-1.4335847067,-0.9390159627
C	2.2538145789,0.849413621,0.9047087849	C	-1.2707016994,-2.1097407228,-2.78910072	C	3.7132328858,-2.1488844142,-1.7179781725
C	3.2542714886,3.3361798397,3.55427656	S	-2.0077687085,-3.2069642778,-3.7034697481	C	2.3776556878,-1.7712082255,-1.7017354494
O	2.5746090211,4.3206825858,4.167693354	H	4.8481946932,-0.2109841765,0.8086985904	C	6.0845241316,-1.7577060258,-0.8862935266
O	4.4135515461,3.0633843849,3.7667781036	H	3.939411766,-3.0903384005,-2.2348268128	O	6.8962081411,-1.1577483495,-0.212042845
N	-0.9418340553,-1.1406310357,0.6980832242	H	1.5797331585,-2.2441967539,-2.2333845338	O	6.4138667543,-2.8064876696,-1.6743143203
C	-2.2551333725,-0.8415499827,0.9105127144	H	7.2437465698,-3.3142278191,-1.3504511272	N	0.8754774491,1.2335485166,0.3924492604
C	-3.0045427959,-1.5475252029,1.8516818795	H	-0.6716487785,2.3473803754,1.1627905374	C	0.2533593529,2.2184619132,1.0771437248
C	-2.4082384296,-2.5759639796,2.57938635	H	0.5646311013,3.6975175015,2.8627496311	C	0.9126525067,3.0646622555,1.9526195383
C	-1.0639398263,-2.8793299691,2.3491130004	H	4.0472164636,1.3419930187,2.0249699265	C	2.2923859483,2.901127124,2.1399223135
C	-0.371757815,-2.1361841084,1.4006974746	H	3.1889745225,4.7572172643,4.7895552261	C	2.9435752311,1.8906308047,1.4350695729
C	-3.2569863574,-3.3069915488,3.579396543	H	-4.0486971498,-1.324097444,2.0348691043	C	2.2235138561,1.0705339139,0.5673335088
O	-4.415964368,-3.0315366872,3.7901213323	H	-0.5678615442,-3.6760269281,2.8899059975	C	3.0972621226,3.7542559275,3.0553732649
O	-2.5779132962,-4.2870933223,4.2004592045	H	0.6692354591,-2.3395969036,1.1795072977	O	2.3547918133,4.7063625776,3.6682532683
N	-1.9111327989,0.8358833119,-0.7671216151	H	-3.1924316496,-4.7181622356,4.8259754121	O	4.2889560127,3.6233447549,3.2453201359
C	-2.3293460578,1.8185971698,-1.586048892	H	-1.5793616766,2.2251992012,-2.2533395821	N	-0.8757527836,-1.2337764193,0.392486137
C	-3.6418112033,2.2800991616,-1.5855761067	H	-3.9388825489,3.0718179799,-2.2627347057	C	-2.2237775569,-1.0705053842,0.5671910014
C	-4.5575138861,1.6986155121,-0.7060526149	H	-4.849035608,0.2192552326,0.8055106104	C	-2.9440877282,-1.8903969598,1.4349156184
C	-4.1282650134,0.671865268,0.135011601	H	-7.2433922868,3.3040291152,-1.38136381	C	-2.2931506895,-2.9009296708,2.1399503644
C	-2.8008029324,0.2503875266,0.0839785496			C	-0.9134271548,-3.0647410868,1.9528119458
C	-5.9964044151,2.1160000862,-0.6181177588	4		C	-0.2538834687,-2.2187513176,1.0773208431
O	-6.2960243605,3.0923146798,-1.4916832928	Charge = 0 Multiplicity = 1		C	-3.0982867042,-3.7538110949,3.0554048356
O	-6.7826415514,1.6213487833,0.157942393	Ru	0.000079439,-0.000303624,-0.9920591133	O	-4.2899779983,-3.6226578686,3.2452014592
N	0.6967514989,1.2905800485,-2.1316068445	N	1.926303944,-0.7406785818,-0.9562990792	O	-2.3560543071,-4.7059602524,3.6685037537
C	1.274730176,2.0860310261,-2.8046660406	C	2.8161730863,-0.0294508511,-0.2023097541	N	-1.9260241186,0.7402314988,-0.9568830724

C -2.3770993678,1.7706454661,-1.7026578184
C -3.7125571532,2.1487335011,-1.7189720912
C -4.6305971167,1.4339762117,-0.9397506395
C -4.1701071944,0.3616889376,-0.1774197433
C -2.8161227839,0.0294660009,-0.2027033789
C -6.0839410947,1.7585840673,-0.88706404
O -6.4129539112,2.8073246299,-1.6752770881
O -6.8957693823,1.1591650589,-0.2125069368
H 4.8821110804,0.1990566485,0.4170633699
H 4.0320723881,-2.9802393142,-2.3348631224
H 1.621149752,-2.2675995502,-2.3000133416
H 7.3764573209,-2.9306244337,-1.5744194404
H -0.8085951388,2.3198845677,0.8906930048
H 0.3663208472,3.8411836839,2.47400513
H 4.0102270883,1.7639355707,1.5762289908
H 2.9710029928,5.207665333,4.2347513573
H -4.0107387501,-1.7635213871,1.575917421
H -0.3672966913,-3.8413163533,2.4743274771
H 0.8080702235,-2.3203809416,0.8909768392
H -2.9724185623,-5.2070807389,4.2349965501
H -1.6204616696,2.2666244554,-2.3011141226
H -4.0311422874,2.9800048692,-2.3361019504
H -4.8821045856,-0.1981945431,0.4168149
H -7.3754842312,2.9318657555,-1.5753051113
Cl 0.7808925401,1.5646018844,-2.6723137975
Cl -0.7801302735,-1.5657384838,-2.6720278184

4+

Charge = 1 Multiplicity = 2

Ru 0.0002292422,-0.0010536697,-1.1248738876
N 1.9931647653,-0.6516903292,-1.0971253154
C 2.8207837564,-0.0010779172,-0.2301339359
C 4.1836485209,-0.2870914489,-0.1834550415
C 4.7160487771,-1.2413072858,-1.0502047305
C 3.8651514321,-1.8847881863,-1.9498906987
C 2.5114726226,-1.5608779941,-1.9430796205
C 6.1891751963,-1.5149837065,-0.9665189898
O 6.9208888672,-0.9660095248,-0.1736356169
O 6.5874387091,-2.4321670651,-1.8646016496
N 0.8407234217,1.1914714799,0.4035676661
C 0.1727645871,2.1213587124,1.1087568879
C 0.7877278709,2.91890991,2.0655504577
C 2.1537344031,2.7397454736,2.3005546779
C 2.8488232428,1.7798085781,1.5677413973
C 2.1737500374,1.0163870363,0.6143986722
C 2.92460696,3.5386061499,3.3123251579
O 2.1529710445,4.4453534335,3.9367172869
O 4.1028979104,3.3710085795,3.5289446185
N -0.8410990114,-1.1916633818,0.4045483828
C -2.1740898011,-1.015787278,0.6149475024
C -2.8496911473,-1.7779905415,1.5688911658
C -2.1551805992,-2.7375610859,2.3027324385

C -0.789218965,-2.9175871658,2.0681385799
C -0.1737059194,-2.1212125133,1.1107158747
C -2.9266265852,-3.5351279074,3.3150845547
O -4.1048744413,-3.366751501,3.5313372823
O -2.1555401055,-4.4416443262,3.9404893791
N -1.9925244027,0.6501559899,-1.0985521163
C -2.5103484601,1.5585664214,-1.9456382686
C -3.863863179,1.8831531197,-1.9529022265
C -4.7151322614,1.2412317322,-1.0524584854
C -4.1832544692,0.2878077451,-0.1845171854
C -2.8205370402,0.0010236949,-0.2308078161
C -6.1881155925,1.5157959274,-0.9691562729
O -6.5858904403,2.4319532883,-1.868501587
O -6.9201527188,0.9681609412,-0.1756460302
H 4.8530223062,0.2183418259,0.5022106149
H 4.2411691801,-2.6221667008,-2.6487756072
H 1.8072188311,-2.0240366745,-2.6237181779
H 7.5507393709,-2.5513085221,-1.7538434828
H -0.8813168379,2.2261360455,0.8815547843
H 0.2173254728,3.6617381834,2.6096028403
H 3.9085845007,1.6548712065,1.7546987249
H 2.7206614731,4.9264128563,4.5699759987
H -3.9094398358,-1.6524264385,1.7554972693
H -0.2192632699,-3.6601768178,2.6129831813
H 0.8803722282,-2.2266723466,0.883800552
H -2.7235840596,-4.921834477,4.5740902379

H -1.8058247781,2.0205598705,-2.626782977
H -4.2394689348,2.6198594532,-2.6527172495
H -4.8529122396,-0.2164311397,0.5017508857
H -7.5491440467,2.5516899026,-1.7579748511
Cl 0.7036160952,1.6287605288,-2.6468322983
Cl -0.7024119983,-1.6327223229,-2.645064528

N3+Br-b

Charge = 0 Multiplicity = 2

Ru -0.8754447871,0.117738974,-0.7741372939
N 1.1934978557,-0.0691218439,-0.6294313744
C 1.8154532345,0.8289571453,0.1871937385
C 3.1977880681,0.8067881889,0.3598201487
C 3.9640119309,-0.1390073762,-0.3198946975
C 3.3197047401,-1.0329486692,-1.1781106442
C 1.9363638298,-0.9636948538,-1.3078435398
C 5.4531359277,-0.1521315445,-0.0738417413
O 5.9728752467,0.6331578141,0.6938808772
O 6.0573334261,-1.1027723036,-0.7723076801
N -0.4105566688,1.634033636,0.5829469803
C -1.2935525027,2.4791548178,1.1502985266
C -0.9160835088,3.4993383654,2.0109777506
C 0.4433248172,3.6592082517,2.3012144871
C 1.3631816488,2.7917465407,1.7153578663
C 0.9187810518,1.7854885566,0.8565376053
C 0.9621649987,4.7251219775,3.2123882303

O -0.0234894686,5.5073913149,3.7022203667
O 2.1333208057,4.870640722,3.4843574143
N -1.4041539726,-1.1754061578,0.7679778308
C -2.7472975778,-1.3276642005,0.9689514656
C -3.2335206995,-2.187974546,1.9527090351
C -2.3422109608,-2.9130236645,2.7419646161
C -0.9688515344,-2.7580993447,2.5237440322
C -0.5484234548,-1.8836937219,1.5317131296
C -2.907134751,-3.8233685868,3.7838943249
O -4.0935315665,-3.9528371646,3.9954319524
O -1.9477348877,-4.4836335254,4.4644089446
N -2.9443677711,0.2858712343,-0.7871775058
C -3.6505701572,1.0409097222,-1.6514755527
C -5.0397311587,1.0414713426,-1.6780554847
C -5.7309438933,0.2240327531,-0.7781595067
C -5.0026434388,-0.5672027227,0.1092944435
C -3.6090820657,-0.525362688,0.0856586355
C -7.22296807,0.1471891794,-0.721342159
O -7.8144925532,0.9369098118,-1.6405147611
O -7.83355289,-0.5457705488,0.0637488873
H 3.7110281391,1.5016817275,1.0142449382
H 3.8859719937,-1.7714365185,-1.7326929461
H 1.3842976491,-1.6287949293,-1.9608330505
H 7.0432810604,-1.1236540768,-0.5737552044
H -2.3325242135,2.3240187759,0.8855932753
H -1.6617653322,4.1578237709,2.4391043459

H 2.4156504297,2.9230332634,1.935630569
H 0.4058669877,6.1712892614,4.2748794767
H -4.295986827,-2.3146881229,2.1220231712
H -0.242574841,-3.3092922934,3.1084332297
H 0.5039613183,-1.7404754582,1.3191698397
H -2.4033392721,-5.0544966184,5.1120996809
H -3.0626070485,1.6419699193,-2.3342276289
H -5.5677091222,1.6614091417,-2.3923119861
H -5.5430594142,-1.2081712016,0.7953785085
H -8.7777348162,0.8170985303,-1.5369923181
Br 9.2023796694,-1.5275302392,-0.2864792778
N -0.6042079235,1.4609611861,-2.2413860815
N -1.086413417,-1.4248105117,-2.0435401795
C -0.4453634434,2.3410206277,-3.0207130282
C -1.3264407103,-2.3955481104,-2.6823992748
S -0.2619988422,3.5468734464,-4.0877041149
S -1.6238411595,-3.7252420749,-3.5586557844

N3+Br-e

Charge = 0 Multiplicity = 2

Ru 1.2573690543,0.7233246802,-0.5266524614
N 0.3063752817,2.460427476,0.1061827303
C -1.0542318084,2.3986975454,0.1788321586
C -1.8058533459,3.5267613481,0.5072889859
C -1.1587956643,4.7366984455,0.7560778593
C 0.2354756703,4.7908079003,0.6653716113

C 0.9286656725,3.6328657139,0.3356108525
C -2.0008658086,5.923765502,1.1020710607
O -3.2080837855,5.890142801,1.1970390306
O -1.2644408133,7.0369604307,1.2989959686
N -0.7433228142,0.1200034498,-0.4975338037
C -1.2009777462,-1.1104212113,-0.7983674999
C -2.5429655245,-1.4566985523,-0.7146928745
C -3.4628002819,-0.4882171324,-0.3041815308
C -2.9977669306,0.7926721554,-0.0123440901
C -1.6379234551,1.0790605847,-0.1171413977
C -4.9370532367,-0.76865251,-0.1402781742
O -5.2282316908,-2.0245604041,-0.4453920595
O -5.703723027,0.0922704437,0.2425103955
N 1.5622383847,-0.1909396685,1.319200882
C 2.1973506225,-1.400192426,1.275385339
C 2.4780779802,-2.1071566917,2.4439448306
C 2.1114387642,-1.5774595405,3.6799285655
C 1.4659649579,-0.3366543263,3.7165835408
C 1.2149528023,0.3166119903,2.5185388122
C 2.4298283371,-2.3705207185,4.9062544985
O 2.9790945142,-3.4504714505,4.8870164955
O 2.0340521217,-1.7499078442,6.0368074757
N 2.1415355306,-1.0669351657,-1.093247299
C 2.4243423981,-1.4170957609,-2.3630457533
C 3.0963196403,-2.5913129972,-2.6801673811
C 3.4998836965,-3.4372917245,-1.6426305702

C 3.2181076602,-3.0719581384,-0.3268943639
C 2.5403340232,-1.8804018484,-0.0730107374
C 4.2295153371,-4.7227506743,-1.8703212114
O 4.4514666991,-4.963414055,-3.1781007988
O 4.5788293575,-5.4661194608,-0.9790513212
H -2.8871507026,3.492561785,0.5644324855
H 0.7737116445,5.7143761534,0.839791336
H 2.0072805916,3.6147362673,0.2382474445
H -1.8918471803,7.7545650781,1.5096929276
H -0.4539534974,-1.8284673849,-1.1155253138
H -2.8714834482,-2.4594252656,-0.9595184402
H -3.7204734303,1.5371446136,0.3009197573
H -6.2073385719,-2.223160448,-0.3027414506
H 2.9792957346,-3.0672662424,2.4204901586
H 1.1685332878,0.1126394021,4.6561233855
H 0.7266444376,1.2833109965,2.498624026
H 2.2798867981,-2.3338718097,6.7795353706
H 2.0998653866,-0.7175746698,-3.1233902017
H 3.3041338328,-2.8340612667,-3.7151083003
H 3.5425996623,-3.7264465261,0.4730754527
H 4.9304580651,-5.8123354489,-3.2318876413
N 1.0025893108,1.3726181095,-2.4049664758
N 3.107615659,1.4953531725,-0.3702040494
C 0.7810269247,1.7405267504,-3.5110745915
C 4.2247720592,1.8354868953,-0.1587914147
S 0.4934091677,2.2209513701,-5.0304226107

S 5.7396198359,2.3321856769,0.1301075177
Br -8.2069922285,-3.075974934,-0.068209021

N3+Br-z

Charge = 0 Multiplicity = 2

Ru 0.3830322842,-1.1049958513,-0.314070368
N 2.348430644,-0.9558875901,0.3672057817
C 2.9703624705,0.2305365034,0.1144077776
C 4.3041944179,0.4256583475,0.4774247705
C 5.0089705301,-0.6057984319,1.095021929
C 4.3630884004,-1.8235472931,1.3332879381
C 3.0345845284,-1.9564725735,0.9510277866
C 6.4359470794,-0.3539186982,1.4664626071
O 7.0097287523,0.6960935505,1.2747855633
O 7.0153651357,-1.4275162148,2.0427924935
N 0.8818613237,0.8316352123,-0.9109869459
C 0.0579622269,1.6872299753,-1.5339810766
C 0.4396041948,2.9946032571,-1.8541056466
C 1.7198795654,3.4159654302,-1.5168914499
C 2.5798246951,2.525931841,-0.8550292738
C 2.1444677881,1.2437385441,-0.561809571
C 2.2321636206,4.7878782947,-1.8085724937
O 1.3423003695,5.5411793215,-2.4839347593
O 3.3307669456,5.1827400835,-1.4763499337
N -0.5907381066,-0.2552122329,1.3337841667
C -1.9333180531,-0.1043976562,1.1987749579

C	-2.7029409999,0.4297468398,2.2369064317	H	-0.925848593,1.3266157271,-1.7920186791	N	0.9898022376,1.7826913433,-0.7545283981
C	-2.0865501028,0.8108132535,3.421945789	H	-0.2769732529,3.6514080636,-2.3288320977	C	1.8586732572,2.1405338097,-1.7232921523
C	-0.6955541154,0.6822247894,3.537819097	H	3.5715594798,2.8698155002,-0.5876211024	C	1.5512334186,3.0576076008,-2.714505869
C	0.0089542965,0.1491528502,2.4728772945	H	1.7564919044,6.4150742843,-2.614039127	C	0.2819806065,3.6519395454,-2.7106310557
C	-2.9442285887,1.3552464026,4.5169597529	H	-3.7718405121,0.5611846482,2.1370657605	C	-0.6217702898,3.2906443577,-1.7122444365
O	-4.1531763047,1.4102496845,4.4710701839	H	-0.1787289906,0.9843576096,4.4400658105	C	-0.2526079926,2.354697779,-0.7463167641
O	-2.2194794891,1.7742442859,5.578768287	H	1.0824378163,0.0136106577,2.5174105387	C	-0.1414061203,4.6597994918,-3.7192494584
N	-1.6009274783,-1.1038092823,-0.9500273713	H	-2.8606832647,2.1131352677,6.2317659764	O	0.8171701972,4.9051022835,-4.6476374486
C	-2.0273373529,-1.6014010694,-2.1272417555	H	-1.2568821231,-2.0034821829,-2.7732106099	O	-1.2198970369,5.2157798519,-3.731473164
C	-3.3672889909,-1.6052060602,-2.4865868595	H	-3.6731930266,-2.0154073035,-3.4409509642	N	0.8500123116,-1.1769748815,-0.2003990351
C	-4.3039346515,-1.0770708721,-1.5906888348	H	-4.5872811899,-0.1360056651,0.3069994013	C	1.8880701494,-1.9275425732,-0.6851885556
C	-3.8633316828,-0.5619178217,-0.3749798524	H	-7.0339462146,-1.4458355766,-3.2068356929	C	1.6576911281,-3.1108498185,-1.383732687
C	-2.5012653085,-0.5877658918,-0.0720234077	Br	-2.5029678274,2.899104957,-0.098716496	C	0.3508972226,-3.5505097394,-1.5966881429
C	-5.7710207161,-1.0443242732,-1.8772897866			C	-0.7072212053,-2.7818432468,-1.0975277267
O	-6.0642913192,-1.5046140915,-3.1132332263	N3+2Br-b		C	-0.411181752,-1.6122362177,-0.4108027258
O	-6.6082484895,-0.6566054007,-1.0926304907	Charge = -1 Multiplicity = 2		C	0.1537352714,-4.8196157951,-2.3513807392
N	1.1149846021,-1.802627132,-2.0281245828	Ru	1.4062661169,0.527925336,0.8330791169	O	1.0568351516,-5.4888365876,-2.8153080253
C	1.6238751447,-2.108424418,-3.0576740908	N	-0.5395899557,1.1021675931,1.2632073394	O	-1.1473532865,-5.1541839729,-2.4716928288
S	2.2888811134,-2.5308621752,-4.4668495717	C	-1.1384125877,1.9000090691,0.3340831217	N	3.2437261666,-0.1778665194,0.224808551
N	0.0669330891,-2.9005518468,0.4903455586	C	-2.5064000239,2.1589568948,0.3785258789	C	4.431715265,0.3948152108,0.515833959
C	-0.1829509399,-3.9094081507,1.0665342554	C	-3.2832895165,1.5699974647,1.3730938146	C	5.6434939661,-0.1773591076,0.159323114
S	-0.4913647201,-5.2852605677,1.8539007415	C	-2.6484570804,0.8129320676,2.3612744064	C	5.6384744931,-1.4011232153,-0.5236489128
H	4.8138273439,1.3614637292,0.2833325733	C	-1.275330943,0.6174509035,2.2823299633	C	4.4142333148,-2.0024642392,-0.8131406754
H	4.8803335712,-2.6523125408,1.8005776285	C	-4.7782258805,1.6517761972,1.2358023502	C	3.2272748562,-1.3790446729,-0.4279156493
H	2.4821097395,-2.8756087561,1.1025207213	O	-5.3136242661,2.370528724,0.4170210092	C	6.8818311649,-2.0976306461,-0.9504099899
H	7.9363304151,-1.1743439743,2.2441457757	O	-5.3955217019,0.810541268,2.0685634141	O	8.0052539543,-1.4290875372,-0.5947910189

O 6.9112752993,-3.1500828257,-1.5559875056
H -3.0075969059,2.7377432545,-0.3881237838
H -3.2242642868,0.3360782838,3.1446613862
H -0.7316285022,0.0157308477,3.000772038
H -6.2264439549,0.4722617473,1.6362079472
H 2.8326319436,1.6690603673,-1.6764358485
H 2.2866050891,3.3133279771,-3.4673271012
H -1.6015199233,3.7525338076,-1.6984423861
H 0.4388215766,5.5749656426,-5.2472168676
H 2.4745630272,-3.7077008117,-1.7712022563
H -1.7469913711,-3.0648305102,-1.2253019992
H -1.2155836565,-1.0078794468,-0.0110866557
H -1.1737977981,-5.9907137441,-2.9720953215
H 4.3739734874,1.3287909427,1.0614240474
H 6.5717522022,0.3163405392,0.4193226778
H 4.4111635916,-2.9549356141,-1.3289535234
H 8.7507278877,-1.9727272203,-0.9110103331
N 2.1781100081,2.1652391452,1.7780117182
N 1.6344578041,-0.6060988065,2.506969078
C 2.7082948182,3.1571361008,2.1451273486
C 1.8838634558,-1.3141171538,3.42248898
S 3.4649886248,4.5120472319,2.653287671
S 2.2013500697,-2.2964271945,4.683579524
Br -4.3585042876,-1.5867903551,-0.6726614659
Br -7.1501023162,-1.190999262,0.2859805262

N3+2Br-e

Charge = -1 Multiplicity = 2

Ru 2.0467407587,0.3861321138,-0.4576612273
N 1.8615600266,2.3289633513,0.2258530205
C 0.6031862218,2.8573016489,0.1890776373
C 0.3736504131,4.1870217094,0.5441364955
C 1.4433269375,4.9912239892,0.9362800902
C 2.7310164117,4.4409271207,0.9574695534
C 2.8962082485,3.1126478339,0.5928455566
C 1.1614971193,6.4072187867,1.3047850001
O 0.0579591294,6.9111483817,1.3076154419
O 2.2765164886,7.0817765655,1.6743400034
N -0.0081358016,0.6930950268,-0.6284354701
C -0.914058619,-0.2165835153,-1.0363928851
C -2.2797735832,0.0331030391,-1.0585693338
C -2.7419817361,1.2855917759,-0.6447942
C -1.8099574589,2.2374885595,-0.2390359256
C -0.4509241375,1.9260705107,-0.2416670999
C -4.2126852916,1.6245416349,-0.5676185179
O -4.9464033098,0.6658128364,-1.0951224224
O -4.591055726,2.6657065943,-0.0612162518
N 1.7983170649,-0.6058460663,1.3221740426
C 1.8901957108,-1.9724435573,1.2586543638
C 1.7631357763,-2.7599546241,2.4012588022
C 1.5344410511,-2.1612791882,3.6389902793
C 1.4379871658,-0.7636111019,3.6969142367

C 1.5779425964,-0.0354862793,2.5277403067
C 1.4015919923,-3.0372913252,4.83275523
O 1.4962631296,-4.2476009578,4.8118970793
O 1.1728657608,-2.3380074871,5.9699892999
N 2.1415146957,-1.5758550816,-1.0799907693
C 2.3324760151,-1.9731872204,-2.3552045625
C 2.4782183222,-3.3078391976,-2.7045569881
C 2.43458851,-4.279917896,-1.6965032317
C 2.2473049915,-3.8715150133,-0.3769893822
C 2.1038477104,-2.5145249469,-0.0885174158
C 2.5870197729,-5.7370687342,-1.965261969
O 2.7505196099,-6.0101043049,-3.2804496525
O 2.5650114988,-6.5991849492,-1.1110059771
H -0.6207872764,4.6152704183,0.5121513396
H 3.5904027444,5.0352379797,1.2423638524
H 3.8676536422,2.633589678,0.5736893554
H 1.9820664874,7.9852563324,1.8949050088
H -0.5130803727,-1.1745313217,-1.3453337759
H -2.9817525549,-0.7319561576,-1.3686526697
H -2.1790051907,3.2016682695,0.0913204466
H -5.9337025534,0.745079488,-0.8698407532
H 1.8344310338,-3.8398897888,2.3527540245
H 1.2605678346,-0.2544726625,4.63627505
H 1.5226272856,1.0459697575,2.5300611004
H 1.0967245721,-3.0001551103,6.6822366751
H 2.3757313133,-1.1751895614,-3.0864201622

H 2.6312835003,-3.5819851091,-3.7410787254
H 2.2217205743,-4.6234371188,0.4024019496
H 2.8381534692,-6.9794026842,-3.3464004566
N 2.2943396238,1.1463364864,-2.3300493708
N 4.0642160594,0.3166732023,-0.1624411872
C 2.4211395666,1.5847790363,-3.4224632406
C 5.2084154325,0.2037504638,0.1188166614
S 2.5899439222,2.1596513531,-4.9375019623
S 6.7885538858,0.0750648758,0.5024874058
Br -7.9855793865,0.3343122628,-0.3912458381
Br -6.6923789561,-2.2592279199,0.3102700052

N3+2Br-z

Charge = -1 Multiplicity = 2

Ru 1.2290101874,-0.9929440449,-0.3736677381
N 2.9700264818,-0.2480115339,0.4343953465
C 3.1921621612,1.0869007815,0.2435149259
C 4.3758374362,1.6860306676,0.6747813541
C 5.3525892468,0.915754571,1.3048565254
C 5.1187154024,-0.4547449451,1.4837003947
C 3.9235731633,-0.9939373373,1.0333860312
C 6.6003132186,1.5901864328,1.7509245885
O 6.8332530017,2.7749178791,1.6166199127
O 7.4761738415,0.7389175215,2.3392703054
N 1.0294923078,1.0240011699,-0.7842339756
C -0.0296844179,1.6134805047,-1.3712186006

C -0.0872566539,2.9777641323,-1.6311068496
C 1.0023386237,3.7766841539,-1.2753489948
C 2.1019505949,3.1754734649,-0.6588726329
C 2.096197323,1.8044888051,-0.4210212758
C 1.0442608279,5.2461354755,-1.5050020823
O -0.0509242646,5.7059021132,-2.149277895
O 1.9580979448,5.9706124584,-1.1605068314
N 0.0110434434,-0.8799791511,1.297318432
C -1.262549154,-1.3403833634,1.1319428264
C -2.1671216326,-1.364585224,2.1941142523
C -1.7718317173,-0.9080915651,3.4480605261
C -0.4704459573,-0.4138829535,3.6044109923
C 0.3794021537,-0.4219932839,2.5114936147
C -2.7533654891,-0.9667734467,4.564354291
O -3.8492108951,-1.4819017088,4.4958522758
O -2.2899849233,-0.3845596728,5.6995557332
N -0.5784411832,-1.655285495,-1.1320011571
C -0.7829901016,-2.0303366258,-2.4110681557
C -1.9935741423,-2.5455697855,-2.8489141021
C -3.0382399388,-2.6914520126,-1.9276773152
C -2.8296978204,-2.3034994491,-0.6064480637
C -1.5908096069,-1.785478048,-0.2295525703
C -4.365925599,-3.256795983,-2.2954923266
O -4.4820714959,-3.4951528438,-3.6254255232
O -5.258653973,-3.4933218055,-1.5090786083
N 2.2325038869,-1.1998126669,-2.1397458885

C 2.8232775062,-1.2437334918,-3.1636734309
S 3.6247013899,-1.3162544835,-4.585069457
N 1.6414885591,-2.9273963665,0.1473038223
C 1.8377573308,-4.0250778786,0.5419848301
S 2.1390539063,-5.5364191911,1.0853014009
H 4.5606496656,2.7429108404,0.526471
H 5.8560907376,-1.0924163313,1.9555327065
H 3.6930538379,-2.0481500924,1.1269197782
H 8.2501087494,1.2805184783,2.5821409317
H -0.8687652166,0.9762535468,-1.6137010926
H -0.9816835162,3.3960973031,-2.074671728
H 2.9410983406,3.7977455435,-0.3725454901
H 0.0655899841,6.6707302166,-2.2290239531
H -3.1815997701,-1.7178249994,2.0626139977
H -0.1267167993,-0.0369790103,4.5597249573
H 1.398565833,-0.0637173062,2.5895230998
H -3.0118410204,-0.4692573016,6.3499072594
H 0.0687418086,-1.9152345714,-3.0700195294
H -2.115604244,-2.8363665755,-3.8849126027
H -3.6418298419,-2.4009272125,0.1023752715
H -5.3805670187,-3.8531447382,-3.7511357607
Br -3.1294304568,1.5326637572,0.0931986968
Br -5.6673509552,3.0006155051,0.2584689318

N3+l-b

Charge = 0 Multiplicity = 2

Ru	-1.3102171747,0.0973012004,-0.7482228613	O	-4.5327197727,-3.9374696978,4.0469916265	H	-9.201390579,0.5168670543,-1.7605902911
N	0.7575347812,-0.0135264399,-0.5483871741	O	-2.38550059,-4.378242423,4.5949379314	I	9.119609024,-1.0966860522,-0.2008868047
C	1.3308693472,0.9498100535,0.2287869225	N	-3.379592176,0.2008784163,-0.8232096602	N	-1.0369846193,1.396419523,-2.2620972953
C	2.7112763746,0.9971359426,0.4141880723	C	-4.0842521874,0.9124469089,-1.7255866577	N	-1.4371084481,-1.4905973157,-1.9806399461
C	3.5248974987,0.0530454131,-0.2099012324	C	-5.470817308,0.8655112953,-1.7934729564	C	-0.8828434826,2.2534939399,-3.0669720114
C	2.9291792749,-0.9133779992,-1.0247161066	C	-6.1622888991,0.0447350465,-0.8962166806	C	-1.6192991754,-2.4864027952,-2.5989032262
C	1.5463009835,-0.9103366201,-1.1708547406	C	-5.4357565483,-0.7005552474,0.0313117767	S	-0.704843089,3.4297856174,-4.1692188702
C	5.0078063713,0.124001709,0.0411613116	C	-4.0442493031,-0.6116015768,0.0493521991	S	-1.8363997117,-3.8567078879,-3.4377705445
O	5.495700636,0.9672415143,0.7662261617	C	-7.6512596495,-0.082105117,-0.884021593		
O	5.6680196274,-0.8305107149,-0.6101710999	O	-8.2401188392,0.6674492753,-1.8385621747	N3+I-e	
N	-0.9324067452,1.6747993016,0.5572360855	O	-8.2640909427,-0.776583138,-0.1017586999	Charge = 0	Multiplicity = 2
C	-1.8585210814,2.5023302902,1.0815235986	H	3.1845187118,1.7487562573,1.0350172532	Ru	1.7340398165,0.595189642,-0.5491466066
C	-1.5379637564,3.5693292219,1.907271667	H	3.5311596768,-1.6543628673,-1.5366707341	N	1.061436776,2.4638560386,0.0592105427
C	-0.1910203007,3.8004134622,2.2091458365	H	1.0303476447,-1.6290694168,-1.7960459633	C	-0.2909500964,2.6005956885,0.1715467013
C	0.7731436686,2.9514057802,1.6690203307	H	6.6438593726,-0.7668490091,-0.413148713	C	-0.8629408529,3.8319817335,0.4903718415
C	0.385418024,1.8952472612,0.8440899542	H	-2.885694027,2.2923302008,0.8089257403	C	-0.0421901874,4.9421969161,0.6864957336
C	0.2674945743,4.9207807065,3.0847063278	H	-2.3179236387,4.2098790009,2.3001924525	C	1.3418876875,4.7933813756,0.552843256
O	-0.7577014383,5.6798749526,3.5288225622	H	1.815635362,3.1354231309,1.8989027902	C	1.8517335583,3.5402863298,0.2366077036
O	1.4271062303,5.1276868097,3.3679289883	H	-0.3646961932,6.38307515,4.0801664001	C	-0.6947861874,6.2446744463,1.0242420702
N	-1.8401596488,-1.164227824,0.8139835659	H	-4.7329566738,-2.3642692438,2.1148135058	O	-1.8905464272,6.3859989057,1.1598619023
C	-3.1836850724,-1.3588113606,0.9799080075	H	-0.680976597,-3.1834482317,3.2561900005	O	0.1979489329,7.2464191867,1.165870819
C	-3.6704508695,-2.2058896022,1.974716613	H	0.0671357576,-1.6451963483,1.4425730471	N	-0.326706263,0.2825467623,-0.4370230639
C	-2.7808082268,-2.8747441522,2.8136712469	H	-2.843090157,-4.9444600665,5.2452061419	C	-0.9635112414,-0.8760554018,-0.6932726918
C	-1.4070921985,-2.6766584842,2.6324183013	H	-3.4954756826,1.5164816856,-2.4050478087	C	-2.3402728534,-1.0197945187,-0.5863649782
C	-0.9859611466,-1.8189403659,1.6271049113	H	-5.9967772581,1.4508023875,-2.537799646	C	-3.1024128208,0.0851921531,-0.1970865724
C	-3.3456245424,-3.7718541444,3.8653892005	H	-5.975008999,-1.344345056,0.7157051709	C	-2.4508906015,1.2906421527,0.0560236351

C	-1.0652430305,1.3720542609,-0.0729713085	H	-0.3332356363,-1.7035039419,-0.9964109686	C	5.1823257263,-0.3306359107,1.1471090781
C	-4.598151472,0.0339852229,-0.0254093049	H	-2.8137014099,-1.9701119706,-0.8009485271	C	4.6331732312,-1.6037972904,1.3325364943
O	-5.0827858162,-1.1731585023,-0.303770901	H	-3.0508467582,2.1425488027,0.3538461426	C	3.323107522,-1.8280595876,0.9296978356
O	-5.2352051852,1.0022207025,0.3354585368	H	-6.0728857292,-1.1920109653,-0.1727864276	C	6.5819820556,0.0190067365,1.5417408193
N	2.0016433207,-0.2889911027,1.3131785373	H	3.0890333088,-3.2869179664,2.4645634073	O	7.0717606905,1.1178565309,1.3955496588
C	2.4730375738,-1.5717586493,1.2896015126	H	1.8177555134,0.176642158,4.6497281281	O	7.2413612606,-1.0265704822,2.0827504056
C	2.7176822199,-2.2692902235,2.4718594858	H	1.4240417257,1.3211543633,2.4685361945	N	0.9611472384,0.8548463504,-0.8279673951
C	2.4843843266,-1.654770457,3.7009929447	H	2.7134304401,-2.3209485298,6.8167671946	C	0.073682723,1.675560669,-1.4137514485
C	2.0068845197,-0.3395827598,3.7165427985	H	2.2525163963,-1.0257513599,-3.1227792066	C	0.3542936292,3.0170229928,-1.6837303483
C	1.7827557173,0.2997768377,2.5058843998	H	3.1498118923,-3.2977712583,-3.6845921152	C	1.6044974739,3.5194672989,-1.3352934067
C	2.7578181615,-2.4405537345,4.9419232118	H	3.4676741585,-4.0791626354,0.5207701932	C	2.5273234964,2.6709335408,-0.7087721475
O	3.1607526159,-3.5835796617,4.942699453	H	4.4151953897,-6.4392430414,-3.1581549787	C	2.1897944714,1.3480438413,-0.4641734769
O	2.5060451004,-1.7347039372,6.0642694482	N	1.4914906419,1.2171134159,-2.4448767005	C	2.015509598,4.9335656102,-1.5811684347
N	2.3437797558,-1.3134750317,-1.0846388196	N	3.6827606828,1.1101232352,-0.5043079973	O	1.0682755723,5.6435078719,-2.2250199061
C	2.5196223929,-1.7374102765,-2.3513140233	C	1.2804010982,1.5648806057,-3.5588118524	O	3.0854696105,5.3943283166,-1.240763708
C	3.0218480225,-2.9975929419,-2.6517813659	C	4.844306338,1.3020299892,-0.3593596765	N	-0.4508717715,-0.5394420052,1.3195619114
C	3.3625352174,-3.8551399174,-1.6009140401	S	0.9972460189,2.015809628,-5.0900946668	C	-1.8029534188,-0.5582113292,1.1743036532
C	3.1918996716,-3.4146023183,-0.2890816158	S	6.4269749695,1.5960059586,-0.1614790437	C	-2.6439730937,-0.2148898178,2.2361624152
C	2.6846966829,-2.1375329188,-0.0521964963	I	-8.4866320075,-1.7873928026,0.0285390231	C	-2.0928682152,0.1484357301,3.4601054396
C	3.9116038079,-5.2298367961,-1.8110441905			C	-0.6993138569,0.1955913571,3.5895478155
O	4.0480169988,-5.5357134359,-3.1172557931	N3+l-z		C	0.0787684344,-0.1522433494,2.497738145
O	4.2034151964,-5.9850359747,-0.9088797485	Charge = 0 Multiplicity = 2		C	-3.0244853202,0.4836320191,4.5788144473
H	-1.9354744554,3.9551991825,0.5805450976	Ru	0.6365697959,-1.1478064356,-0.3606516799	O	-4.2296680454,0.3858558235,4.5112306456
H	2.0118219826,5.6342706412,0.6841151675	N	2.5641986958,-0.8639855945,0.374771628	O	-2.3706179629,0.9012522292,5.6856059718
H	2.9128046338,3.3652473724,0.1070659327	C	3.0913207336,0.3773656147,0.1767027914	N	-1.3236574996,-1.3050212603,-1.0483947557
H	-0.3141844329,8.0504517737,1.3760063093	C	4.4020755054,0.664643257,0.5614313327	C	-1.673151386,-1.7323715496,-2.2767476583

C -2.9992711772,-1.8633300812,-2.6659910817
C -4.0039628068,-1.543739239,-1.7466134029
C -3.6431041776,-1.1013135044,-0.4763152665
C -2.2920739864,-0.9930907168,-0.1455881838
C -5.4611296132,-1.6592332292,-2.0617348191
O -5.6831717945,-2.0295363983,-3.3414828937
O -6.346566908,-1.4507380433,-1.2620103008
N 1.472855674,-1.6594809284,-2.0978706635
C 2.0155798779,-1.8660394663,-3.1339255631
S 2.7312442708,-2.1565929208,-4.5537547287
N 0.4878585936,-3.0283964533,0.2966874853
C 0.3376497002,-4.1062642787,0.7724197902
S 0.1625606969,-5.5735248192,1.4281089445
H 4.8369099975,1.6447957879,0.4084854983
H 5.2113594757,-2.4062504283,1.7736853398
H 2.8457214463,-2.7944754449,1.0367681539
H 8.138098545,-0.7091312144,2.3015867797
H -0.8822069606,1.2505096919,-1.6831490275
H -0.4076014493,3.6373626055,-2.1374513353
H 3.4930691835,3.0752714281,-0.4307088017
H 1.4173123325,6.5489296587,-2.3280872385
H -3.7206333651,-0.2185264396,2.1291002309
H -0.2333815544,0.4894016035,4.5218576229
H 1.1604313124,-0.1486717644,2.552892526
H -3.0557539548,1.0985353509,6.3520540336
H -0.8519633815,-1.9739381405,-2.9400208649

H -3.2409105002,-2.2113973249,-3.662644983
H -4.4227568495,-0.8383605206,0.226751325
H -6.651698644,-2.0779286194,-3.4517415719
I -2.8503808452,2.775880327,0.0833623284

N3+2I-b

Charge = -1 Multiplicity = 2

Ru 1.9229540281,0.550578511,0.8187873436
N -0.003227737,1.1930918219,1.2263061843
C -0.5652808981,2.013802942,0.2935108708
C -1.9077059833,2.378613105,0.3675293668
C -2.700197164,1.8726607208,1.3947738678
C -2.1025996473,1.0758930379,2.3747903937
C -0.7512041297,0.7742848233,2.2657567736
C -4.1801437981,2.1187332724,1.3271461646
O -4.6810979792,2.8762986297,0.5228406878
O -4.848160854,1.3513674064,2.1966832771
N 1.5421898935,1.7576737886,-0.8111905942
C 2.4117431584,2.0343933922,-1.8061482089
C 2.1327863441,2.9238833892,-2.8300159984
C 0.892799313,3.5772438125,-2.8341165482
C -0.0121334541,3.2988535615,-1.8108927785
C 0.3269937004,2.3863975025,-0.8119398071
C 0.5015401293,4.5626516043,-3.8772690268
O 1.4551448467,4.7229845573,-4.829056932
O -0.5489768757,5.1695475822,-3.8964169487

N 1.3513200471,-1.1772689952,-0.1586931857
C 2.3806565649,-1.9684278727,-0.595923627
C 2.1365592329,-3.1744273667,-1.2495910247
C 0.8243657777,-3.5955353497,-1.4656503188
C -0.224578275,-2.7838282984,-1.0173173598
C 0.0844889974,-1.5935999927,-0.3742017926
C 0.611989387,-4.8905076966,-2.1702254627
O 1.5073328945,-5.5956848061,-2.5941210891
O -0.6939667662,-5.2054158432,-2.2944734195
N 3.755277365,-0.2066488279,0.2568129961
C 4.9494177183,0.3583043466,0.5372298232
C 6.1553834103,-0.2511213786,0.2256374664
C 6.1373075258,-1.5051999915,-0.3995431492
C 4.9066133765,-2.0974812291,-0.6796979858
C 3.7261186431,-1.4354571823,-0.3417610191
C 7.3736788797,-2.2430713285,-0.7744821441
O 8.503864161,-1.5780313879,-0.4344689588
O 7.3922704945,-3.3219564697,-1.3319935556
H -2.3804143115,2.9895209165,-0.3919902723
H -2.6900169545,0.6627727995,3.1851535715
H -0.2370831036,0.1497939637,2.9864782325
H -5.7654100585,1.1995458339,1.8597458045
H 3.3630232539,1.5192458978,-1.753775859
H 2.8676563209,3.1135873522,-3.6025610307
H -0.9699941206,3.8044913927,-1.8058516772
H 1.0990360952,5.3849912232,-5.4505715818

H	2.9467470762,-3.8027538655,-1.5994273599	C	2.2172947124,6.3528076284,1.4482450419	C	2.2215570214,-2.5953305431,-0.1580232913
H	-1.2679840558,-3.0472400386,-1.1553310045	O	1.1916356266,6.9957812318,1.3651367934	C	2.4639941682,-5.7862718817,-2.1321618238
H	-0.7136415026,-0.9544166345,-0.0172270147	O	3.3788297249,6.8821970225,1.9018215609	O	2.6592543697,-6.0314812113,-3.4487045976
H	-0.7291341709,-6.0605760679,-2.7617354267	N	0.4977863006,0.8491284558,-0.677008145	O	2.3229100135,-6.6697192867,-1.3118034346
H	4.9020709193,1.3175882987,1.037905179	C	-0.4877900115,0.0505391749,-1.1305932723	H	0.2940793085,4.8097842814,0.4852093924
H	7.0887969703,0.2378281314,0.475840214	C	-1.8100258088,0.4624675463,-1.2346193457	H	4.4555692895,4.6892577106,1.5364359948
H	4.8933594892,-3.0729246101,-1.1504228138	C	-2.1349845151,1.7696264755,-0.8598659351	H	4.4867302546,2.2844652572,0.8279978024
H	9.2437734784,-2.1481182411,-0.7151713004	C	-1.1226247494,2.6027909562,-0.3905820082	H	3.1840435278,7.8150090547,2.1103341041
I	-7.0705140161,-0.6912992131,0.4754064649	C	0.185439107,2.1270637036,-0.3082771846	H	-0.1917242954,-0.9541409549,-1.4074937051
N	2.7118584208,2.202690996,1.7172041301	C	-3.5525728911,2.2751159171,-0.8672002416	H	-2.583918016,-0.2239882254,-1.5583263627
N	2.1175435227,-0.5338941354,2.5267285032	O	-4.3460348524,1.462449892,-1.5542921706	H	-1.3879350626,3.604624254,-0.0734479965
C	3.255355662,3.1974662907,2.0565677126	O	-3.873872845,3.2990500972,-0.2952539263	H	-5.3030870629,1.5716584198,-1.2955397769
C	2.3545654677,-1.2315068595,3.4536867224	N	2.0399902064,-0.714191867,1.3093783945	H	1.6857935569,-3.9661920179,2.2140087909
S	4.0273835967,4.555793643,2.5298899477	C	1.9941252647,-2.0794058883,1.1973550488	H	1.3431968285,-0.4173999984,4.5986660098
S	2.6531832626,-2.1980342384,4.7311341479	C	1.722802609,-2.8869698905,2.3002984035	H	1.8616183424,0.9174372065,2.5624823603
I	-4.0705607367,-1.3476335175,-0.8698088139	C	1.484722534,-2.3082957219,3.5456587444	H	0.7707212872,-3.1956175934,6.5223474281
		C	1.5253995299,-0.9111574571,3.6520884103	H	2.768229269,-1.1924802226,-3.0884187795
N3+2I-e		C	1.8075496765,-0.1634397221,2.5213002092	H	2.8071110461,-3.5893468236,-3.8220880545
Charge = -1 Multiplicity = 2		C	1.1965205437,-3.2046224728,4.6968252854	H	2.1002854858,-4.7202125137,0.2574136708
Ru	2.4904270025,0.3059416216,-0.4160895015	O	1.1735685566,-4.4169000882,4.6357574063	H	2.6538459107,-7.0020769715,-3.5458456457
N	2.4902483517,2.2359812522,0.3252746996	O	0.9595036511,-2.5222549178,5.8423362133	N	2.9180489469,1.1011966603,-2.2410753247
C	1.3122280582,2.9169836678,0.2099808242	N	2.4031604595,-1.6330880016,-1.110155027	N	4.4706539666,-0.004157312,-0.0288461701
C	1.2226078907,4.259853495,0.5786362199	C	2.6103467848,-2.0053526574,-2.3902627649	C	3.1843686373,1.5666953828,-3.2964741951
C	2.3498745498,4.9185165533,1.068016906	C	2.6354523152,-3.3355888689,-2.7833268242	C	5.5782474799,-0.2354413514,0.3184130503
C	3.5542167307,4.2114004765,1.1730710732	C	2.4469249192,-4.3308460191,-1.8155924457	S	3.535084412,2.1836766713,-4.7634121423
C	3.5819604425,2.8787812965,0.788801003	C	2.2398489713,-3.949554725,-0.4909392895	S	7.1106753395,-0.5311050169,0.7938041179

I -7.4062852148,0.5914053007,-0.34706066
I -5.0632615627,-1.7380584206,0.3759349975

N3+2I-z

Charge = -1 Multiplicity = 2

Ru 1.8904457601,-0.8704982649,-0.3747453643
N 3.4482859162,0.1955344474,0.4517206992
C 3.4082071852,1.548828997,0.2649347216
C 4.4552685912,2.3641643839,0.6949889341
C 5.56449255,1.7949544122,1.3190893954
C 5.5995905919,0.4047825398,1.4950210317
C 4.5291438751,-0.3538301697,1.0467539267
C 6.6625050109,2.6962140323,1.7604222317
O 6.6609144185,3.9039287427,1.6306554808
O 7.6899432466,2.0276538393,2.3386192116
N 1.3032195979,1.0716602507,-0.7732655711
C 0.1501641953,1.4481121563,-1.3594595844
C -0.1743411234,2.7763426037,-1.6077099429
C 0.7369281474,3.7706725258,-1.2406395177
C 1.9314244204,3.3907199957,-0.6250839968
C 2.1948511443,2.0430818547,-0.3987875933
C 0.4886105566,5.2222859337,-1.4556272228
O -0.676100533,5.4628693801,-2.0961446833
O 1.2429600429,6.1083001981,-1.1032248045
N 0.6605652893,-1.018297372,1.2836661966
C -0.4906088855,-1.72933244,1.1033416614

C -1.3749789942,-1.9555956456,2.158690141
C -1.0873995781,-1.446227458,3.4221454855
C 0.0822596213,-0.6950079949,3.5934235608
C 0.920471705,-0.5110797897,2.5064726166
C -2.03887033,-1.72671541,4.5314106933
O -3.0068791701,-2.45187523,4.4442171233
O -1.7076728274,-1.0838041555,5.6794408224
N 0.2542351774,-1.8657884541,-1.1601255961
C 0.1310635229,-2.2480508913,-2.4474869287
C -0.9556815795,-2.979281935,-2.9034124813
C -1.955172439,-3.3439284559,-1.9928231871
C -1.8306780913,-2.9493388223,-0.6627883605
C -0.7163381403,-2.2092625031,-0.2673276798
C -3.1481651954,-4.1479293993,-2.3798826237
O -3.2180864141,-4.3690383272,-3.7154522001
O -3.9779670297,-4.5692907294,-1.6022455357
N 2.9321058769,-0.8633275677,-2.1287966749
C 3.5269555748,-0.7815815342,-3.1483084939
S 4.3363485169,-0.6842459305,-4.562616091
N 2.6688005256,-2.6883075064,0.1446187873
C 3.1023665018,-3.7103526229,0.5531652762
S 3.7236547611,-5.1042000281,1.1353333004
H 4.4329942263,3.4370975466,0.548129349
H 6.4480383482,-0.0802103757,1.9617670545
H 4.5081835576,-1.432868561,1.1374595565
H 8.3477389705,2.7065410352,2.5788928383

H -0.5431869486,0.6581494271,-1.6150136555
H -1.1322482928,3.0150204814,-2.0520959638
H 2.6316830831,4.1626486725,-0.3297347252
H -0.7546868155,6.4322855739,-2.1669068026
H -2.291061363,-2.5144424235,2.0172485984
H 0.3368899383,-0.2691843855,4.5560530234
H 1.8431489998,0.0488906197,2.5980770939
H -2.3980422163,-1.3255555656,6.3246315558
H 0.9467987381,-1.9568840559,-3.097877095
H -1.0163445768,-3.2665609681,-3.9458008813
H -2.6093464562,-3.2208784104,0.0382775577
H -4.0321199336,-4.8878157662,-3.8554938107
I -3.2135136259,0.8556183116,0.0615876821
I -6.3724844634,1.8863570401,0.1937505519

N3+At-b

Charge = 0 Multiplicity = 2

Ru -2.0036864253,0.0972710054,-0.7329968012
N 0.0623567825,0.0300438148,-0.5183943004
C 0.6121973156,1.0190110313,0.2434656117
C 1.9914818402,1.104121671,0.425261543
C 2.8273084595,0.1713745479,-0.1865227366
C 2.2547831338,-0.823330587,-0.9841081989
C 0.8722389113,-0.8571904113,-1.1274025189
C 4.3075999537,0.2879059106,0.0535994246
O 4.7827350967,1.1539647214,0.7590327424

O 4.9918944913,-0.6637486418,-0.5829813935
N -1.6678462506,1.6957930519,0.5541373506
C -2.6146271921,2.5077205427,1.066198775
C -2.3218306174,3.5904710551,1.8815879983
C -0.9817299907,3.855820085,2.1864557854
C 0.0036777313,3.0230719877,1.6593792847
C -0.3565046956,1.9497932432,0.8442939624
C -0.5524648019,4.9949177821,3.0518758578
O -1.5960037008,5.7367893695,3.4826255206
O 0.6008547187,5.2304061391,3.3393475643
N -2.5254737865,-1.1580403392,0.8347429086
C -3.8665395589,-1.3801131042,0.9863953617
C -4.3474880506,-2.2280677736,1.9833437015
C -3.4543498442,-2.8698274554,2.8395337354
C -2.0829304507,-2.6434993292,2.6732556742
C -1.6678488686,-1.7864844674,1.6650183503
C -4.0126276609,-3.7689604004,3.8925256209
O -5.1980634658,-3.9564987384,4.0640608929
O -3.0489573688,-4.3472839042,4.6405270983
N -4.0728880876,0.1598780148,-0.8316130789
C -4.78055127,0.8478132781,-1.7498341159
C -6.1644990873,0.768150329,-1.8369945158
C -6.8497522029,-0.0610977736,-0.9426344882
C -6.1198274768,-0.781706305,0.0015949709
C -4.7310998698,-0.6603874172,0.0384573672
C -8.3351785366,-0.2228320892,-0.95136392

O -8.9271682924,0.5029630748,-1.9224058785
O -8.9438513995,-0.9250270403,-0.1726094603
H 2.445766789,1.878943307,1.0314501456
H 2.8733486829,-1.5568905809,-1.486793492
H 0.3731325893,-1.5975333358,-1.7410008083
H 5.9607139803,-0.5606182866,-0.3935824788
H -3.635633616,2.2710374091,0.7923779146
H -3.117920413,4.2169953365,2.264660487
H 1.0406101852,3.2330660549,1.8921367305
H -1.220686272,6.4539777068,4.0281597365
H -5.4080272513,-2.4078411063,2.111956918
H -1.3539984501,-3.1284158556,3.310961256
H -0.6164992118,-1.591469446,1.4921188449
H -3.5033064633,-4.9154934352,5.2912651564
H -4.1957889132,1.4589680323,-2.4263907704
H -6.6930496891,1.334703347,-2.5938551689
H -6.6538767521,-1.4326407543,0.683286409
H -9.8854786702,0.3292920956,-1.8575755585
At 8.6120488941,-0.7189540115,-0.1263353666
N -1.7395232308,1.3837143095,-2.2627507193
N -2.0895180179,-1.5084996829,-1.9503874947
C -1.5927884926,2.2336827663,-3.0761891749
C -2.2560415951,-2.5108652369,-2.5620587788
S -1.4240418823,3.3988369797,-4.192865579
S -2.4519690432,-3.8853750449,-3.4009179662

N3+At-e

Charge = 0 Multiplicity = 2

Ru 2.4192915914,0.5433766875,-0.5488714467
N 1.8665958854,2.4487800133,0.0577470833
C 0.5247262133,2.6709037541,0.1666808157
C 0.0303841035,3.9358242842,0.4838215525
C 0.9183457135,4.9924225765,0.682641433
C 2.2908459634,4.7565998584,0.5529106765
C 2.7221015065,3.4743230966,0.2376448848
C 0.3479357722,6.3327701442,1.0186037445
O -0.8370814829,6.5494122036,1.1509873188
O 1.3009645517,7.2774384127,1.1615328168
N 0.3465851378,0.3573512831,-0.4346008858
C -0.3627988279,-0.7600687289,-0.6868149747
C -1.7458804217,-0.8161658409,-0.5837394323
C -2.4385050317,0.3371780841,-0.2034837134
C -1.7126415386,1.500049426,0.0459683484
C -0.324028533,1.4929738223,-0.0775223158
C -3.933172284,0.3841439078,-0.0418858434
O -4.4971104333,-0.7947126581,-0.3089994205
O -4.5148990112,1.3927568857,0.2999099035
N 2.6448599384,-0.3474382065,1.3125972482
C 3.0437497345,-1.6554124184,1.2922399233
C 3.2543867481,-2.3621674704,2.4755126595
C 3.061565464,-1.732741735,3.7040162212
C 2.6589464725,-0.3923053358,3.7169764695

C 2.4654177899,0.2551867948,2.5058659565
C 3.2960540281,-2.528614549,4.9455363241
O 3.6317657226,-3.6933834884,4.9492186203
O 3.0906921016,-1.8063951185,6.0674969956
N 2.9160688426,-1.3966488313,-1.0813203127
C 3.0631472837,-1.8335665975,-2.3477804097
C 3.4956221947,-3.1193823936,-2.6467331347
C 3.7945759548,-3.9916554609,-1.5949522366
C 3.6540685675,-3.5389365788,-0.2838477367
C 3.2176098112,-2.235724401,-0.0482114589
C 4.2680303925,-5.3938542452,-1.8037752456
O 4.3826991613,-5.7100119541,-3.1099821869
O 4.5194023325,-6.1635004815,-0.9014308433
H -1.0325164212,4.1263807313,0.5707206049
H 3.0120038759,5.553673973,0.686066046
H 3.770457135,3.2332583263,0.1104976853
H 0.8387734526,8.1117001714,1.3694141734
H 0.2132594792,-1.6282248198,-0.9843426285
H -2.2762291646,-1.7365275517,-0.7956193527
H -2.2570996409,2.3912361735,0.3350014567
H -5.4813881622,-0.734242979,-0.1831972211
H 3.5688618999,-3.3987750318,2.4689185657
H 2.5041938355,0.1367660408,4.6493141229
H 2.1651967969,1.2952535501,2.4681436322
H 3.2685727919,-2.4022655771,6.8199129264
H 2.8316650526,-1.1103876681,-3.1200589307

H 3.6031009823,-3.4282978448,-3.6792899647
H 3.8979204149,-4.2147906755,0.526914229
H 4.6999751256,-6.6322880005,-3.1490091294
N 2.2059548034,1.1736301302,-2.4479632566
N 4.3969065936,0.9424774706,-0.5188669459
C 2.0043069491,1.5259939272,-3.5620419892
C 5.5686562427,1.063843938,-0.3810823098
S 1.7332460878,1.9828734871,-5.0944587006
S 7.1679824632,1.2610413135,-0.1928387551
At -8.0991317394,-1.0376856524,0.030251898

N3+At-z

Charge = 0 Multiplicity = 2

Ru 1.0383183416,-1.2088402295,-0.3531975627
N 2.8877621927,-0.6609489266,0.4302372238
C 3.2481722374,0.638343574,0.228881524
C 4.5065290412,1.0979312865,0.6209645798
C 5.4081429923,0.2170849924,1.2150511492
C 5.0299051023,-1.1164228031,1.4053895528
C 3.7632733372,-1.5130982195,0.9972935651
C 6.7474043198,0.7494159006,1.6131982391
O 7.0854881502,1.9049786095,1.4745220362
O 7.5351403396,-0.1972709896,2.1654357771
N 1.0779054856,0.8235083856,-0.7849436494
C 0.0866801072,1.5236750869,-1.3639730582
C 0.1869088796,2.8895017688,-1.6347930557

C 1.3632023723,3.5531802363,-1.2929022943
C 2.3882158215,2.8339541217,-0.6656683877
C 2.229270905,1.4775593778,-0.4197657668
C 1.5847266444,5.0071305949,-1.5440637289
O 0.5485945272,5.5854412207,-2.1840481058
O 2.5864046979,5.6058863909,-1.2105550979
N -0.1729959287,-0.823917118,1.304992035
C -1.4964145984,-1.0963348036,1.1327109407
C -2.40369833,-0.9424140311,2.1820811293
C -1.9547169541,-0.4964993347,3.4211822173
C -0.5993625566,-0.1867588963,3.5790217201
C 0.2510645502,-0.3650788964,2.4987826647
C -2.953035485,-0.3638343473,4.5251766425
O -4.1185630416,-0.6775192424,4.4268496168
O -2.4088228418,0.1453255976,5.6522022659
N -0.8498797054,-1.6548938044,-1.1018020774
C -1.0970054093,-2.081476838,-2.3549146001
C -2.3714793583,-2.430700033,-2.7820136906
C -3.432332857,-2.3408602639,-1.8754769526
C -3.1773560621,-1.9017402719,-0.5780437337
C -1.8750010841,-1.5667064707,-0.2100902945
C -4.8395026083,-2.7009857699,-2.2299799484
O -4.9684639411,-3.0591482641,-3.5255955181
O -5.7617214578,-2.683857447,-1.4448057199
N 1.9943027997,-1.5601460137,-2.0738750136
C 2.6058871515,-1.6697483723,-3.08559336

S	3.4174431371,-1.8274462376,-4.4758970413	C	-0.234670418,2.1261546796,-0.2125594037	N	-4.4860446379,-0.2275868816,-0.3123293131
N	1.1591826403,-3.1101323728,0.2626701173	C	1.0895361473,2.5552684211,-0.2682793522	C	-5.6911108292,0.3109259665,-0.597417363
C	1.1464174044,-4.2132276299,0.7018814912	C	1.9048914085,2.1331673675,-1.3156104328	C	-6.8838141259,-0.3413690603,-0.3229125998
S	1.1568674794,-5.7113111904,1.3121948615	C	1.3482658224,1.3428010415,-2.3248119656	C	-6.8395960973,-1.6109694579,0.2683823784
H	4.8091466009,2.1265119421,0.4669793015	C	0.0126180493,0.9720335873,-2.2298539063	C	-5.5968889564,-2.1757802493,0.5523352222
H	5.7063076567,-1.833884625,1.8532388635	C	3.3687752377,2.4589057175,-1.2397177577	C	-4.4308541279,-1.4720168085,0.2508696504
H	3.416993227,-2.5336071438,1.1061599262	O	3.8278427425,3.2160980579,-0.4099887128	C	-8.060056781,-2.3940961065,0.6021584394
H	8.3790024332,0.2383480997,2.3910389793	O	4.0738945402,1.7844574702,-2.1545267947	O	-9.2030189398,-1.7541632783,0.257475244
H	-0.8054069836,0.9749547563,-1.6313462272	N	-2.339830155,1.7490598686,0.8657614114	O	-8.0555072215,-3.4887162301,1.1282103194
H	-0.648926861,3.4036259696,-2.0914503003	C	-3.2222359176,1.9508931263,1.8676961141	H	1.5323637497,3.1588435865,0.5148729384
H	3.2927273486,3.3614746176,-0.3880379991	C	-2.9777464446,2.8027787887,2.9318511404	H	1.9554403548,0.9886498691,-3.1485094819
H	0.776742052,6.5280647331,-2.2917184667	C	-1.7611494296,3.4970757094,2.9724388099	H	-0.4719849729,0.3517844737,-2.9743890947
H	-3.4565025715,-1.1590396501,2.0560917573	C	-0.8430236376,3.2950736239,1.9430762672	H	5.012292931,1.714380204,-1.8512681678
H	-0.214344201,0.17630141,4.5237720042	C	-1.1465247841,2.4177930012,0.9020239569	H	-4.156405638,1.4082193074,1.7885379763
H	1.3112247977,-0.1576750807,2.5780002994	C	-1.4069077881,4.447629262,4.0602731604	H	-3.7223962177,2.9325988672,3.7074565083
H	-3.130776598,0.2009889993,6.3065998844	O	-2.3708952192,4.5378979707,5.0105948135	H	0.0974625737,3.8318808454,1.9667946332
H	-0.2344260485,-2.1430528727,-3.0068903658	O	-0.3761836398,5.0856474357,4.1117788472	H	-2.0396380434,5.1834870396,5.6624463193
H	-2.529285575,-2.7704729861,-3.7981259803	N	-2.0613641043,-1.1485663012,0.1010464037	H	-3.6022986856,-3.8558396692,1.4459920037
H	-4.0027640101,-1.8242918504,0.117774518	C	-3.074365325,-1.9775390796,0.5045659327	H	0.5942677827,-2.9996583489,1.0398786123
H	-5.9102144068,-3.2770325446,-3.6607153474	C	-2.8053827846,-3.1977753392,1.1211119076	H	-0.0056073122,-0.8732745817,-0.0302747332
At	-3.0396263645,2.334135969,0.0944652357	C	-1.4849331316,-3.595778939,1.3301524784	H	0.1231591575,-6.0630847209,2.554336078
		C	-0.4531172587,-2.7477420567,0.9108206185	H	-5.6634031047,1.2851157743,-1.0700152952
		C	-0.7865935765,-1.5435534326,0.3066750426	H	-7.8268458071,0.1275062944,-0.5755385581
		C	-1.2450936032,-4.9071928824,1.9947907811	H	-5.5629070362,-3.1634245642,0.9958289914
		O	-2.1258665894,-5.6465649869,2.3894018918	H	-9.9309719592,-2.353086343,0.5078905912
		O	0.0674516665,-5.1937438996,2.1160269956	At	6.564894095,-0.1653330626,-0.5191081288

N3+2At-b

Charge = -1 Multiplicity = 2

Ru	-2.6678450562,0.6005226418,-0.819561794
N	-0.7562436208,1.3185541695,-1.1794598468

N -3.4922229065,2.266150538,-1.6663204236
N -2.8076429682,-0.4212573868,-2.5744015472
C -4.0697094568,3.2477269319,-1.9873604386
C -3.0003273828,-1.0986860045,-3.5263121058
S -4.8855536731,4.5885217678,-2.4361090296
S -3.2395439195,-2.033617601,-4.8390640262
At 3.5021177563,-1.2585693627,0.8100642634

N3+2At-e

Charge = -1 Multiplicity = 2

Ru 3.2503733955,0.2623016015,-0.4069422
N 3.3573803834,2.180948921,0.3555402088
C 2.2269084439,2.9361424862,0.2252741886
C 2.2148219167,4.2787640348,0.6057327773
C 3.3719944191,4.8608125939,1.1216847332
C 4.5274797163,4.0781733323,1.2408233661
C 4.4789029951,2.7498597627,0.8441803166
C 3.3230769428,6.2972219095,1.5128276689
O 2.3412303362,7.0041272323,1.4185330979
O 4.5078481197,6.7493225141,1.9895238997
N 1.3070896334,0.9394603006,-0.7216398947
C 0.28599665,0.2142189792,-1.2168857511
C -1.0080086261,0.7057842763,-1.3320047014
C -1.2641119247,2.0170995814,-0.9199715252
C -0.2131903293,2.7776416781,-0.4136467547
C 1.0640155508,2.2250916766,-0.3263368778

C -2.6528885917,2.593745237,-0.916817051
O -3.4881702188,1.8313729893,-1.6154450945
O -2.9279837004,3.6182849694,-0.3230292368
N 2.6676902348,-0.7380609595,1.2917117742
C 2.5188377576,-2.0943438368,1.1621068942
C 2.1415928427,-2.8870875632,2.2444765783
C 1.9012687847,-2.3019851751,3.4863338672
C 2.0492761562,-0.9136475427,3.6108732285
C 2.4333757219,-0.1810541807,2.5005092996
C 1.4974637552,-3.1818352952,4.6152031891
O 1.3837478228,-4.3881297904,4.5406424934
O 1.2603085191,-2.4905471729,5.7557145042
N 3.0505165737,-1.6622070523,-1.1237232263
C 3.2762502475,-2.0393709219,-2.3991658501
C 3.2116270865,-3.3642693906,-2.8057216775
C 2.9090266309,-4.3493504257,-1.8568004372
C 2.6825481827,-3.9635450641,-0.5366788456
C 2.7579973515,-2.6149563507,-0.1896308609
C 2.8236928881,-5.7991335187,-2.188368039
O 3.0423670327,-6.0478178057,-3.5006436277
O 2.5869829327,-6.6754204595,-1.3825960629
H 1.324672814,4.8867776736,0.4996328618
H 5.4503636706,4.4955813748,1.6241246464
H 5.3436808394,2.0991562874,0.8941083023
H 4.3683667,7.6908795757,2.2028688334
H 0.5258560327,-0.7991733669,-1.5150239283

H -1.8128284796,0.0731216181,-1.6883784776
H -0.4249176673,3.7827346949,-0.0676758982
H -4.4330893098,1.9886381905,-1.3525904133
H 2.0214582107,-3.9589685479,2.1436535749
H 1.8701136924,-0.4152975677,4.5556321007
H 2.5709616609,0.891760151,2.555978892
H 0.989731967,-3.1522710358,6.4193176672
H 3.5215030007,-1.2354585943,-3.0823683648
H 3.4010636293,-3.6222558295,-3.8403409048
H 2.4536224367,-4.7266594317,0.1972937327
H 2.9634011593,-7.0140606852,-3.6087239577
N 3.7938827953,1.0416353545,-2.2092985794
N 5.1912843277,-0.1851757801,0.0446203778
C 4.0989466557,1.5050266595,-3.2550132079
C 6.2654711103,-0.503198751,0.4264885727
S 4.5067023651,2.1196412668,-4.7083302885
S 7.754555901,-0.9180132893,0.9484488662
At -6.6194479424,0.8783129847,-0.3182285761
At -4.1580851212,-1.5591646678,0.3437243158

N3+2At-z

Charge = 0 Multiplicity = 2

Ru 1.0383183416,-1.2088402295,-0.3531975627
N 2.8877621927,-0.6609489266,0.4302372238
C 3.2481722374,0.638343574,0.228881524
C 4.5065290412,1.0979312865,0.6209645798

C 5.4081429923,0.2170849924,1.2150511492
C 5.0299051023,-1.1164228031,1.4053895528
C 3.7632733372,-1.5130982195,0.9972935651
C 6.7474043198,0.7494159006,1.6131982391
O 7.0854881502,1.9049786095,1.4745220362
O 7.5351403396,-0.1972709896,2.1654357771
N 1.0779054856,0.8235083856,-0.7849436494
C 0.0866801072,1.5236750869,-1.3639730582
C 0.1869088796,2.8895017688,-1.6347930557
C 1.3632023723,3.5531802363,-1.2929022943
C 2.3882158215,2.8339541217,-0.6656683877
C 2.229270905,1.4775593778,-0.4197657668
C 1.5847266444,5.0071305949,-1.5440637289
O 0.5485945272,5.5854412207,-2.1840481058
O 2.5864046979,5.6058863909,-1.2105550979
N -0.1729959287,-0.8239171118,1.304992035
C -1.4964145984,-1.0963348036,1.1327109407
C -2.40369833,-0.9424140311,2.1820811293
C -1.9547169541,-0.4964993347,3.4211822173
C -0.5993625566,-0.1867588963,3.5790217201
C 0.2510645502,-0.3650788964,2.4987826647
C -2.953035485,-0.3638343473,4.5251766425
O -4.1185630416,-0.6775192424,4.4268496168
O -2.4088228418,0.1453255976,5.6522022659
N -0.8498797054,-1.6548938044,-1.1018020774
C -1.0970054093,-2.081476838,-2.3549146001

C -2.3714793583,-2.430700033,-2.7820136906
C -3.432332857,-2.3408602639,-1.8754769526
C -3.1773560621,-1.9017402719,-0.5780437337
C -1.8750010841,-1.5667064707,-0.2100902945
C -4.8395026083,-2.7009857699,-2.2299799484
O -4.9684639411,-3.0591482641,-3.5255955181
O -5.7617214578,-2.683857447,-1.4448057199
N 1.9943027997,-1.5601460137,-2.0738750136
C 2.6058871515,-1.6697483723,-3.08559336
S 3.4174431371,-1.8274462376,-4.4758970413
N 1.1591826403,-3.1101323728,0.2626701173
C 1.1464174044,-4.2132276299,0.7018814912
S 1.1568674794,-5.7113111904,1.3121948615
H 4.8091466009,2.1265119421,0.4669793015
H 5.7063076567,-1.833884625,1.8532388635
H 3.416993227,-2.5336071438,1.1061599262
H 8.3790024332,0.2383480997,2.3910389793
H -0.8054069836,0.9749547563,-1.6313462272
H -0.648926861,3.4036259696,-2.0914503003
H 3.2927273486,3.3614746176,-0.3880379991
H 0.776742052,6.5280647331,-2.2917184667
H -3.4565025715,-1.1590396501,2.0560917573
H -0.214344201,0.17630141,4.5237720042
H 1.3112247977,-0.1576750807,2.5780002994
H -3.130776598,0.2009889993,6.3065998844
H -0.2344260485,-2.1430528727,-3.0068903658

H -2.529285575,-2.7704729861,-3.7981259803
H -4.0027640101,-1.8242918504,0.117774518
H -5.9102144068,-3.2770325446,-3.6607153474
At -3.0396263645,2.334135969,0.0944652357

4+Br-b

Charge = 0 Multiplicity = 2

Ru -0.91149766,0.0192878949,-1.0641939935
N 1.1597802505,-0.1479666412,-0.8547164459
C 1.755261325,0.8107945066,-0.0886071142
C 3.1344817543,0.8269517079,0.1056082759
C 3.9284002907,-0.1453429198,-0.5006930847
C 3.3118408031,-1.1041912876,-1.3063238151
C 1.9289111813,-1.0704687438,-1.4611890164
C 5.4144101441,-0.1122199727,-0.2367414672
O 5.9089653616,0.7336007413,0.4824848339
O 6.0461190751,-1.092576104,-0.8649428428
N -0.4845603799,1.6058557523,0.2174252057
C -1.3939547209,2.4664799263,0.7142309261
C -1.0503396186,3.540163377,1.5213709454
C 0.3009143177,3.7378597195,1.8292918376
C 1.2462178235,2.8533341533,1.3140875663
C 0.8352711958,1.7919254015,0.5058568356
C 0.7830983616,4.8626709188,2.6875303099
O -0.2251770945,5.6556226112,3.1115760965
O 1.9455243442,5.0464158731,2.9741042801

N	-1.5004555352,-1.1558281228,0.5462181318	H	-4.4321846314,-2.2146246972,1.8741530783	C	-2.1072582884,-1.6968771111,-0.6569266859
C	-2.8480728064,-1.3034574981,0.7067335652	H	-0.4107496975,-3.1008048353,3.0757130244	C	-3.1580654784,-0.8298533372,-0.3443534372
C	-3.3649937879,-2.0922693466,1.7338982148	H	0.3912088095,-1.6612155105,1.2023240981	C	-2.8829756565,0.5284673165,-0.1985608975
C	-2.4983927815,-2.7495852324,2.6058424423	H	-2.6331655154,-4.7096848447,5.1245324385	C	-1.5788800805,0.9941706351,-0.3538604017
C	-1.1182981119,-2.6000388255,2.426290022	H	-3.0415351393,1.3948611858,-2.8239324586	C	-4.580345234,-1.2966434552,-0.1419256933
C	-0.6669088372,-1.7974889283,1.3888810492	H	-5.5497672963,1.3761864984,-2.9899004363	O	-4.691559124,-2.6031126463,-0.3201900002
C	-3.0946939842,-3.5853521281,3.6910070748	H	-5.6318167717,-1.230942993,0.4141059321	O	-5.4628206137,-0.512714459,0.1467761945
O	-4.2870688001,-3.7136303429,3.8684601426	H	-8.7853610745,0.559156929,-2.2038044258	N	1.782529821,0.3189286861,1.1082889888
O	-2.156546672,-4.1845216076,4.4538311093	Cl	-0.5068953657,1.520652845,-2.8636087746	C	2.5980937806,-0.7739908636,1.1642209306
N	-2.9838165476,0.172194228,-1.1710302779	Cl	-1.1374980879,-1.9127460947,-2.4344743589	C	2.9890829951,-1.3132298393,2.3893105083
C	-3.6588839758,0.8445122597,-2.1227315008	Br	9.1938566618,-1.4099300468,-0.3729113017	C	2.5464058703,-0.7307320546,3.5758050828
C	-5.0463592132,0.8224768862,-2.206776131			C	1.7138750308,0.3922624801,3.5072056652
C	-5.7677715471,0.0710889091,-1.2745173922	4+Br-e		C	1.3605039296,0.8805724285,2.2578886623
C	-5.0701310587,-0.6381454019,-0.2976172951	Charge = 0 Multiplicity = 2		C	2.9876409819,-1.3432188788,4.8654192289
C	-3.6775404011,-0.5787231268,-0.267856186	Ru	1.3320145076,1.0061321092,-0.8040668742	O	3.7016948179,-2.3196635599,4.9400441932
C	-7.2594966921,-0.0201879429,-1.2742047109	N	0.1456870425,2.6558818494,-0.336212933	O	2.4961346789,-0.6912677059,5.939915312
O	-7.8204319136,0.686636974,-2.2773017972	C	-1.1903367289,2.4076787935,-0.2229490446	N	2.4773028078,-0.6802914023,-1.2228601897
O	-7.89817551,-0.6632478757,-0.4688804177	C	-2.0988014003,3.4440436764,-0.0095076437	C	2.8115965382,-1.0956644396,-2.4589797675
H	3.6246110401,1.5730884199,0.719994849	C	-1.6360123428,4.7565177346,0.0762038128	C	3.6655155357,-2.1712462447,-2.676260793
H	3.8989229796,-1.8669731236,-1.8034859277	C	-0.2667256918,5.000841684,-0.0606167814	C	4.2020180406,-2.8412012519,-1.573396685
H	1.3959298798,-1.7860838994,-2.0765414474	C	0.588874098,3.925344994,-0.2687520342	C	3.8670371362,-2.4045241445,-0.2922913132
H	7.0323912792,-1.0790834407,-0.6600875927	C	-2.6407022361,5.8408277112,0.3028474409	C	3.0062424445,-1.3187140059,-0.1397874138
H	-2.423053264,2.2787344139,0.4331708375	O	-3.8295159884,5.6456119171,0.4312554205	C	5.1298176879,-4.0072258377,-1.6954068612
H	-1.8144118321,4.2103512802,1.8954932055	O	-2.0766844482,7.0666318302,0.3428486765	O	5.3812891208,-4.3337587303,-2.9797390586
H	2.291633015,3.0130708031,1.5483741095	N	-0.5579022128,0.1359818233,-0.6393370581	O	5.5983582638,-4.5999475539,-0.7474808443
H	0.1828280032,6.3575261807,3.6535796201	C	-0.8289294973,-1.1736229025,-0.7950487623	H	-3.1622075224,3.2584129681,0.0806236766

H	0.1305037097,6.007416373,-0.0138721824	C	4.4932515902,-2.2083507755,0.9206897934	C	-4.3592209018,-1.376778471,-1.3969504393
H	1.6583548906,4.0495870086,-0.3944648087	C	3.1323251175,-2.3112946341,0.6605327243	C	-3.8378448189,-0.8175528392,-0.233873115
H	-2.8034552798,7.7029654987,0.4832795415	C	6.6064647776,-0.7936885587,0.8540577484	C	-2.4602782269,-0.8524164002,-0.0148479762
H	0.0160065773,-1.8048151812,-1.043058903	O	7.1897142425,0.2381561764,0.6004435552	C	-5.8402342655,-1.3360137223,-1.5940189471
H	-2.2888140683,-2.7568082935,-0.7875973122	O	7.2093085093,-1.8776868077,1.3871399012	O	-6.2158581135,-1.8426136947,-2.7896772702
H	-3.7072758317,1.1904747502,0.0398045727	N	0.9002836898,0.5173765121,-1.0324324699	O	-6.6244237335,-0.9040149954,-0.7779724328
H	-5.6409141242,-2.9225513726,-0.169037264	C	0.0404725384,1.3883104659,-1.5797247812	H	4.9262771439,0.9566478612,-0.1918752766
H	3.6340097842,-2.1816303721,2.4477063697	C	0.4180751822,2.6889666368,-1.9283427224	H	5.029265017,-3.0473911233,1.3467912875
H	1.3514808016,0.876963073,4.4054361912	C	1.7324131939,3.0826487132,-1.7054871047	H	2.5690461095,-3.2135549589,0.8685485837
H	0.7276233872,1.7533340309,2.1528738861	C	2.6290524988,2.1745134397,-1.1216507347	H	8.1502087512,-1.6444432345,1.50090565
H	2.8300793001,-1.1592754602,6.7288351806	C	2.1950457824,0.900497172,-0.7918567875	H	-0.9705087228,1.050198833,-1.7478042963
H	2.3734577209,-0.5269893424,-3.271319789	C	2.2447591896,4.4445198075,-2.0396760813	H	-0.3268315692,3.3605761077,-2.3336394364
H	3.90882783,-2.4729065924,-3.6877102086	O	1.3145510714,5.2185121709,-2.6326747114	H	3.6467618785,2.4979482349,-0.9401206129
H	4.2939721797,-2.9194018533,0.5598712087	O	3.3767241099,4.8167120803,-1.8070503219	H	1.7343875547,6.0839530882,-2.7963023005
H	5.9888158117,-5.0975829044,-2.9613643224	N	-0.4701540835,-0.5010578228,1.2618856963	H	-3.583100457,0.3874977127,2.2278377954
Cl	0.843160016,1.4853494252,-3.0782957944	C	-1.8141990221,-0.3358069823,1.2019159584	H	0.1488443356,0.8180185267,4.2981959148
Cl	3.3874656752,2.2128076848,-0.7453248097	C	-2.5122074022,0.2426214229,2.2673829687	H	1.2782410207,-0.2250343427,2.3312483993
Br	-7.5055504206,-3.9830661131,0.1117780969	C	-1.8196957568,0.6453516652,3.4019573704	H	-2.4041873911,2.044929571,6.2099209533
		C	-0.425674787,0.4987152841,3.4376869259	H	-1.3971779351,-2.3882332629,-2.7254459281
4+Br-z		C	0.2061107533,-0.0736056722,2.3483813698	H	-3.8535744049,-2.4047415697,-3.2370510822
Charge = 0	Multiplicity = 2	C	-2.6011258945,1.2323171483,4.5304489657	H	-4.5113856986,-0.3512312412,0.4728819925
Ru	0.4043125452,-1.4131461361,-0.4090112287	O	-3.8102675134,1.2972601203,4.561877701	H	-7.1885516004,-1.7718557924,-2.8238848533
N	2.4211938216,-1.2976176511,0.1325173772	O	-1.8070676065,1.6778142995,5.5310346353	Br	-2.4339172434,2.6977385011,-0.0433765586
C	3.0493041104,-0.1301190311,-0.1840445591	N	-1.6186320334,-1.4095268283,-0.9263052109	Cl	0.0374259966,-3.5021212497,0.6309065212
C	4.4143975516,0.0348865241,0.0559382538	C	-2.1241389376,-1.9531825171,-2.0503347011	Cl	1.1560847531,-2.2402731083,-2.4878433674
C	5.1463184088,-1.0101625091,0.6158161591	C	-3.4850928041,-1.9564315231,-2.3227057869		

4+2Br-b

Charge = -1 Multiplicity = 2

Ru -1.710115804,0.3322350865,-1.0536011044
N 0.3631522474,0.5327233673,-1.0065116772
C 0.8434796034,1.4788552812,-0.1490748928
C 2.2119745511,1.7020166134,-0.0078686962
C 3.1161954248,0.9477783161,-0.7523488817
C 2.6131957453,-0.0005722062,-1.6471910172
C 1.236554612,-0.1721895265,-1.7517396672
C 4.5922752848,1.1744242255,-0.5250238396
O 4.9846185532,2.0133516086,0.2653930756
O 5.3270689203,0.3698216058,-1.2715736114
N -1.4699211033,1.7699383593,0.3954358813
C -2.4731357541,2.3723153493,1.069740494
C -2.265987904,3.3898708294,1.9848164075
C -0.954679204,3.825906301,2.2215663853
C 0.0866314819,3.2137836852,1.5257629762
C -0.1871571445,2.1895328231,0.6185831306
C -0.6254171063,4.9149497127,3.1777029322
O -1.7244512728,5.4230368439,3.7927423315
O 0.4943168644,5.3243784609,3.4045202904
N -1.8569695585,-1.2205126504,0.2641574896
C -3.1232033096,-1.6987658961,0.4821150132
C -3.3508563683,-2.7858438014,1.3239917077
C -2.27978003,-3.4140414726,1.9575876973
C -0.985538356,-2.9259413988,1.7219260564

C -0.8231746484,-1.8415178029,0.8772845904
C -2.5644170945,-4.5684526759,2.8470993682
O -3.6744840613,-5.007300297,3.077680455
O -1.4431739546,-5.095563146,3.3946430113
N -3.74512831,0.0925011295,-0.9648504689
C -4.6487800885,0.8186847038,-1.6600324521
C -6.0076809795,0.5464987572,-1.6261854485
C -6.4691825663,-0.5259937552,-0.8493101536
C -5.5383358743,-1.2886697294,-0.1451975982
C -4.1832667785,-0.9679487957,-0.2195962995
C -7.9041318944,-0.8957736381,-0.7450562931
O -8.7099132759,-0.0905821332,-1.4811395923
O -8.337791298,-1.8125756498,-0.0754105025
H 2.6107133401,2.4373578075,0.6813072836
H 3.2886155684,-0.6027482166,-2.2430123478
H 0.7851697632,-0.8855787476,-2.4324513625
H 6.3080758087,0.4136523643,-1.0308484323
H -3.4702978896,2.0164972698,0.841990344
H -3.1069725026,3.8412866343,2.4968270382
H 1.1015618066,3.5501875883,1.6991584748
H -1.3925374442,6.1224785239,4.3859932946
H -4.3513586153,-3.1632000322,1.4985489447
H -0.1198913252,-3.3874667875,2.1814565584
H 0.1601578627,-1.4459180806,0.6571509269
H -1.7390649642,-5.8412125354,3.9491455338
H -4.2233688342,1.6186480172,-2.2571028046

H -6.6943945449,1.1541835299,-2.2029263036
H -5.8899687426,-2.1264345543,0.4448562848
H -9.6152709965,-0.4260033412,-1.3435079824
Cl -1.7963764248,2.1824832656,-2.6324268585
Cl -1.7226461277,-1.3178694025,-2.8293542837
Br 8.437855367,0.0435764027,-0.7106919957
Br 7.3094693226,-2.4077202342,0.5344740302

4+2Br-e

Charge = -1 Multiplicity = 2

Ru 2.2797926564,0.5469059595,-0.766438439
N 1.9904136886,2.5180989308,-0.2256151758
C 0.6923712904,2.944078124,-0.1998373862
C 0.3765908768,4.2801487597,0.0474860223
C 1.3998194681,5.2018287089,0.267008785
C 2.727190086,4.7559315617,0.2271174207
C 2.978682791,3.4151771436,-0.0241823924
C 1.028902593,6.6192804388,0.5244352179
O -0.1083978654,7.0419064597,0.5642682724
O 2.1087473521,7.4195218216,0.7096316778
N 0.2123830101,0.665339161,-0.7278456248
C -0.6375762768,-0.3539805965,-0.9614763425
C -2.0173687648,-0.2158964347,-0.9033422827
C -2.5581491344,1.0372699577,-0.5980238528
C -1.6852786249,2.0981414789,-0.3717465036
C -0.3072585828,1.8950449486,-0.4427438897

C	-4.0433325684,1.2821382382,-0.4790550405	H	-2.6679464025,-1.0636737438,-1.0825817111	O	7.3954410881,1.8607115645,0.9390532878
O	-4.7306718314,0.1879772489,-0.7513007298	H	-2.1114422318,3.0654971499,-0.1320312433	O	7.887327497,-0.2294063772,1.6200877216
O	-4.4810281577,2.3737498885,-0.1630593947	H	-5.7228505538,0.2963301539,-0.5941416351	N	1.2515519707,0.6965859367,-0.9150143755
N	2.3832657268,-0.2965528891,1.083096367	H	3.0065064533,-3.3831455161,2.3509090014	C	0.1900292645,1.3903833224,-1.3731906075
C	2.6517655663,-1.6413005917,1.1173592891	H	2.2685201709,0.3126391741,4.4018456338	C	0.2246565597,2.7594324055,-1.5991106502
C	2.7939766947,-2.3211319576,2.3253335874	H	2.0562037294,1.4200402369,2.1859050214	C	1.4144374454,3.4538320502,-1.3543912831
C	2.6604101158,-1.6366838473,3.5325353261	H	2.7681540786,-2.2187618115,6.6616997342	C	2.5142108869,2.7449639233,-0.8666288974
C	2.3811271059,-0.2620249378,3.4905720227	H	2.4047649456,-1.2026544513,-3.2912708514	C	2.4122931156,1.3743354777,-0.6480599499
C	2.2558638469,0.3584620533,2.2607026562	H	2.8711278958,-3.6235150984,-3.7925853938	C	1.5608519331,4.9168741084,-1.5666551795
C	2.8187148403,-2.3961332427,4.7973562668	H	3.2048039583,-4.3020509964,0.4315622199	O	0.4445003581,5.4876607054,-2.0740935421
O	3.0687208821,-3.5833210351,4.8666994022	H	3.5774561929,-6.9208017119,-3.1701232142	O	2.5666274429,5.5553670181,-1.318334041
O	2.6527776185,-1.6219678778,5.8990561167	Cl	2.1722604488,1.3008600891,-3.0757994887	N	0.1974731654,-1.1804692269,1.1479565875
N	2.5135939145,-1.4399371851,-1.2525533809	Cl	4.7158181346,0.681391619,-0.7284811187	C	-1.1203004222,-1.5203722854,1.0448905521
C	2.568903963,-1.9344096583,-2.5075613653	Br	-7.8653388596,0.0171400105,-0.2557747044	C	-1.9657771479,-1.487239376,2.1538968863
C	2.8358446862,-3.2702075777,-2.7692880774	Br	-6.924913566,-2.6325861625,0.6948911691	C	-1.4642942506,-1.1038109697,3.3947146016
C	3.0660966701,-4.1412536537,-1.6958535132			C	-0.1134298847,-0.7418064089,3.4894927749
C	3.0195793298,-3.6318158533,-0.3991145761	4+2Br-z		C	0.6728039196,-0.797587817,2.3522783148
C	2.7433250292,-2.2797604557,-0.199166238	Charge = -1 Multiplicity = 2		C	-2.384436972,-1.1002989179,4.5608147419
C	3.3652313923,-5.5873349999,-1.8720361753	Ru	1.3047381761,-1.3239496799,-0.5763425113	O	-3.5243844656,-1.5161522118,4.5490955073
O	3.3758442111,-5.9665556893,-3.1729894242	N	3.1520492691,-0.7591522482,0.1224529981	O	-1.8105821168,-0.5879870866,5.6811036676
O	3.58245677,-6.3645193219,-0.9639806266	C	3.489625645,0.5492255414,-0.0906626323	N	-0.5837322013,-1.8144471801,-1.2575707137
H	-0.6509701426,4.6224871438,0.0637317096	C	4.7593174764,1.0282740879,0.2305348971	C	-0.8876057955,-2.1343493932,-2.5323750711
H	3.5519570729,5.4413102165,0.3797224555	C	5.7090376943,0.1631941623,0.7733690039	C	-2.1571430921,-2.5421617743,-2.9128831583
H	3.982120148,3.0083809829,-0.0888691696	C	5.3556445797,-1.1786874523,0.9771250957	C	-3.1602505196,-2.6376158176,-1.9399733752
H	1.7503414049,8.3143399436,0.8584923386	C	4.0786479792,-1.5970775383,0.6375894687	C	-2.8496476589,-2.3080109335,-0.6227863704
H	-0.1759052028,-1.3043213271,-1.2003309173	C	7.050502156,0.7062548754,1.1015686824	C	-1.5554923464,-1.8972729051,-0.3047580196

C	-4.5432463905,-3.0890465633,-2.2474864335	Ru	-1.3696184582,0.0082582058,-1.0336969663	O	-4.7545815245,-3.7320448703,3.8833766533
O	-4.75474102,-3.2665378758,-3.5770882076	N	0.6981581808,-0.0994436578,-0.7845279016	O	-2.6263252231,-4.1344838974,4.5238380014
O	-5.4082905716,-3.2937812173,-1.4210739076	C	1.2561441339,0.9029896435,-0.046878801	N	-3.4385886525,0.1084951429,-1.188521346
H	5.0304643991,2.0634107815,0.0619997227	C	2.6332875735,0.9722483898,0.1533501462	C	-4.1086110913,0.7504574463,-2.1649460785
H	6.0660508084,-1.8881321861,1.383880875	C	3.4624945748,0.0078173307,-0.4169429757	C	-5.492150366,0.6886784121,-2.2822056342
H	3.7479180265,-2.6246596317,0.7454368245	C	2.8830755078,-0.9994443233,-1.1915033382	C	-6.2157937409,-0.0717155314,-1.3584414064
H	8.72638146,0.2377698768,1.788937481	C	1.5012318022,-1.0166712208,-1.3544176136	C	-5.5230946141,-0.7490277969,-0.3557663495
H	-0.7216532971,0.8324015456,-1.5363870076	C	4.9424688532,0.1054057071,-0.1563766636	C	-4.1338371841,-0.6501762797,-0.2926494846
H	-0.6742676072,3.2626680019,-1.931943375	O	5.4182106714,0.991500484,0.5244879395	C	-7.7030567,-0.2056516519,-1.3950405738
H	3.4303456891,3.2843400182,-0.6580270991	O	5.616477031,-0.8757491815,-0.7514547433	O	-8.2589161567,0.4775723323,-2.4178922417
H	0.6391109132,6.4400653419,-2.148050024	N	-1.0113142464,1.6326894074,0.2105914481	O	-8.3458969787,-0.8520093299,-0.5953488259
H	-3.0151270454,-1.7380386495,2.0682285554	C	-1.9531176004,2.4754474968,0.6783009618	H	3.0920302345,1.7572886621,0.7427742644
H	0.3156522744,-0.4272756006,4.4329328286	C	-1.6535419725,3.5781820914,1.4632546668	H	3.496500957,-1.7584802636,-1.6617328488
H	1.7243061272,-0.5400579888,2.3810528798	C	-0.3131710983,3.8285279383,1.7810768885	H	0.9948564013,-1.7677056385,-1.9500196996
H	-2.5049129172,-0.6219683773,6.3649116468	C	0.6656403482,2.9626994061,1.2970696025	H	6.5903133244,-0.7938974997,-0.5525107739
H	-0.0609962785,-2.0626870769,-3.2304227937	C	0.2987587701,1.8700491268,0.5104351506	H	-2.9724205381,2.2479319577,0.3911009188
H	-2.357750112,-2.7896776559,-3.9480918544	C	0.122225109,4.9871946577,2.6168106068	H	-2.4436865876,4.230998516,1.813298944
H	-3.625197071,-2.3674124402,0.129987512	O	-0.9154009972,5.7584332022,3.0104367008	H	1.7025149476,3.1611989745,1.5396864481
H	-5.6848379961,-3.5487266343,-3.6555601737	O	1.2746656937,5.2155182883,2.9134040861	H	-0.5348224691,6.4847043815,3.5399841915
Br	-2.9304591774,1.6038259353,0.2248090891	N	-1.9608843395,-1.1555517235,0.5770277699	H	-4.8938999948,-2.2714698404,1.8567607398
Cl	1.6116772185,-3.6923706946,-0.0467224027	C	-3.3080456512,-1.3378052126,0.7108136661	H	-0.8793313965,-3.0282449051,3.1648465763
Cl	2.3795973402,-1.5718733771,-2.7544806605	C	-3.8271950521,-2.1233836603,1.7391996743	H	-0.0730665028,-1.6003058547,1.28505882
Br	-5.3600214167,3.2489942895,0.5155332213	C	-2.9644905839,-2.7425525903,2.6422648674	H	-3.106265164,-4.6585663698,5.1928942686
		C	-1.5848664,-2.5580173355,2.4908307612	H	-3.488491535,1.3076794936,-2.8583956187
		C	-1.1311712109,-1.761544252,1.4503187386	H	-5.9911687825,1.2181402421,-3.0846797041
		C	-3.5623775042,-3.5749139283,3.7275969692	H	-6.0851336039,-1.3495026498,0.3492439226

4+1-b

Charge = 0 Multiplicity = 2

H -9.2215294096,0.3258465697,-2.3635908228
Cl -0.9590402014,1.4781289759,-2.8703459677
Cl -1.5176148819,-1.9578628783,-2.3817356598
I 9.0784463502,-1.0177261146,-0.2743841223

4+l-e

Charge = 0 Multiplicity = 2

Ru 1.9401230445,0.7900490133,-0.8021822857
N 1.1646300633,2.6631963744,-0.3329897208
C -0.1941135443,2.7325708378,-0.235614271
C -0.8397936023,3.9505191463,-0.0255429359
C -0.0860634587,5.1193702925,0.0749086127
C 1.3045417867,5.0385964048,-0.0426746133
C 1.8896036033,3.7947901189,-0.2483335591
C -0.8135656078,6.4061909026,0.2954059634
O -2.0171233177,6.4940835095,0.4076733434
O 0.0192357599,7.4676239267,0.3519651326
N -0.0943789055,0.3780700182,-0.6519821254
C -0.6566080189,-0.8348078416,-0.8131774279
C -2.0215910884,-1.0525746862,-0.6902435551
C -2.8502859309,0.0324989122,-0.3885899187
C -2.2742485838,1.2921184553,-0.2364974571
C -0.8959219318,1.4470559367,-0.3762969283
C -4.3396275553,-0.0980978589,-0.2050109767
O -4.7478196489,-1.3508548988,-0.3880834663
O -5.036603083,0.8537181774,0.0819620847

N 2.2408020224,0.032129783,1.1044165369
C 2.7894863328,-1.2171531568,1.1641285963
C 3.0632060984,-1.822446355,2.3900650541
C 2.7810870966,-1.1463124661,3.575909414
C 2.22500847,0.1366173971,3.5042259569
C 1.9748073013,0.6830412692,2.2546350782
C 3.0887078655,-1.8318331785,4.8660545645
O 3.5665895738,-2.9431416105,4.9460457619
O 2.7801598562,-1.0733849013,5.9398884235
N 2.6669918167,-1.1119872869,-1.2209539007
C 2.8857148206,-1.5993413067,-2.4570964611
C 3.4706687394,-2.8416374085,-2.6737405946
C 3.8516553361,-3.6112008603,-1.570539438
C 3.6379818574,-3.1028549542,-0.2899334195
C 3.0487167136,-1.8485563359,-0.1381573054
C 4.4875254675,-4.9579726052,-1.692069518
O 4.6508692435,-5.3382807185,-2.9764723808
O 4.8184963833,-5.6387010893,-0.7448685448
H -1.9183477566,4.0168773651,0.0506369423
H 1.9239711991,5.925133395,0.0166246066
H 2.9601018759,3.6656511255,-0.3609676132
H -0.5426290838,8.2541752854,0.4872885137
H 0.0253121533,-1.6414644786,-1.0533344411
H -2.4364817727,-2.0440183991,-0.8249923163
H -2.9251926166,2.1271419811,-0.0055622571
H -5.733193526,-1.4257589298,-0.2391013767

H 3.4947954639,-2.8143071789,2.4494105894
H 1.9958831418,0.6985767253,4.4013332705
H 1.5581994327,1.6770879456,2.1479604042
H 3.0157417077,-1.5978988744,6.7286423101
H 2.581207252,-0.9489058489,-3.269279733
H 3.629747462,-3.1956992358,-3.6849570027
H 3.9446600448,-3.6964353432,0.5627023798
H 5.0705922001,-6.2192283716,-2.9556957144
Cl 1.5733207269,1.3709538712,-3.0850146324
Cl 4.2225367267,1.5023530272,-0.7690095566
I -8.072027622,-2.1867763464,0.129783315

4+l-z

Charge = 0 Multiplicity = 2

Ru 0.6227455474,-1.4385763928,-0.5709567973
N 2.6162342558,-1.2848996193,0.0342479331
C 3.1953188841,-0.066735261,-0.1621649778
C 4.5454004072,0.1379637548,0.1273219433
C 5.3131462604,-0.9184729773,0.6134253363
C 4.7103755445,-2.1669804099,0.796011818
C 3.3621620831,-2.307867268,0.491573583
C 6.7551925289,-0.658326562,0.9091899958
O 7.2949203272,0.4171944392,0.7629942601
O 7.3962035731,-1.7568149691,1.3625594521
N 1.0229269592,0.5643972554,-0.9651514583
C 0.1314648779,1.4509621142,-1.4368283134

C	0.4636787986,2.7851209745,-1.6861588511	H	5.2755523099,-3.0152771562,1.1619096778	C	1.9911645523,0.3962748054,-1.7133703945
C	1.76800149,3.2038200234,-1.4413855637	H	2.8371847146,-3.2498474577,0.6016597744	C	0.6275518895,0.1350153437,-1.7976483283
C	2.6932172097,2.2847230426,-0.9257373503	H	8.3220311727,-1.4919143612,1.5215494376	C	3.9043002128,1.6738958142,-0.598130192
C	2.3041578693,0.9748513882,-0.6929781767	H	-0.8656523815,1.0868561876,-1.6355351822	O	4.2690478886,2.485393504,0.2311150917
C	2.2367230365,4.5993019533,-1.6839859263	H	-0.3006542097,3.4614477413,-2.0457156597	O	4.6780953641,0.9643771983,-1.4087304721
O	1.2779258438,5.3840264519,-2.2151693654	H	3.701129729,2.6263991176,-0.7238402723	N	-2.1591057049,1.8243621414,0.4549347236
O	3.359364076,4.9889597827,-1.4349176376	H	1.6706442826,6.2707341695,-2.3224894959	C	-3.1859736581,2.3269916982,1.1743359122
N	-0.3279906353,-0.8244315523,1.188079313	H	-3.5128470666,-0.3692382091,2.2260548701	C	-3.0302965067,3.3255044639,2.1198795789
C	-1.6838277277,-0.7787116224,1.1343707504	H	0.1605482849,0.1121863837,4.3865220832	C	-1.7488758968,3.850214601,2.3407950017
C	-2.4327709861,-0.4203948574,2.258849754	H	1.3838379043,-0.542387402,2.3106883569	C	-0.6835325833,3.3395691256,1.6008424845
C	-1.7818656926,-0.1149105514,3.4486704836	H	-2.4993140962,0.8240319289,6.4137782038	C	-0.9046799949,2.328443496,0.6652077071
C	-0.3815911443,-0.1366599459,3.4827679413	H	-1.074097827,-2.1252535891,-3.0641586061	C	-1.476242607,4.9290035443,3.325662691
C	0.3022908348,-0.4923389494,2.3326073529	H	-3.5188226359,-2.2612902825,-3.61780921	O	-2.5929735473,5.3317545277,3.9852547732
C	-2.6169457083,0.2377912759,4.6353259642	H	-4.368312692,-0.9468286247,0.3766016681	O	-0.3846121741,5.4149467056,3.5385039131
O	-3.8272781259,0.1933174229,4.6531535772	H	-6.8994842273,-2.0167607439,-3.1573922067	N	-2.3569966371,-1.1806504792,0.2094442897
O	-1.8699896239,0.6072520844,5.7001667024	I	-2.5789190113,2.6684423487,0.2860031652	C	-3.5835718133,-1.758677688,0.4104482727
N	-1.3866067269,-1.4858322245,-1.1321165912	Cl	0.355341999,-3.6734063207,0.1678379855	C	-3.7247165847,-2.8985986362,1.1998794503
C	-1.8391777196,-1.8712062198,-2.3400705509	Cl	1.4648554329,-1.9790881266,-2.7138372409	C	-2.6057529434,-3.4753135777,1.7986828569
C	-3.1945087564,-1.9457551098,-2.6338736186			C	-1.3528651786,-2.8810391998,1.5852214944
C	-4.1191277234,-1.6147091006,-1.6388015846	4+2I-b		C	-1.2766026756,-1.7491199194,0.7921125229
C	-3.6520464765,-1.2161743237,-0.3887030306	Charge = -1 Multiplicity = 2		C	-2.7982906743,-4.6903374368,2.6311574885
C	-2.2778669806,-1.1624701018,-0.1559767056	Ru	-2.3316136386,0.4314475005,-1.0443581233	O	-3.8713434074,-5.2217135908,2.8413517709
C	-5.5975088311,-1.6757727423,-1.8498495766	N	-0.2767702287,0.7624693951,-1.0204537475	O	-1.6377806254,-5.1582731458,3.1484407768
O	-5.924424487,-2.0038050926,-3.119383724	C	0.155659487,1.7153911944,-0.1448435593	N	-4.3461944356,0.0530593446,-0.9411595059
O	-6.4175826386,-1.4611266692,-0.984323071	C	1.5085124357,2.0270094682,-0.0221760884	C	-5.3062063356,0.7474924449,-1.5914230292
H	5.0183929098,1.1005089383,-0.0235648785	C	2.4455788924,1.3559671489,-0.8046020111	C	-6.6421690173,0.3784788535,-1.5612462154

C -7.0181194803,-0.76146096,-0.8361425308
C -6.0283610669,-1.4904614346,-0.17818625
C -4.700027943,-1.0714590512,-0.2467633634
C -8.4224897641,-1.2364966269,-0.740040583
O -9.2904745413,-0.4565546345,-1.4312732372
O -8.7834275516,-2.2135762608,-0.1140036005
H 1.8690426996,2.7667845924,0.6830396704
H 2.6932064527,-0.148295157,-2.3330440828
H 0.2125126158,-0.5912421455,-2.487737129
H 5.6406281941,1.0312080349,-1.1445468301
H -4.159565492,1.9053358898,0.9572527782
H -3.8883885173,3.695411719,2.6676061041
H 0.3084244739,3.743090197,1.7636325081
H -2.2982536585,6.0341220677,4.5944706781
H -4.6933120019,-3.35700817,1.359729149
H -0.4525627538,-3.2971278169,2.0209062641
H -0.3269593057,-1.2703332812,0.59028683
H -1.8720465049,-5.9515030733,3.6651105841
H -4.9448411137,1.6035923766,-2.1516255539
H -7.3764080543,0.9637354199,-2.1014078876
H -6.3138337071,-2.3790353294,0.3718602599
H -10.1683763913,-0.8620733286,-1.304733488
Cl -2.5595590203,2.3298548463,-2.5495722558
Cl -2.2732202995,-1.1425724432,-2.8870523324
I 7.9692594907,0.320400326,-0.6363245502
I 6.1540658475,-2.2362002305,0.5895514488

4+2I-e

Charge = -1 Multiplicity = 2

Ru 2.9634514575,0.4412131436,-0.7643397963
N 2.8646023604,2.4172668353,-0.1762534762
C 1.6143079423,2.9674793,-0.1459399151
C 1.4285607574,4.3198496554,0.141312412
C 2.534930842,5.129691129,0.3956483206
C 3.8126812892,4.557515064,0.3491658576
C 3.9341160258,3.2067050833,0.0581339908
C 2.3014027432,6.5676848402,0.6965315193
O 1.2096786553,7.0957907132,0.7505371991
O 3.4515948725,7.2506829979,0.9224307909
N 0.9175080598,0.7594851792,-0.7313037405
C -0.0264928961,-0.1655357522,-0.9950701916
C -1.3863394236,0.1084406363,-0.9511650455
C -1.8029972393,1.4041233653,-0.6280739427
C -0.8324258732,2.3675214746,-0.3670238726
C 0.5192864335,2.0287009332,-0.4248292515
C -3.2556830256,1.7958053403,-0.5264793598
O -4.0479738198,0.7848203007,-0.8459124936
O -3.5929253346,2.9140467969,-0.1841718714
N 2.9786215709,-0.4514996458,1.0672238176
C 3.1166165454,-1.8159063275,1.0689376664
C 3.1913221864,-2.5346758011,2.2603728823
C 3.122757561,-1.8690638605,3.4833634403

C 2.9767340749,-0.473501861,3.4743784023
C 2.9133336222,0.1850690096,2.2594601649
C 3.2047999445,-2.6697930299,4.7301961697
O 3.3442641281,-3.8761175519,4.7712896499
O 3.1116272835,-1.9090497972,5.8495478488
N 3.0006528095,-1.5469579715,-1.2960534664
C 3.0035740271,-2.0156433807,-2.5619723944
C 3.1329938624,-3.3653807558,-2.8548191398
C 3.2764952418,-4.2793899581,-1.8022948943
C 3.2841275511,-3.7974704282,-0.4942606572
C 3.1452753976,-2.4294485127,-0.2626172062
C 3.4273500791,-5.7441011556,-2.012251185
O 3.3847828065,-6.0936955342,-3.3206700127
O 3.5663515379,-6.5594603956,-1.1226411723
H 0.4393605298,4.7607012908,0.16371216
H 4.6991941142,5.1538302882,0.527406059
H 4.8932116208,2.7049537212,-0.0126811547
H 3.1804114918,8.1698135204,1.1040309315
H 0.3411629128,-1.1525167102,-1.2483948637
H -2.1147879198,-0.6675388964,-1.1547791609
H -1.1621214765,3.3680981448,-0.1126159115
H -5.0178952279,0.9968894459,-0.6978731156
H 3.2996662748,-3.6126318304,2.2606682454
H 2.9182651517,0.0874652567,4.3991687626
H 2.8168939602,1.2623720007,2.2092077029
H 3.1694713969,-2.5313175636,6.5982811026

H 2.9135832294,-1.2534554919,-3.3285408377
H 3.1296971168,-3.6969945996,-3.8859645982
H 3.4019996284,-4.5016675356,0.3204650682
H 3.4847972637,-7.0636828,-3.340437865
Cl 2.9467793413,1.2547900487,-3.0554823713
Cl 5.4008194056,0.3396504351,-0.712285077
I -7.4511512919,0.7924677059,-0.4060885218
I -6.4028716052,-2.1984947975,0.7443630701

4+2I-z

Charge = -1 Multiplicity = 2

Ru 2.047893071,-1.1929655725,-0.6497448703
N 3.7934602867,-0.3100270854,-0.0136123675
C 3.8479473301,1.050079619,-0.1482358436
C 5.0206508716,1.755500828,0.1195049471
C 6.1628884756,1.0687176266,0.5300959205
C 6.097834706,-0.326216702,0.6575426983
C 4.9048623535,-0.9729985402,0.3744990666
C 7.3943566916,1.8511042624,0.8044951971
O 7.4895586896,3.0589149157,0.7061522102
O 8.4385527638,1.0743815094,1.1919553638
N 1.5693552281,0.791745633,-0.8194753294
C 0.3547357524,1.2829436381,-1.1398065928
C 0.0893834015,2.641980956,-1.2295523575
C 1.1293899608,3.5485675948,-0.9925020445
C 2.387117964,3.0486196933,-0.6499227213

C 2.585828176,1.6735071521,-0.5618283467
C 0.9550955605,5.0231712791,-1.063534244
O -0.2919400006,5.3840769016,-1.4386884732
O 1.8271843465,5.8346675203,-0.8152546583
N 1.0392777475,-1.3617130816,1.127565531
C -0.2007631747,-1.9322150405,1.0651495383
C -0.9824789432,-2.0917707941,2.2094963242
C -0.4939039914,-1.6752358976,3.4458957808
C 0.7773415111,-1.0870194554,3.5007748208
C 1.5019083956,-0.9541481521,2.3292890161
C -1.3406301919,-1.880751629,4.6492099184
O -2.3952146747,-2.4805171431,4.6630897976
O -0.805546775,-1.3258620566,5.7683382446
N 0.2523205704,-2.0095625541,-1.2717570067
C -0.0594919643,-2.3151795395,-2.5478188138
C -1.2494280037,-2.9399495916,-2.8914891575
C -2.1562480668,-3.2793970961,-1.8800857335
C -1.8376899595,-2.9639726884,-0.56108925
C -0.6289817815,-2.3275594879,-0.2811256626
C -3.4452953446,-3.9728826299,-2.1468731721
O -3.704544604,-4.1072875541,-3.4719496229
O -4.19691708,-4.3916124742,-1.2912082603
H 5.0687718393,2.8319596071,0.0083929493
H 6.9646427117,-0.9004365262,0.9613669487
H 4.7936427787,-2.0508951283,0.4267882743
H 9.1812655285,1.6895250337,1.3365327901

H -0.4337388959,0.5610042362,-1.3064113243
H -0.9192163585,2.967765486,-1.4524190608
H 3.1876442772,3.749520232,-0.4453993579
H -0.3077458627,6.3588670603,-1.4310940116
H -1.9741626957,-2.5225610086,2.157097871
H 1.1937049437,-0.7436501561,4.4398835118
H 2.4934367029,-0.5185249726,2.3252750496
H -1.4461750514,-1.5097507707,6.4802450004
H 0.6949083768,-2.0469522629,-3.2789164554
H -1.4612431135,-3.1648354963,-3.9296352637
H -2.5417773095,-3.213320473,0.2222378796
H -4.5697802481,-4.5541522118,-3.5243597517
I -3.1062377419,0.9074523112,0.3844976215
Cl 2.8503734871,-3.4768812136,-0.3104758054
Cl 3.0054331203,-1.0806581081,-2.8904004445
I -6.175587194,2.1781802406,0.045748174

4+At-b

Charge = 0 Multiplicity = 2

Ru -2.1003041984,0.0327754712,-1.0225959368
N -0.0340528841,-0.025278541,-0.7743243485
C 0.5003095484,0.9882873666,-0.0338807652
C 1.8758608873,1.0909279916,0.1648249311
C 2.7276506673,0.1494924891,-0.4103803143
C 2.1721762202,-0.8701851561,-1.1871201631
C 0.7914397641,-0.9214860653,-1.347307569

C 4.2026746334,0.2820962678,-0.1524717784
O 4.6646174413,1.1672769774,0.5383144304
O 4.9038698818,-0.6794991412,-0.7569695495
N -1.7851783117,1.6542626016,0.2288262555
C -2.7480703062,2.4705867618,0.7024602608
C -2.4768920585,3.5773385646,1.4915387597
C -1.1432089445,3.8634139957,1.8085461499
C -0.1425864143,3.0259973399,1.3189716887
C -0.4811810381,1.9273114656,0.528594784
C -0.7378801953,5.0290652033,2.6478663883
O -1.7948638683,5.7711607291,3.0474526184
O 0.4085699452,5.287742185,2.9443837082
N -2.6611311371,-1.168354099,0.5654261284
C -4.0033604205,-1.3919750747,0.6932787835
C -4.5024775447,-2.2080573909,1.7076762557
C -3.6253839929,-2.816430245,2.6041060058
C -2.2509730211,-2.5896048989,2.4594380605
C -1.8175345491,-1.7649649713,1.4329290686
C -4.2015273676,-3.6812933359,3.6743706581
O -5.3891235495,-3.8752956508,3.8258080217
O -3.2519407098,-4.227083077,4.4652798727
N -4.168041432,0.0842691736,-1.1787387286
C -4.8544902968,0.7297475135,-2.1422879456
C -6.2354881193,0.6347953776,-2.2628660992
C -6.9407065733,-0.1637723183,-1.356718209
C -6.2317402168,-0.8435353239,-0.3673016371

C -4.8455724771,-0.7099061411,-0.2995255104
C -8.4232638423,-0.3352340813,-1.3991330875
O -8.9958695187,0.3548149673,-2.4087464721
O -9.0513945459,-1.0154867291,-0.6156808702
H 2.3139786724,1.8855480774,0.7569705918
H 2.8025916938,-1.6126435483,-1.6612362347
H 0.3023620039,-1.68270915,-1.9445449221
H 5.8676146853,-0.5675482196,-0.55025751
H -3.7615540969,2.2172299054,0.416553205
H -3.2840252356,4.2067977866,1.8456104168
H 0.8890108163,3.2514933703,1.560588337
H -1.431513579,6.5042729813,3.5795387889
H -5.564942375,-2.3877535223,1.8193667867
H -1.5340301463,-3.0496212003,3.1284373527
H -0.7639165568,-1.5714599965,1.2739267834
H -3.7201329451,-4.7739387313,5.1242653179
H -4.248273877,1.3165381828,-2.8235410703
H -6.7470422211,1.1680548445,-3.0548475747
H -6.7785362358,-1.4728737417,0.3244046589
H -9.9539675412,0.175834847,-2.358772842
Cl -1.7231776607,1.532113925,-2.8505851291
Cl -2.1952487533,-1.9198507641,-2.4042665454
At 8.5127090635,-0.6750216987,-0.1761232226

4+At-e

Charge = 0 Multiplicity = 2

Ru 2.6651379795,0.6636291331,-0.8138351699
N 2.092096458,2.6082085876,-0.3568299369
C 0.7483163862,2.818363784,-0.2490135336
C 0.2326523165,4.0971612414,-0.0414551201
C 1.1020973796,5.183638679,0.0450023925
C 2.4759393232,4.9600316271,-0.0860773278
C 2.928948308,3.6620430559,-0.2885128207
C 0.5116413076,6.5380752663,0.2652518921
O -0.6754437403,6.7486562801,0.3921939691
O 1.4482683629,7.5101059277,0.3095835573
N 0.6042997551,0.4611774902,-0.6379623223
C -0.0839891363,-0.688837309,-0.7786370779
C -1.4635446205,-0.7609983221,-0.6506299842
C -2.1745827677,0.4091320816,-0.365424571
C -1.4691728636,1.6029552336,-0.2308854366
C -0.0823386191,1.6109603158,-0.3739351607
C -3.6670482653,0.4413946939,-0.1870206936
O -4.2115067882,-0.7654405733,-0.3523754377
O -4.2659879398,1.462711024,0.0800347209
N 2.9332045456,-0.0929052581,1.0932634724
C 3.3699963415,-1.3859175267,1.1611370176
C 3.6168940768,-1.9973169024,2.3897091777
C 3.4203856755,-1.2850417418,3.5716480822
C 2.9756095507,0.0405063159,3.4922536906
C 2.7481171343,0.5915284742,2.2408135164
C 3.6947574846,-1.9781705926,4.8641298835

O 4.072799999,-3.1270091262,4.9518155926
O 3.4741167717,-1.1834138225,5.934116388
N 3.1943599097,-1.3012000015,-1.2205906807
C 3.3324638989,-1.8252606293,-2.4541300066
C 3.7932912561,-3.1191731197,-2.6655496971
C 4.1326517247,-3.9057087077,-1.5603664146
C 4.0035746939,-3.3613980915,-0.2834048165
C 3.5374849521,-2.0557035852,-0.1364738811
C 4.6373598637,-5.3065860877,-1.676671161
O 4.7309559415,-5.7182424346,-2.9589017305
O 4.9303824633,-6.0031227696,-0.7281643385
H -0.8325969962,4.2741227676,0.0441560096
H 3.1837186403,5.7786352784,-0.0397180022
H 3.9796998128,3.4255843986,-0.4126138548
H 0.9698889066,8.3494594211,0.4482798102
H 0.5058769401,-1.5682608783,-1.0072608134
H -1.9781295336,-1.7064211092,-0.7714180861
H -2.0268133816,2.5061460288,-0.0132747531
H -5.194929059,-0.7148574066,-0.2196870717
H 3.9616639107,-3.0223135138,2.4533323788
H 2.8144853758,0.6312383813,4.3856784681
H 2.4163478774,1.6166078536,2.1297342963
H 3.6792639955,-1.7184723883,6.7242031206
H 3.0686614788,-1.1601995367,-3.2687379295
H 3.8907306845,-3.500149984,-3.6748032788
H 4.2783459561,-3.9684438647,0.5706598346

H 5.0693028182,-6.6333477718,-2.9332098023
Cl 2.3249931827,1.2559697173,-3.1044713987
Cl 5.0120882776,1.1459835542,-0.8370007603
At -7.7824401294,-1.1936141863,0.1084273018

4+At-z

Charge = 0 Multiplicity = 2

Ru 0.9957699445,-1.5522694933,-0.5744695645
N 2.9508339795,-1.2063581388,0.068475661
C 3.4151932546,0.0597024412,-0.1313070074
C 4.7342434918,0.3951250166,0.1774034672
C 5.5913670351,-0.578852768,0.6859601261
C 5.1073681514,-1.8775812618,0.8708644909
C 3.7837617944,-2.1495301936,0.5470624963
C 6.9967932893,-0.1795944122,0.9999883773
O 7.4346354228,0.9409080731,0.8496455526
O 7.7330686415,-1.207381207,1.4747164991
N 1.2070780571,0.472895999,-0.9768193147
C 0.2500632762,1.2682921367,-1.4866626193
C 0.4660950623,2.6197628791,-1.7607996913
C 1.720590628,3.1634256942,-1.4941844616
C 2.7115979406,2.3426724093,-0.9394378478
C 2.4391315804,1.0057013547,-0.6902949622
C 2.0644353129,4.5905192926,-1.756524011
O 1.049268456,5.2732712493,-2.3242462689
O 3.1399230591,5.0880331411,-1.491841914

N -0.0429983519,-1.059955082,1.1679999111
C -1.3947401401,-1.1887032011,1.0991737108
C -2.1947119935,-0.9426853767,2.2176945924
C -1.6019796902,-0.5631466193,3.4173269459
C -0.2115606173,-0.4040579515,3.4674036587
C 0.5252248021,-0.6601891398,2.3227327657
C -2.4882469843,-0.3324094716,4.5966997476
O -3.6841057304,-0.5260447341,4.5972581719
O -1.8057025665,0.1120654731,5.6757861624
N -0.9849935351,-1.803611746,-1.1762025617
C -1.3733020215,-2.2028084721,-2.4014457354
C -2.7066445074,-2.4294536516,-2.7191991823
C -3.6763320994,-2.2437424532,-1.729755596
C -3.2757989795,-1.8309076265,-0.4608722103
C -1.9213720007,-1.6185605596,-0.2054093481
C -5.1339417378,-2.4745621823,-1.9649013914
O -5.4042859893,-2.806919738,-3.2464488738
O -5.9846418692,-2.3786581817,-1.1073779408
H 5.1168383675,1.3966129811,0.0233720094
H 5.745161874,-2.6653498451,1.2523944045
H 3.3500330321,-3.1372342441,0.6550262342
H 8.6267219301,-0.8530276712,1.6431656891
H -0.7043286564,0.8087842293,-1.6996315319
H -0.3427595616,3.2164667845,-2.1617040845
H 3.6799215235,2.7772798414,-0.7231764282
H 1.3617287467,6.1900226278,-2.4421686923

H -3.2717833146,-1.0369350252,2.175212727
H 0.2842103049,-0.0947934334,4.3790976796
H 1.6046528525,-0.5731619077,2.314014847
H -2.4651266345,0.2390286888,6.3838752297
H -0.5728313233,-2.3428686242,-3.118549856
H -2.9785658679,-2.7506889691,-3.7171074164
H -4.030035766,-1.6804555653,0.3009223653
H -6.3703905837,-2.9342658412,-3.2993967551
At -2.6641927826,2.3244427095,0.2563956575
Cl 0.9405643581,-3.815099389,0.143678577
Cl 1.9365495546,-2.0219989499,-2.6998857149

4+2At-b

Charge = -1 Multiplicity = 2

Ru -2.9848232571,0.6527566712,-1.1503931888
N -1.0035231363,1.2368644301,-1.3683932526
C -0.5360643903,2.1036275593,-0.4219894174
C 0.8075204306,2.4712194476,-0.3745593895
C 1.7027491726,1.9376173277,-1.2981625836
C 1.2065528495,1.0885932634,-2.2923627754
C -0.1470019896,0.7775976658,-2.3047788999
C 3.1673036951,2.2149015041,-1.102533697
O 3.5768031407,2.9704705734,-0.2450533708
O 3.9173496312,1.5183239255,-1.9588362485
N -2.7536713763,1.9063086607,0.4545156305
C -3.7224213286,2.2321337468,1.3408814006

C -3.5448854708,3.1605459669,2.3503465074
C -2.3056883335,3.8080920516,2.4636724912
C -1.3004091587,3.4799523676,1.5554639522
C -1.5378475757,2.5289689088,0.5634487139
C -2.020370913,4.8314274322,3.5006766536
O -3.0720962906,5.0416168015,4.3349351754
O -0.9686537982,5.4261359821,3.6193743007
N -2.5947053191,-1.0563325992,-0.0978246614
C -3.6894670257,-1.8209432546,0.2185144164
C -3.5515989071,-3.0468654466,0.8680258047
C -2.2856843923,-3.5188257202,1.2096045125
C -1.169978393,-2.7316975023,0.8870423617
C -1.3695795846,-1.523351027,0.2426908962
C -2.1827412932,-4.8320270553,1.8967695718
O -3.1321928328,-5.5282239936,2.2017099597
O -0.9028867197,-5.1847955146,2.1549303805
N -4.8865620327,-0.0083111413,-0.7744953342
C -6.0287468029,0.6096683574,-1.1586278839
C -7.2836493132,0.0665590242,-0.9387112833
C -7.3869006444,-1.1786420386,-0.3003907719
C -6.2146024055,-1.8268638246,0.0847505373
C -4.97761852,-1.2318158532,-0.1620185852
C -8.6838277287,-1.8445179026,-0.0213723656
O -9.7501044759,-1.1220344022,-0.4492778815
O -8.8088739204,-2.9163867729,0.538044222
H 1.1959501982,3.1254648364,0.3972955083

H 1.8720420312,0.6435846767,-3.0215636897
H -0.5877892578,0.1185065681,-3.0443243231
H 4.8337267713,1.4110798883,-1.5976881366
H -4.6695036071,1.7250633848,1.2056384352
H -4.3567390915,3.3857280425,3.0311001724
H -0.3412754102,3.9778211122,1.6311782714
H -2.7717703688,5.7219186777,4.9659423554
H -4.4153086666,-3.6534950665,1.1132296787
H -0.1628059688,-3.0540162096,1.1232902667
H -0.5285072148,-0.9015428742,-0.0344995641
H -0.9423047032,-6.0531428474,2.5967243326
H -5.8806551792,1.5555330596,-1.6690684126
H -8.1671508175,0.5989845519,-1.269592009
H -6.2873914869,-2.7939324185,0.567413524
H -10.5356176604,-1.6521206739,-0.21903049
Cl -3.6914185796,2.6243238337,-2.3923906069
Cl -3.0256200534,-0.707452854,-3.1523302573
At 6.7691669841,0.0091453591,-0.381499995
At 3.7883765903,-1.5172185724,0.7250293963

4+2At-e

Charge = -1 Multiplicity = 2

Ru 3.8848878008,0.4355958212,-0.7411277342
N 3.8539272483,2.3898633881,-0.0791683626
C 2.6264378039,2.989446246,-0.0508014922
C 2.4899044288,4.3380824045,0.278486

C 3.623080016,5.0932760731,0.578555581
C 4.8773930113,4.4713073636,0.5344711931
C 4.9498226404,3.1271245201,0.1999705663
C 3.4421500803,6.5289171727,0.9238486732
O 2.3722943293,7.1006848959,0.9706319531
O 4.6149416048,7.1575116639,1.1878500332
N 1.853537805,0.8329419702,-0.7257924499
C 0.8776237931,-0.0437960258,-1.0356689956
C -0.4707905509,0.2825175499,-1.0017667686
C -0.8413051082,1.5814774314,-0.6379047896
C 0.1621495618,2.4953621589,-0.3276486139
C 1.5002489557,2.1053596725,-0.3790788805
C -2.2775922546,2.0269861782,-0.5431289851
O -3.104989709,1.0614839311,-0.9187175561
O -2.5798889522,3.1418926622,-0.1617638864
N 3.8343857292,-0.5312225085,1.0520451943
C 3.926075474,-1.8983522465,0.9996132417
C 3.9560117759,-2.6669209373,2.1616226179
C 3.8878050675,-2.0493849671,3.409568365
C 3.7872917492,-0.6506353936,3.4557777609
C 3.7679394507,0.0584153306,2.2679842778
C 3.9215228199,-2.9027644069,4.6235862899
O 4.0230443342,-4.1135021527,4.6167326392
O 3.83230548,-2.185714022,5.7714902885
N 3.8560653031,-1.5296983726,-1.3538217791
C 3.8608608843,-1.947208188,-2.6377001575

C 3.9465412337,-3.2878578214,-2.9833825358
C 4.042165622,-4.2480254978,-1.9672469202
C 4.0481526202,-3.819729566,-0.6407107418
C 3.9544795387,-2.45795231,-0.3555262908
C 4.1435482748,-5.7077401652,-2.2341209979
O 4.1113925025,-6.0030597724,-3.5561194991
O 4.2442746978,-6.5619021836,-1.376359847
H 1.5190933197,4.8181554943,0.2992006087
H 5.7836913821,5.0247790817,0.7478741625
H 5.8893301363,2.589812502,0.1282606397
H 4.378240081,8.0814364566,1.3919902682
H 1.2090980006,-1.0355549692,-1.3183653616
H -1.2251786152,-0.4567505861,-1.2435189874
H -0.1310164249,3.4984684432,-0.0406550131
H -4.0631868571,1.308078899,-0.7741516219
H 4.0282222085,-3.7470775312,2.1196983632
H 3.7298217345,-0.1260718935,4.4017437119
H 3.7073060964,1.1395311081,2.2603818154
H 3.8567279741,-2.8392205913,6.4950278748
H 3.8095575509,-1.1527238312,-3.3743702736
H 3.9466092531,-3.5772384183,-4.0271659886
H 4.1288201063,-4.5597477177,0.1462856091
H 4.1797192676,-6.9742917573,-3.6137017495
Cl 3.9380524773,1.341298169,-2.9969467261
Cl 6.3148939266,0.2332976711,-0.6523702232
At -6.6223038401,1.1213943983,-0.4922839044

At -5.5316198722,-1.9842850934,0.7122120547

4+2At-z

Charge = -1 Multiplicity = 2

Ru -2.8815839134,0.9990316114,-0.1440396948
N -4.0124788639,-0.601777351,0.4816102294
C -3.7182494004,-1.8010630196,-0.1053248391
C -4.4816931061,-2.9388480462,0.1558067605
C -5.5675528878,-2.8583373469,1.026649439
C -5.8668676042,-1.6207863362,1.6139676479
C -5.0739507194,-0.5241783519,1.3139272145
C -6.3590380174,-4.089454349,1.2818748069
O -6.1370834071,-5.1757619558,0.78494009
O -7.3825977576,-3.8875425122,2.1504885412
N -1.9578657409,-0.5495932954,-1.1256168913
C -0.8463385596,-0.449858991,-1.8811096227
C -0.2738943387,-1.5349992732,-2.5303110328
C -0.8838178904,-2.7882317024,-2.4131215651
C -2.0303887694,-2.9024332385,-1.6257676125
C -2.5471389351,-1.7784218596,-0.988105185
C -0.3546589665,-4.0151928745,-3.0670521997
O 0.7377810844,-3.7729985765,-3.8242179715
O -0.8414749364,-5.1232700168,-2.9492711554
N -1.4631372046,1.0441726356,1.3409056317
C -0.565765523,2.0725887599,1.2789278149
C 0.4110680219,2.2413643067,2.2582032593

C	0.4977300115,1.3387224832,3.3149629707	H	2.3473976413,0.7719360914,5.8461238563
C	-0.4071096593,0.2711259774,3.3572950217	H	-2.6991570022,2.960808382,-2.5121460822
C	-1.3657777895,0.1685237152,2.3630101042	H	-1.2927925709,4.9586911298,-3.1058920649
C	1.5516025664,1.5530012743,4.3423144352	H	0.9104048631,4.3237129586,0.5222418118
O	2.2865322913,2.5176338014,4.3874916624	H	1.1779502119,7.3102213487,-2.795966647
O	1.6085619196,0.5481263483,5.2503179931	At	2.7792213159,0.3482788259,-0.5970908816
N	-1.6882037537,2.5702794936,-0.7652994224	Cl	-4.1223142071,2.6447343599,1.1706399566
C	-1.8809724769,3.2973133028,-1.8850262099	Cl	-4.4062797313,1.1537114289,-2.0427018615
C	-1.1024219079,4.4020360961,-2.196465046	At	5.0620986881,-2.0879851965,0.4264240174
C	-0.0823765773,4.7844807611,-1.3158015396		
C	0.1176133924,4.0369819923,-0.1567723171		
C	-0.7012040211,2.9376715093,0.1018747279		
C	0.7945707383,5.962123855,-1.5553895829		
O	0.5508950142,6.564931909,-2.7470472957		
O	1.6417031706,6.3656794835,-0.785644653		
H	-4.2530489328,-3.8902041209,-0.3089049932		
H	-6.7084762743,-1.5112411032,2.2871037255		
H	-5.2636950052,0.4660477241,1.7142072454		
H	-7.8265573507,-4.7514605765,2.2375899576		
H	-0.3999391052,0.5321681296,-1.9511377529		
H	0.6406678074,-1.3970269913,-3.0925332098		
H	-2.4937298176,-3.8759741502,-1.5200536304		
H	1.0257756506,-4.6371233162,-4.1720152562		
H	1.1215639911,3.0565749136,2.2103032395		
H	-0.3677597116,-0.464660955,4.1511015511		
H	-2.0979611629,-0.6291273705,2.3704014384		