Structures, Electronic Properties and Solid State Luminescence of Cu(I) Iodide Complexes with 2,9-dimethyl-1,10-phenanthroline and Aliphatic Aminomethylphosphines or Triphenylphosphine

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The luminescent complexes of triphenylphosphine and two interesting aminomethylphosphines: $P(CH_2N(CH_2CH_2)_2NCH_3)_3$ and $P(CH_2N(CH_2CH_2)_2O)_3$ with copper(I) iodide and 2,9-dimethyl-1,10-phenanthroline (dmp): $[CuI(dmp)PPh_3]$, $[CuI(dmp)P(CH_2N(CH_2CH_2)_2NCH_3)_3]$ and $[CuI(phen)P(CH_2N(CH_2CH_2)_2O)_3]$ are presented in this work. These complexes were characterized in solutions by means of the NMR spectroscopy and their structures were crystallographically determined in the solid state. All complexes crystallize as the discrete dimers bound by π-stacking interactions between dmp rings. The coordination geometry about the Cu(I) centre is pseudo-tetrahedral showing the small flattening and the large rocking distortions. Investigated compounds exhibit intense orange photoluminescence in the solid state (emission peaks at r.t.: $\lambda_{max} = 588\text{-}592$ nm; $\tau = 1.7\text{-}2.2$ and $6.4\text{-}10.0$ μs; at 77 K: $\lambda_{max} = 605\text{-}612$ nm; $\tau = 4.8\text{-}6.5$ and $32\text{-}47$ μs) which is several orders higher than the luminescence of the analogous complexes with 1,10-phenanthroline (phen). To interpret the photophysics of the $[CuI(dmp/phen)PR_3]$ complexes electronic and structural properties of the dmp and phen complexes were characterized using DFT methods. On the basis TDDFT calculations the broad CT bands observed in UV-Vis spectra are interpreted as the two mixed transitions (S_5 and S_6 (or S_4 and S_5): HOMO-2→LUMO and HOMO-2→LUMO+1) from σ(CuI) and σ(CuP) bond to π* phen or dmp ligand (MX, MPR_3)LCT, while the emissions the most probably occur from two triplet states (T_1: HOMO→LUMO and T_2: HOMO-1→LUMO) which are in thermal equilibrium.

Table S1. NMR spectra in CDCl₃ at 298 K.

	dmp	1	3	4 (PPh₃)		1N	1N1	3N	3N3	4N	4N4
P		-60.87	-62.77			-28.5*	-29*; -60*	-28.5*	-29*; -60*	-6*	-6*
C^{2,9}	159.07				157.45	159.08	159.08	159.14	159.02	159.43	159.31
C^{3,8}	123.29				125.51	124.86	124.78	124.92	124.84	124.89	124.83
C^{4,7}	136.07				137.14	136.45	136.35	136.59	136.55	136.27	136.33
C^{5,6}	125.22				125.97	125.33	125.27	125.41	125.36	125.29	125.28
C^{11,12}	145.03				142.86	142.94	142.90	142.88	142.79	143.09	142.99
C^{13,14}	126.58				127.44	127.05	127.00	127.09	127.02	127.00	126.96
C^{Me}	25.64				25.80	27.59	27.65	27.60	27.55	26.84	26.68**
H^{3,8}	7.42 (8.16)				7.79 (8.36)	7.62 (8.36)	7.58 (8.16)	7.64 (8.16)	7.62 (8.32)	under PPh₃	7.43 (8.36)
H^{4,7}	8.04 (8.16)				8.54 (8.14)	8.23 (8.36)	8.20 (8.16)	8.25 (8.16)	8.24 (8.32)	8.16 (8.16)	8.16 (8.16)
H^{5,6}	7.62				8.04	7.77	7.74	7.79	7.77	7.75	7.74
H^{Me}	2.90				2.41	3.20	3.20	3.24	3.23	2.84	2.81
C^{1-P}		58.69 (3.5)	59.31 (4.3)	137.14 (10.8)		not observed	58-55	55.8s*	56.6s*	134.24 (28.5)	136.29 (6.81)
C^{2-P}		55.21 (7.9)	56.11 (8.1)	133.71 (19.8)		55.0-55.2	55.1-54.8	55.53 (4.7)*	55.47 (6.1)*	133.55 (14.4)	133.63 (16.8)
C^{3-P}		55.73	67.57	128.46 (7.06)		54.92	55.02	66.71	66.77	128.21 (9.0)	128.34 (7.7)
C^{4-P}		46.25		128.68		45.79	46.91			129.25 (1.2)	128.99*
H^{1-P}		2.58 (3.03)	2.64(2.95)			2.87	2.73	2.88	2.77		
H^{2-P}		2.50	2.49			2.52	2.53	2.52	2.51		
H^{3-P}		2.31	3.58			2.18	2.27	3.48	3.36		
H^{4-P}		2.15				2.17	2.20				

* - broadened signal, ** - signal of a very low intensity

Fig S1. X-ray structures - view of 1N along dmp plane
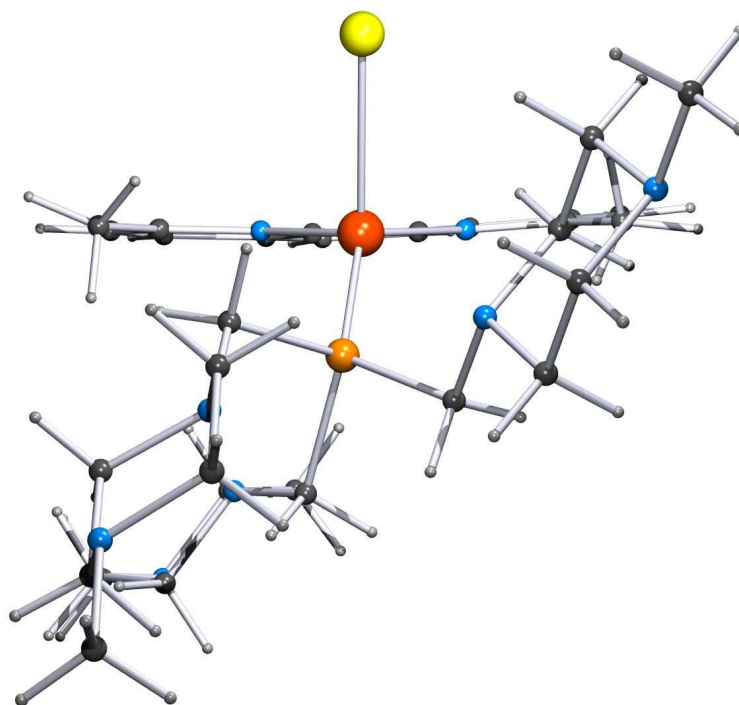
Fig S2. X-ray structures - crystal packing of 1N
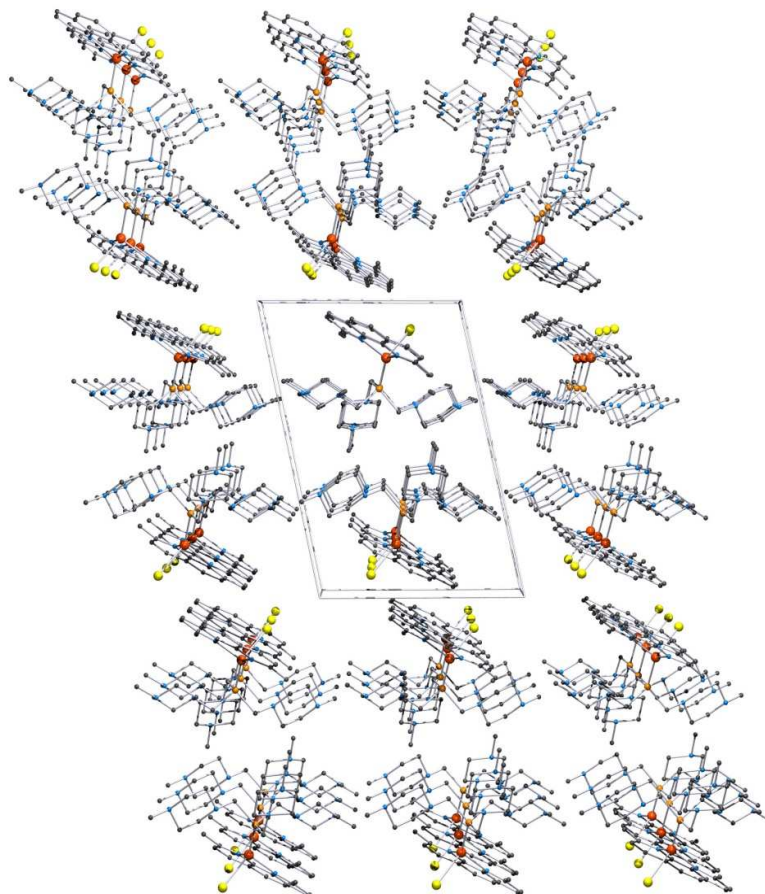
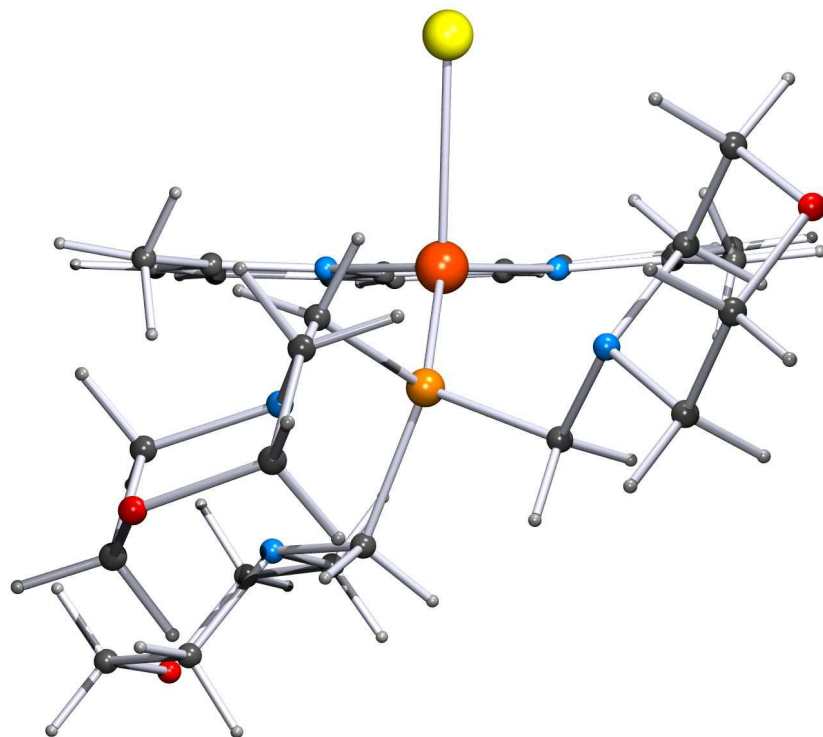**Fig S3. X-ray structures - view of 3N along dmp plane**

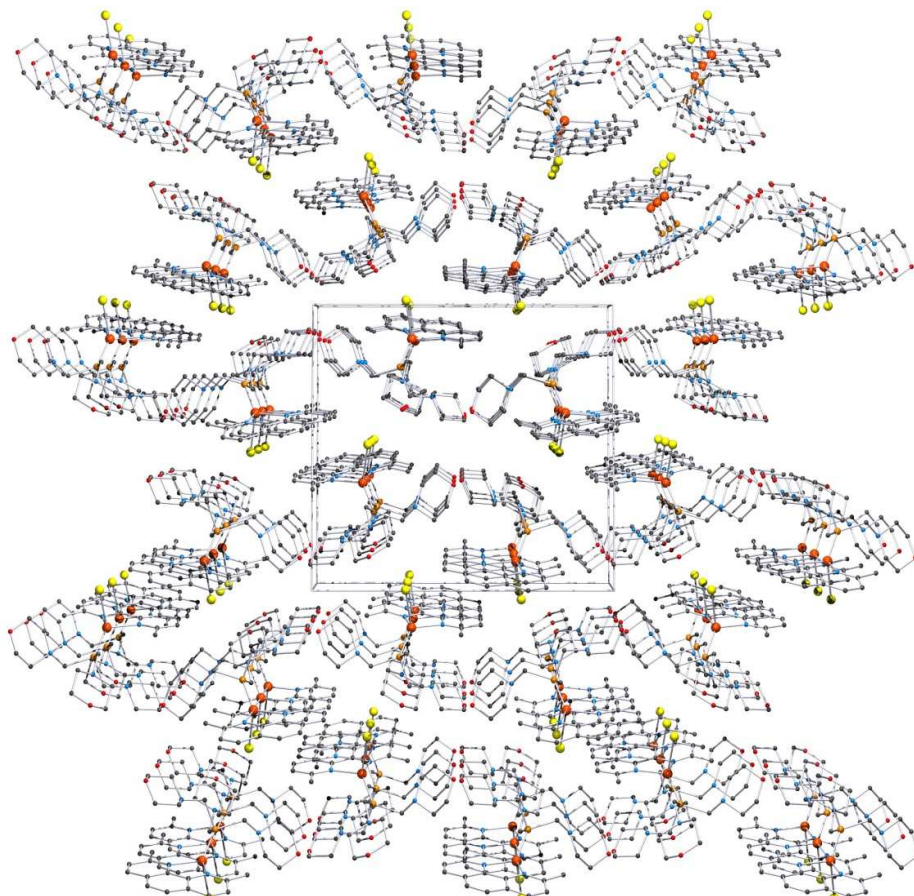**Fig S4. X-ray structures - crystal packing of 3N**

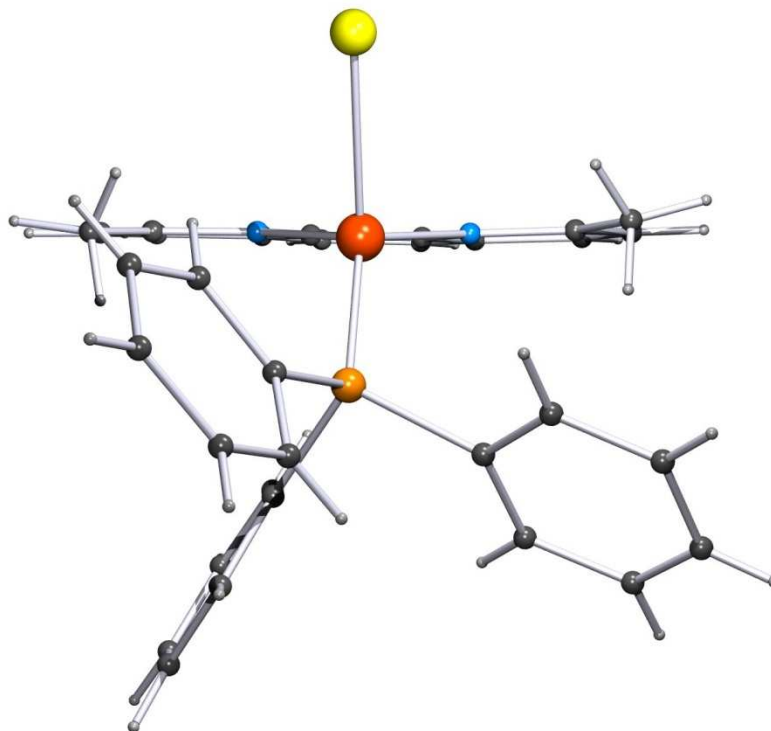**Fig S5. X-ray structures - view of 4N along dmp plane**
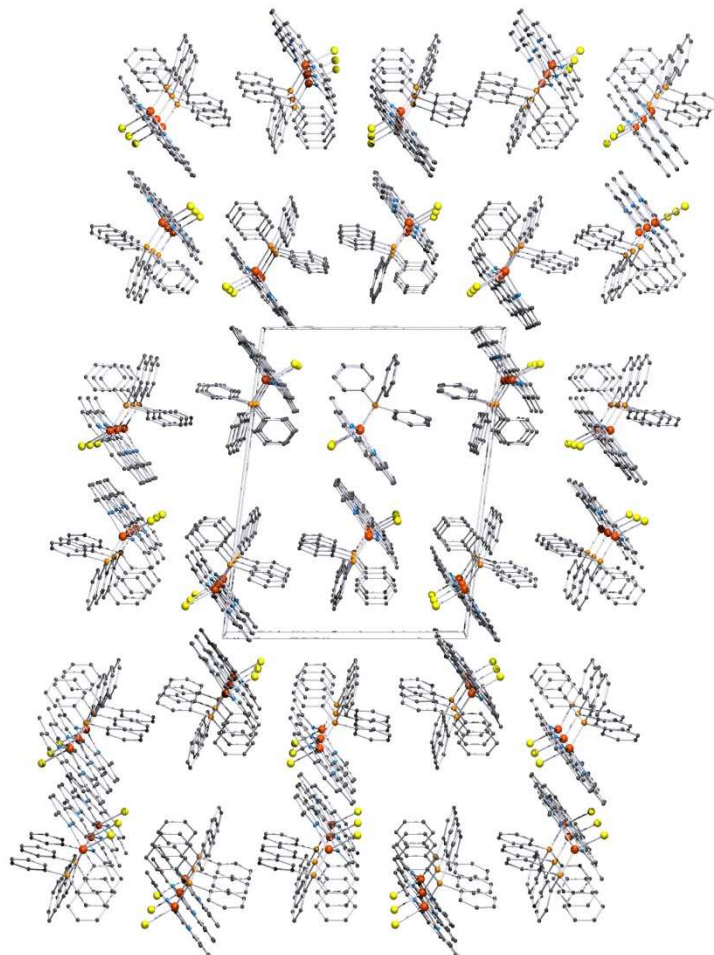

Fig S6. X-ray structures - crystal packing of 4N

Table S2. 1N – molecular orbitals energy and contributions.

	176	177	178	179	180	181	182	183	184
	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O
Energy:	-0.30553	-0.29295	-0.26096	-0.25725	-0.2505	-0.24915	-0.2398	-0.23114	-0.22455
%									
Cu:	4.8	40.3	77.0	32.9	88.9	73.3	13.0	49.4	17.0
I:	0.1	0.3	17.7	1.3	1.6	1.4	0.7	4.1	2.3
phosphine:	1.6	51.9	2.5	1.7	3.6	2.6	6.5	34.8	72.8
dmp:	93.5	7.5	2.7	64.1	5.9	22.7	79.8	11.7	7.9

185	186	187	188	189	190	191	192	193	194	195
(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--V	(A)--V
-0.22122	-0.21705	-0.21294	-0.21149	-0.20884	-0.20393	-0.18546	-0.17952	-0.17581	-0.06963	-0.06532
51.9	0.2	4.1	6.9	6.5	0.5	32.1	10.0	11.9	2.4	0.2
2.5	0.1	0.1	0.6	2.5	0.1	50.4	83.4	76.6	1.7	0.1
27.0	99.1	94.4	90.4	89.4	98.4	11.1	1.7	9.9	1.4	0.7
18.6	0.6	1.4	2.1	1.5	0.9	6.5	4.8	1.6	94.5	99.0

196	197	198	199	200
(A)--V	(A)--V	(A)--V	(A)--V	(A)--V
-0.0201	0.00636	0.02168	0.03153	0.04369
2.1	1.8	47.7	16.1	63.5
1.2	0.2	4.5	3.4	4.1
3.1	0.9	33.6	72.4	23.9
93.6	97.1	14.2	8.0	8.5

Fig S7. 1N UV-VIS spectrum (blue lines – singlet transitions; red lines – triplet transitions)
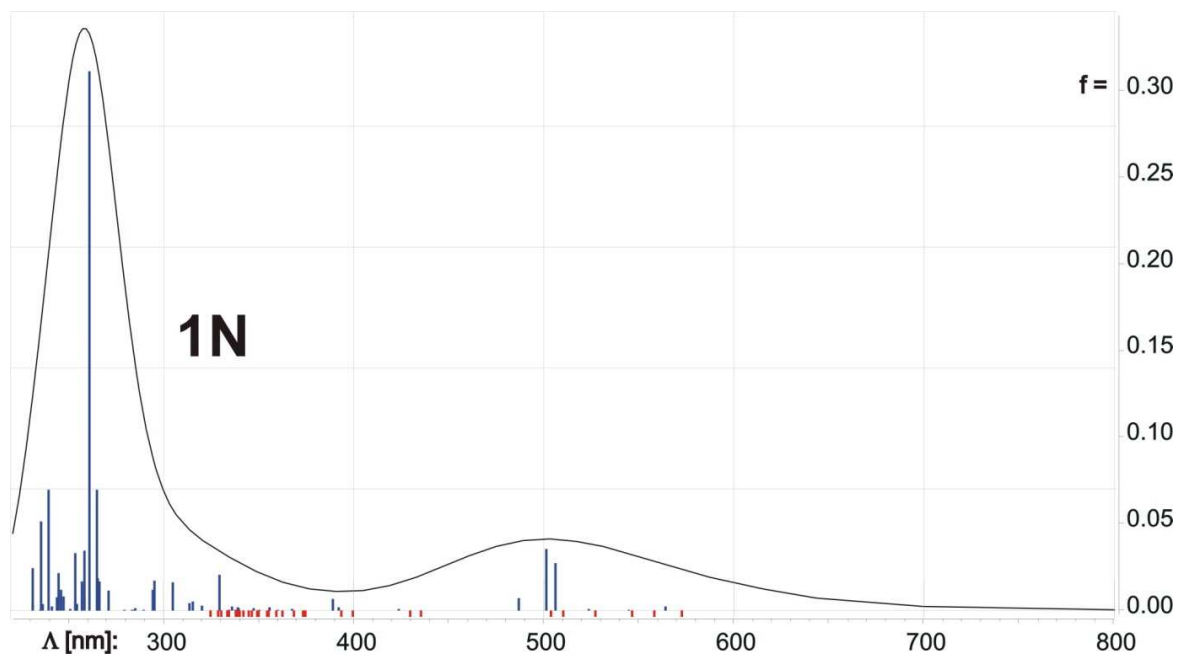
No: λ [nm] osc. str.	Orbitals	%					
S1: 564.17 f=0.0021	193->194	100.00	S5: 501.30 f=0.0353	191->194	37.38	192->195	2.10
S2: 544.91 f=0.0005	192->194	100.00		192->195	62.62	193->194	5.36
S3: 523.96 f=0.0006	193->195	100.00	S6: 487.22 f=0.0072	191->195	100.00	T3: 546.11 f=0.0000 191->194	83.55
S4: 506.47 f=0.0274	191->194	59.27	T1: 572.23 f=0.0000	192->194	5.09	192->194	16.45
	192->195	40.73		193->194	94.91		
			T2: 557.84 f=0.0000	191->194	17.89		
				192->194	74.65		

Table S3. 3N – molecular orbitals energy and contributions.

	166	167	168	169	170	171	172	173	174
	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O
Energy:	-0.26194	-0.25984	-0.2561	-0.25434	-0.24902	-0.24536	-0.24181	-0.2399	-0.23242
%									
Cu:	8.5	9.4	13.5	52.5	11.1	13.4	86.3	75.5	5.5
I:	1.3	1.2	3.3	17.3	1.2	2.1	3.3	1.8	0.2
phosphine:	41.6	55.8	82.4	27.4	82.1	20.2	5.0	9.9	90.1
dmp:	48.5	33.5	0.8	2.8	5.6	64.3	5.4	12.8	4.2

175	176	177	178	179	180	181	182	183	184	185
(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--V	(A)--V	(A)--V	(A)--V
-0.22654	-0.22087	-0.21652	-0.21365	-0.18651	-0.18277	-0.17894	-0.07429	-0.07018	-0.02502	0.00132
39.9	16.1	22.3	57.2	37.2	15.7	18.0	2.6	0.2	2.0	1.6
3.6	1.7	5.3	3.5	47.4	77.2	69.6	1.7	0.1	1.1	0.1
52.8	77.9	69.0	23.6	8.7	1.4	10.7	1.5	0.7	3.2	0.9
3.7	4.3	3.4	15.7	6.7	5.7	1.8	94.3	99.0	93.8	97.4

186	187	188	189	190
(A)--V	(A)--V	(A)--V	(A)--V	(A)--V
0.01703	0.02705	0.03892	0.04294	0.04599
46.8	13.8	63.9	58.0	5.6
4.4	3.2	3.9	2.2	0.2
35.0	75.5	24.0	29.0	14.0
13.9	7.5	8.2	10.8	80.2

Fig S8. 3N UV-VIS spectrum (blue lines – singlet transitions; red lines – triplet transitions)
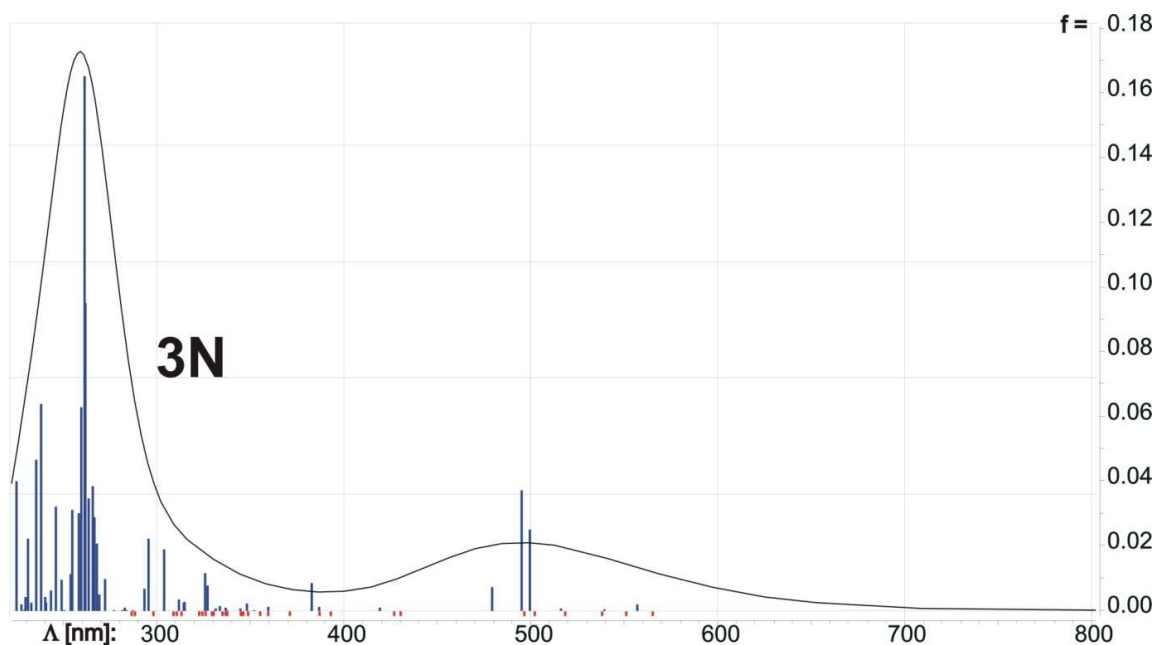
No: λ [nm] osc. str.	Orbitals	%						
S1: 557.20 f=0.0021	181->182	100.00	S5: 495.06 f=0.0373	179->182	41.01		179->182	10.79
S2: 539.43 f=0.0005	180->182	100.00		180->183	58.99		180->182	78.90
S3: 516.16 f=0.0006	181->183	100.00	S6: 479.43 f=0.0074	179->183	100.00		181->182	8.07
S4: 499.78 f=0.0252	179->182	55.85	T1: 565.52 f=0.0000	180->182	7.03	T3: 538.46 f=0.0000	179->182	89.60
	180->183	44.15		181->182	92.97		180->182	10.40
			T2: 551.36 f=0.0000	178->182	2.24			

Table S4. 4N – molecular orbitals energy and contributions.

	141	142	143	144	145	146	147	148	149
	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O
Energy:	-0.31017	-0.30723	-0.30508	-0.30368	-0.26374	-0.2611	-0.25808	-0.2563	-0.25422
%									
Cu:	0.7	16.4	10.5	21.5	3.5	3.5	9.7	3.1	7.2
I:	0.1	0.0	0.0	0.1	0.4	0.2	0.2	0.3	0.2
phosphine:	0.5	1.2	2.2	51.5	93.1	93.8	88.4	17.3	76.7
dmp:	98.7	82.4	87.2	26.9	3.0	2.5	1.7	79.3	15.9

150	151	152	153	154	155	156	157	158	159	160
(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O
-0.25051	-0.24995	-0.24591	-0.23959	-0.23617	-0.23376	-0.21348	-0.20878	-0.18396	-0.17688	-0.17171
45.7	38.5	12.9	6.7	87.8	91.6	60.0	68.1	38.4	18.8	19.7
13.6	12.3	0.4	3.2	3.6	2.3	10.6	8.3	46.4	73.6	68.4
34.3	47.7	83.6	5.1	3.5	3.2	19.7	5.2	9.3	0.7	9.7
6.4	1.5	3.1	85.0	5.1	2.9	9.7	18.3	5.9	6.8	2.2

161	162	163	164	165
(A)--V	(A)--V	(A)--V	(A)--V	(A)--V
-0.06918	-0.06541	-0.02866	-0.02328	-0.02064
2.7	0.2	3.2	1.4	2.9
1.3	0.1	0.2	0.1	0.7
1.5	0.3	94.6	96.1	16.1
94.6	99.4	1.9	2.5	80.3

Fig S9. 4N UV-VIS spectrum (blue lines – singlet transitions; red lines – triplet transitions)

No: λ [nm] osc. str.	Orbitals	%							
S1: 569.93 f=0.0034	160->161	100.00	S4: 501.97 f=0.0007	159->162	100.00			159->161	93.61
S2: 544.49 f=0.0001	157->161	2.17	S5: 485.72 f=0.0543	158->161	100.00			160->161	2.55
	159->161	97.83	S6: 467.35 f=0.0075	158->162	100.00	T3: 530.96 f=0.0000	160->162	100.00
S3: 528.83 f=0.0005	160->162	100.00	T1: 579.74 f=0.0000	160->161	100.00				
			T2: 554.05 f=0.0000	157->161	3.83				
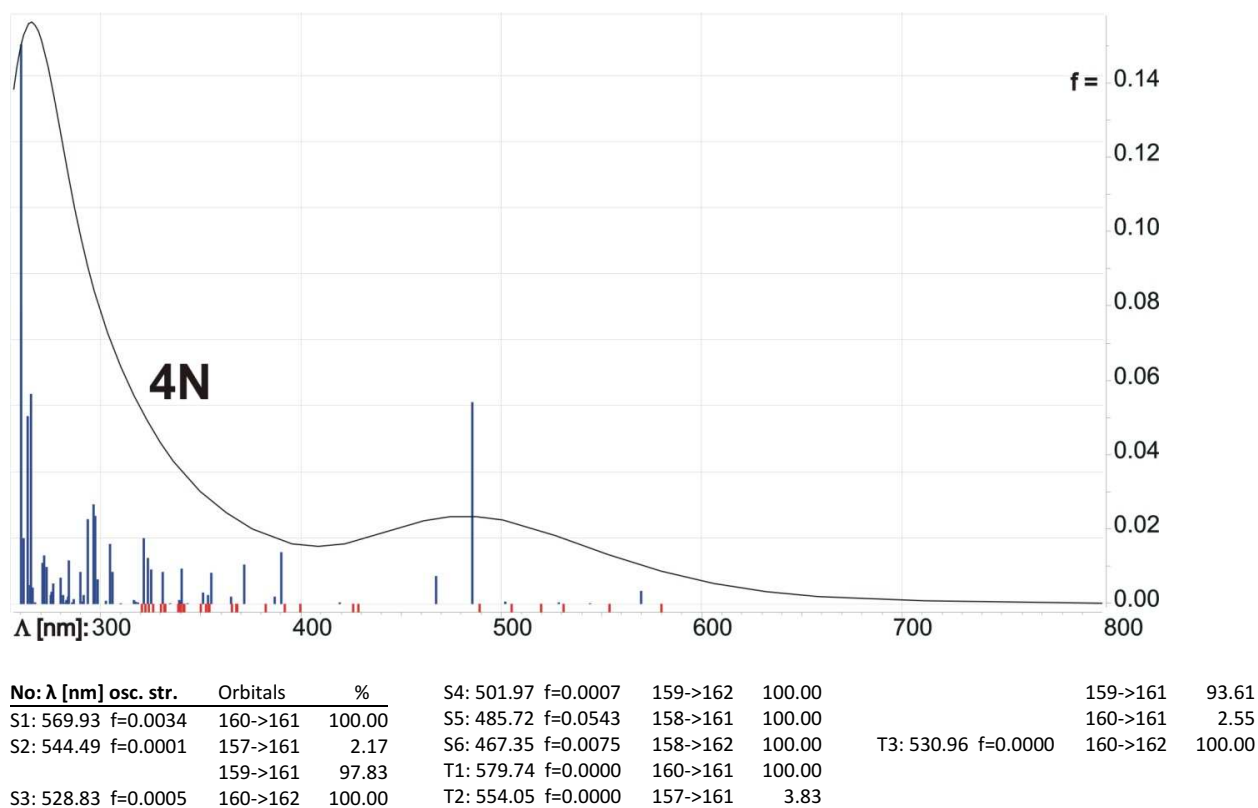
Table S5. 1P – molecular orbitals energy and contributions.

	166	167	168	169	170	171	172	173	174
	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O
Energy:	-0.31692	-0.31466	-0.31166	-0.28685	-0.26619	-0.25426	-0.24946	-0.23831	-0.2382
%									
Cu:	2.6	16.8	1.8	36.7	2.4	19.7	63.1	90.3	88.2
I:	0.1	0.0	0.0	0.4	0.1	3.4	21.0	2.6	2.7
phosphine:	70.1	17.2	91.7	57.4	0.2	1.2	2.2	4.1	4.5
dmp:	27.2	66.0	6.5	5.5	97.3	75.7	13.7	3.1	4.7

175	176	177	178	179	180	181	182	183	184	185
(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O
-0.22442	-0.21877	-0.21465	-0.21239	-0.21224	-0.20923	-0.20814	-0.20398	-0.17828	-0.17369	-0.16981
34.3	35.9	0.3	27.7	20.6	3.6	14.4	12.1	31.9	14.2	19.2
1.3	5.6	0.1	1.9	2.4	0.9	1.9	1.3	52.1	80.1	65.5
61.9	51.5	99.5	63.4	72.4	94.7	80.3	83.6	10.3	1.1	13.6
2.4	7.0	0.2	7.1	4.6	0.8	3.4	3.0	5.7	4.6	1.6

186	187	188	189	190
(A)--V	(A)--V	(A)--V	(A)--V	(A)--V
-0.07599	-0.07478	-0.02931	-0.00119	0.02279
2.3	0.6	2.8	0.7	41.1
1.3	0.3	0.6	0.1	4.4
1.1	0.6	2.4	1.1	35.8
95.3	98.5	94.2	98.0	18.7

Fig S10. 1P UV-VIS spectrum (blue lines – singlet transitions; red lines – triplet transitions)
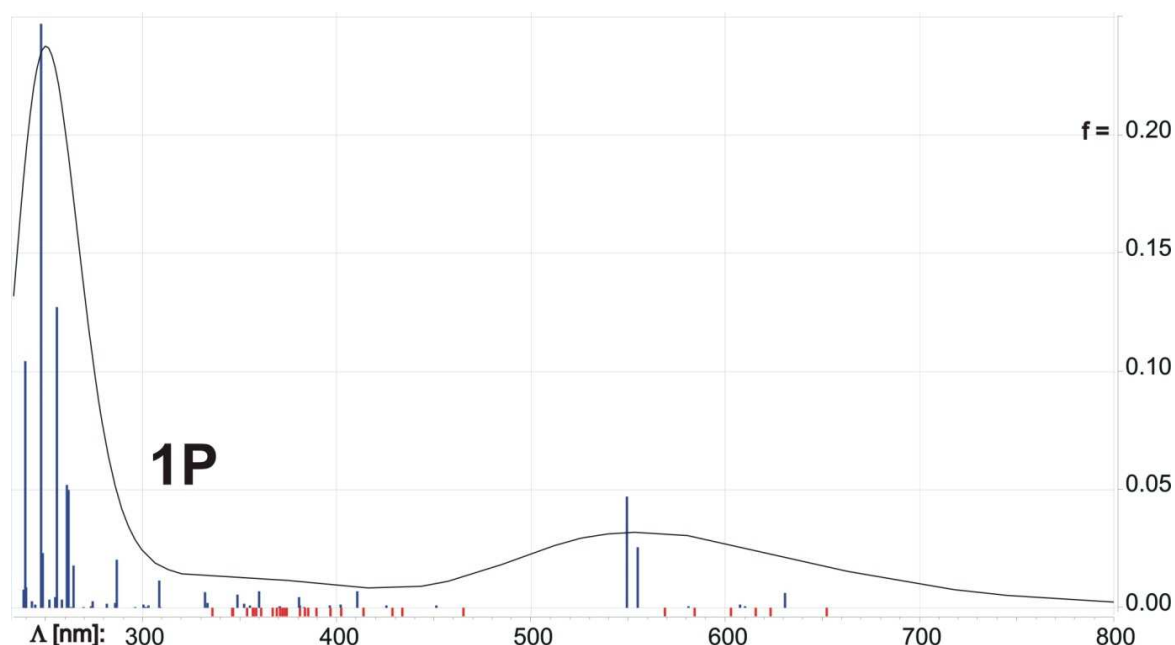
No: λ [nm] osc. str.	Orbitals	%					
						185->187	8.08
S1: 630.85 f=0.0064	183->186	3.29	S4: 581.15 f=0.0006	184->186	14.47	T2: 623.39 f=0.0000	183->186	3.12
	185->186	87.38		184->187	85.53		183->187	2.07
	185->187	9.33	S5: 555.05 f=0.0257	183->186	70.61		184->186	69.44
S2: 610.42 f=0.0006	184->186	77.77		183->187	29.39		184->187	18.27
	184->187	12.90	S6: 549.58 f=0.0470	183->186	24.55		185->186	3.65
	185->187	9.34		183->187	75.45		185->187	3.45
S3: 607.73 f=0.0014	184->186	8.04	T1: 652.43 f=0.0000	183->186	4.41	T3: 615.66 f=0.0000	183->187	6.30
	185->186	8.91		184->186	3.37		185->186	9.53
				185->186	84.14		185->187	84.17

Table S6. 3P – molecular orbitals energy and contributions.

		156	157	158	159	160	161	162	163	164
		(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O
Energy:		-0.30203	-0.29543	-0.2718	-0.26143	-0.2579	-0.25674	-0.25526	-0.2521	-0.24552
%										
Cu:		0.7	29.5	2.7	32.6	6.8	16.5	34.0	7.4	87.7
I:		0.1	0.3	0.1	6.2	1.2	4.0	12.2	0.6	2.8
phosphine:		98.7	65.6	0.3	25.6	59.3	79.1	41.5	90.7	6.1
dmp:		0.5	4.5	97.0	35.6	32.7	0.3	12.4	1.3	3.4

165	166	167	168	169	170	171	172	173	174	175
(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--V	(A)--V
-0.24518	-0.23136	-0.22665	-0.21927	-0.21705	-0.21166	-0.1858	-0.18019	-0.17623	-0.08169	-0.08032
84.0	20.0	42.4	48.8	20.3	10.7	32.4	14.6	19.0	2.4	0.4
2.0	0.7	6.4	4.9	2.4	1.3	51.5	79.5	65.7	1.2	0.2
10.6	77.7	43.5	35.3	72.2	85.2	10.8	1.2	13.7	1.3	0.6
3.5	1.6	7.7	11.0	5.1	2.7	5.3	4.7	1.7	95.1	98.8

176	177	178	179	180
(A)--V	(A)--V	(A)--V	(A)--V	(A)--V
-0.03505	-0.00695	0.01567	0.03083	0.038
2.8	0.7	39.8	61.7	6.8
0.6	0.2	4.4	5.5	1.4
2.8	1.8	38.7	24.1	6.3
93.9	97.3	17.1	8.7	85.5

Fig S11. 3P UV-VIS spectrum (blue lines – singlet transitions; red lines – triplet transitions)
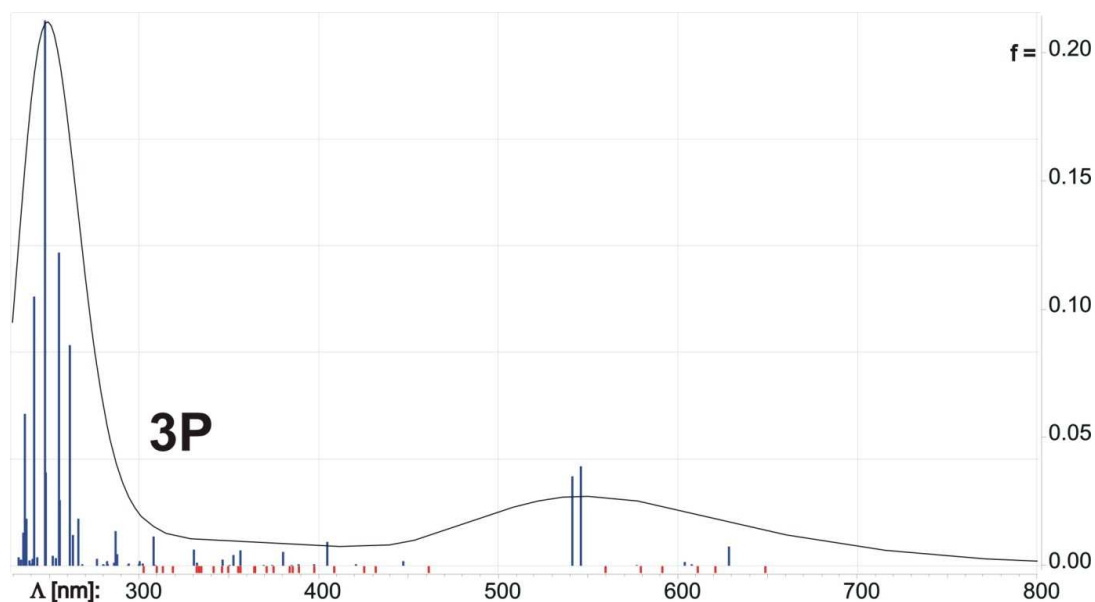
No: λ [nm] osc. str.	Orbitals	%						
S1: 628.66 f=0.0074	171->174	2.49	S4: 577.03 f=0.0004	172->174	10.28	T2: 620.83 f=0.0000	172->174	79.12
	173->174	91.34		172->175	89.72		172->175	12.50
	173->175	6.17	S5: 545.92 f=0.0388	171->174	81.66		173->174	3.07
				171->175	18.34		173->175	5.31
S2: 607.87 f=0.0007	172->174	86.23	S6: 541.21 f=0.0349	171->174	14.53	T3: 611.14 f=0.0000	171->175	5.34
	172->175	9.56		171->175	85.47		172->175	2.55
	173->175	4.21	T1: 648.83 f=0.0000	171->174	3.27		173->174	5.88
S3: 603.90 f=0.0014	172->174	3.35		172->174	3.70		173->175	86.22
	173->174	6.28		173->174	88.52			
	173->175	90.37		173->175	4.51			

Table S7. 4P – molecular orbitals energy and contributions.

	136	137	138	139	140	141	142	143	144
	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O
Energy:	-0.3041	-0.26517	-0.26148	-0.25886	-0.25689	-0.25427	-0.25167	-0.24984	-0.24781
%									
Cu:	25.8	2.8	3.0	6.8	7.9	27.1	7.0	52.8	9.1
I:	0.5	0.1	0.5	0.2	0.1	5.1	2.6	17.7	1.6
phosphine:	59.1	1.5	94.4	91.3	83.9	18.6	86.1	9.2	83.3
dmp:	14.6	95.7	2.1	1.8	8.1	49.2	4.3	20.3	6.0

145	146	147	148	149	150	151	152	153	154	155
(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--O	(A)--V	(A)--V	(A)--V
-0.24507	-0.23867	-0.23607	-0.2142	-0.21152	-0.18205	-0.17388	-0.1691	-0.07454	-0.07389	-0.02853
16.6	89.7	89.9	58.9	70.4	36.2	15.1	17.4	2.5	0.2	4.2
0.5	3.0	1.8	9.2	5.4	47.9	79.4	71.6	1.4	0.1	0.5
78.1	4.0	4.2	22.7	6.6	10.0	0.8	9.1	1.0	0.2	16.9
4.8	3.2	4.1	9.2	17.5	5.9	4.7	1.9	95.1	99.5	78.4

156	157	158	159	160
(A)--V	(A)--V	(A)--V	(A)--V	(A)--V
-0.0259	-0.02257	-0.01343	-0.00714	-0.00082
1.2	1.5	5.0	5.2	2.0
0.4	0.4	0.2	1.5	0.3
85.7	95.9	92.0	91.6	74.9
12.8	2.2	2.8	1.8	22.8

Fig S12. 4P UV-VIS spectrum (blue lines – singlet transitions; red lines – triplet transitions)
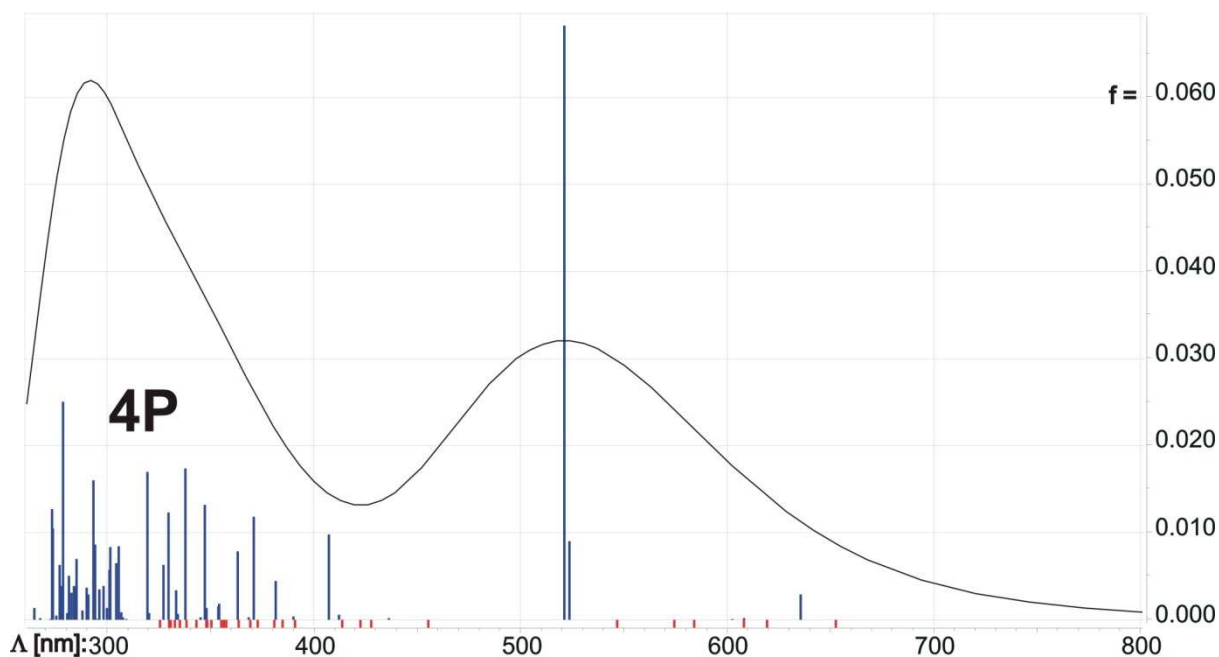
No: λ [nm] osc. str.	Orbitals	%						
S1: 635.48 f=0.0029	152->153	100.00	S5: 523.54 f=0.0090	150->153	11.59	T1: 652.70 f=0.0000	152->153	100.00
S2: 608.33 f=0.0002	151->153	7.72		150->154	88.41	T2: 619.63 f=0.0000	149->153	3.01
	152->154	92.28	S6: 520.99 f=0.0682	150->153	87.52		151->153	82.06
S3: 602.57 f=0.0001	151->153	91.83		150->154	12.48		152->154	14.93
	152->154	8.17	S7: 436.31 f=0.0002	148->153	9.07	T3: 608.51 f=0.0000	151->153	14.36
S4: 574.44 f=0.0000	151->154	100.00		149->153	88.71		152->154	85.64
				149->154	2.22			

Fig S13. 1N - selected orbitals
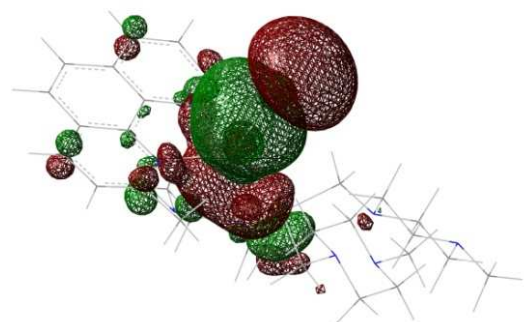
191
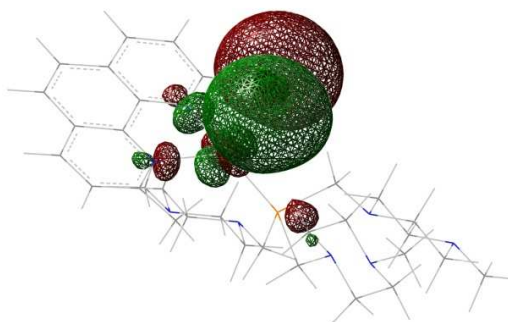
192
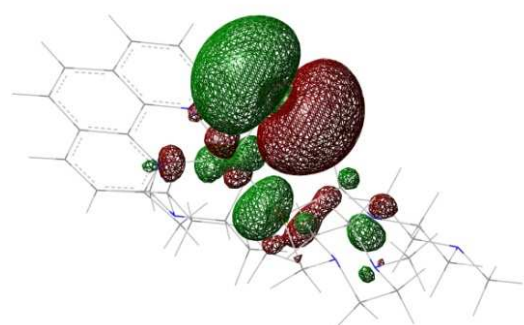
193 - HOMO
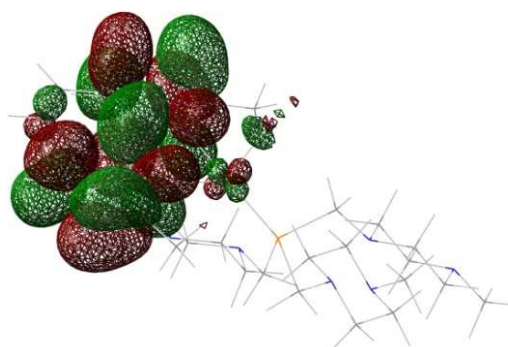
194 - LUMO
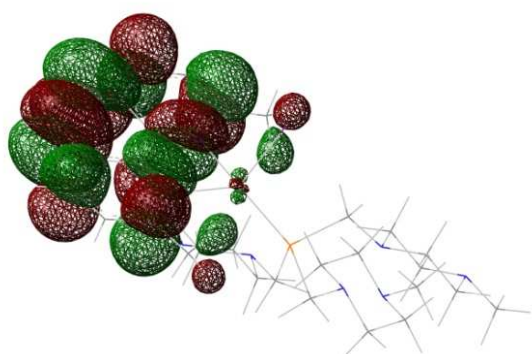
195

Fig S14. 3N - selected orbitals

179

180

181 - HOMO

182 - LUMO

183

Fig S15. 4N - selected orbitals

158
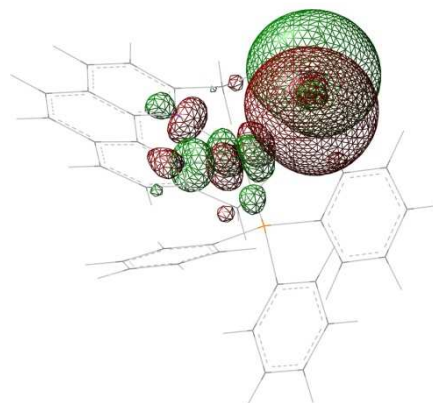
159
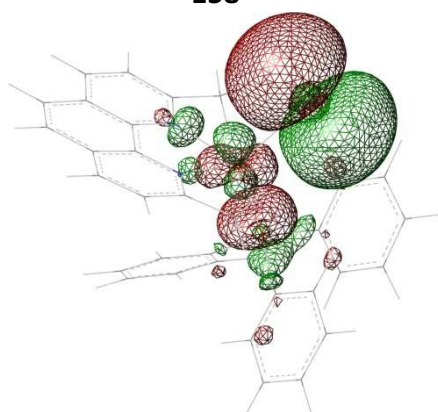
160 - HOMO
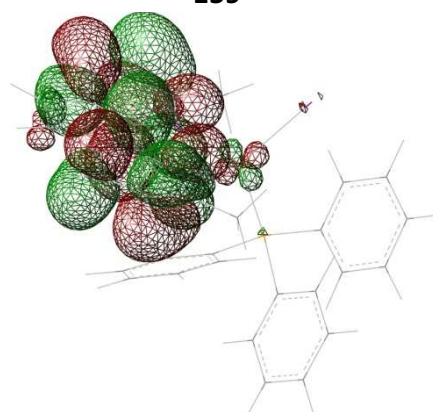
161 - LUMO
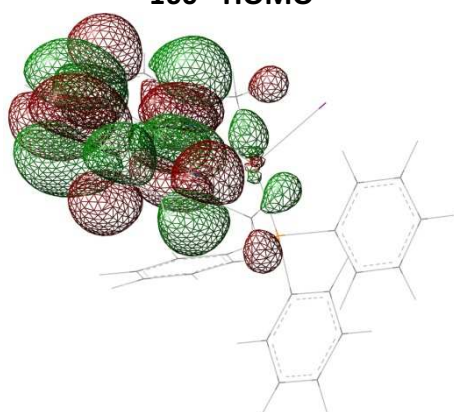
162

Fig S16. 1P - selected orbitals
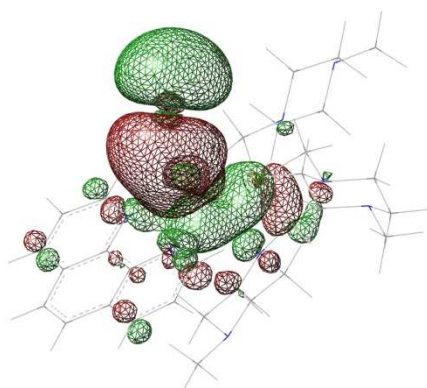
183
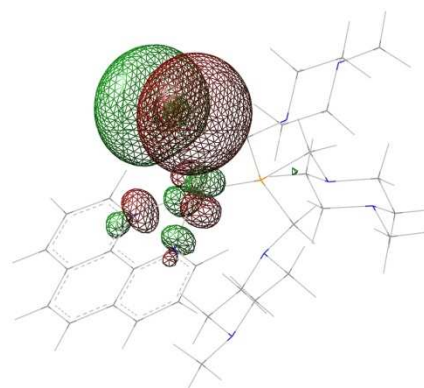
184
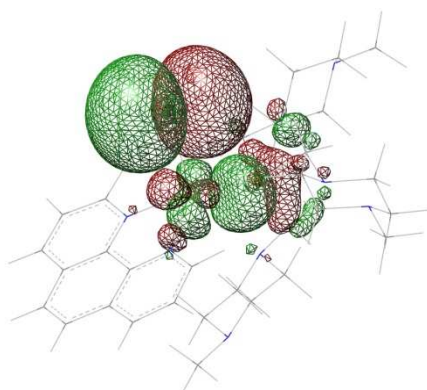
185 - HOMO
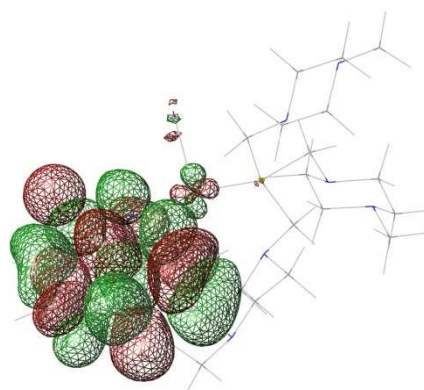
186 - LUMO
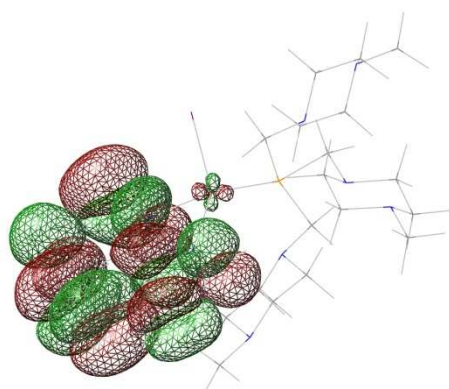
187

Fig S17. 3P - selected orbitals
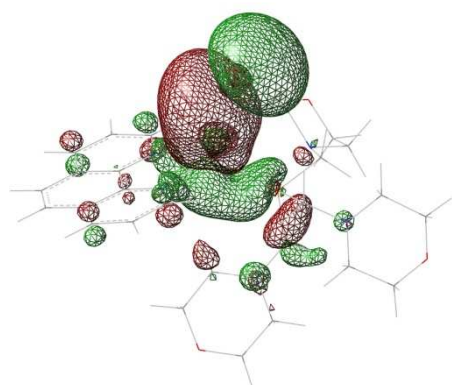
171
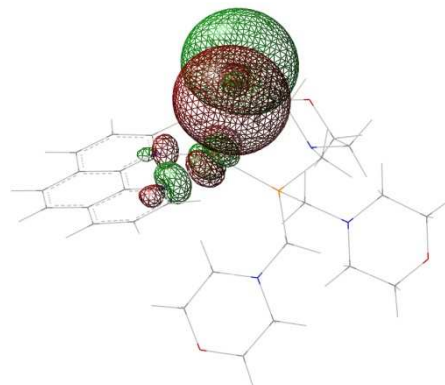
172
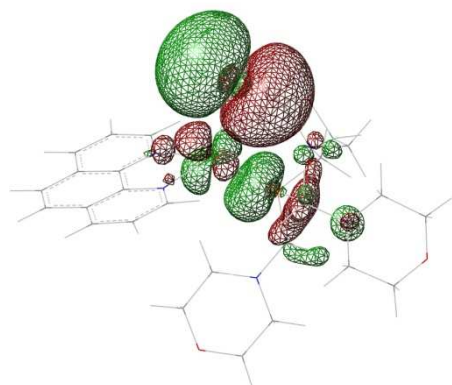
173 - HOMO
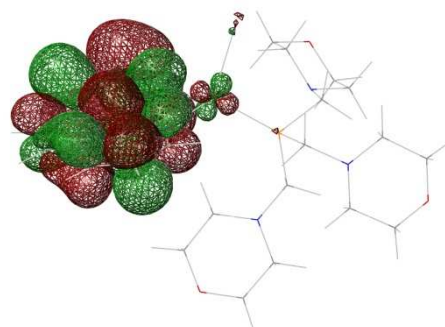
174 - LUMO
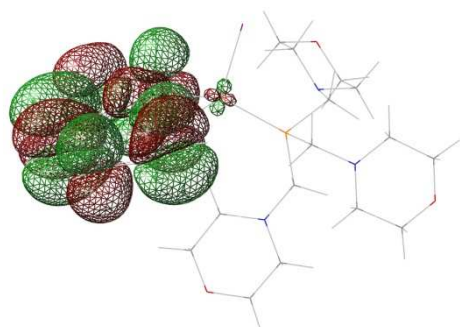
175

Fig S18. 4P - selected orbitals

150

151

152 - HOMO

153 - LUMO

154
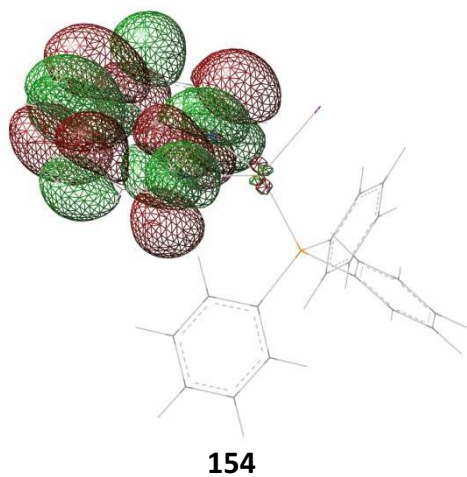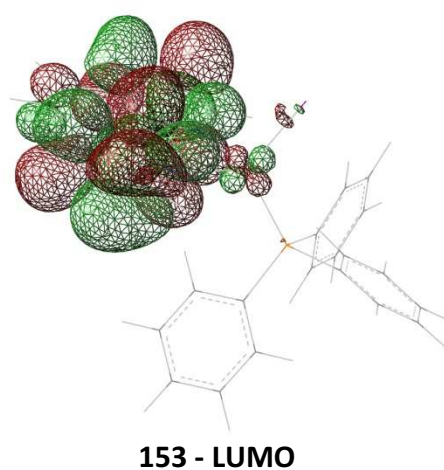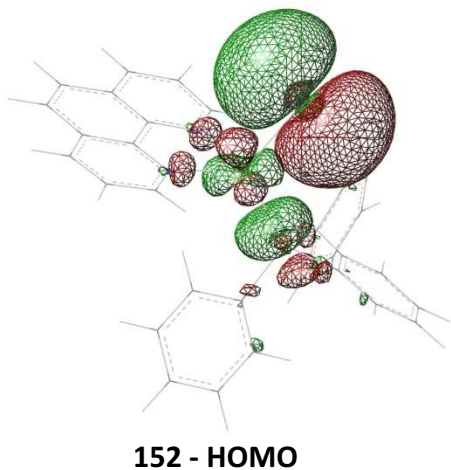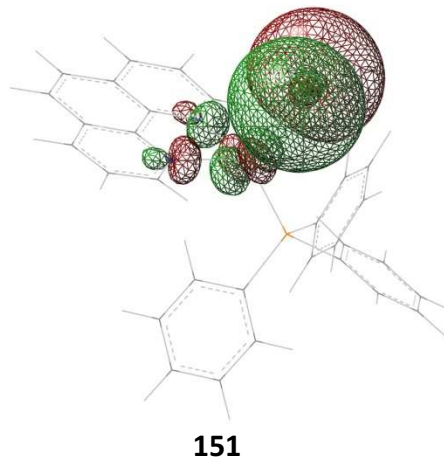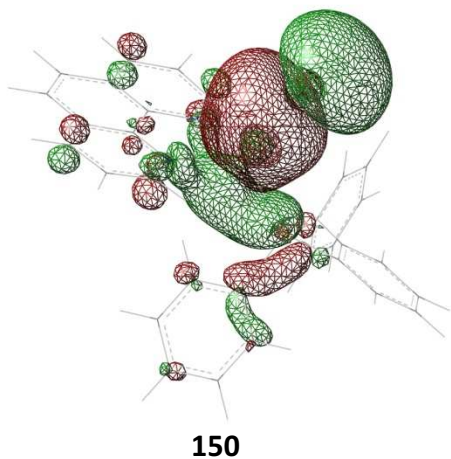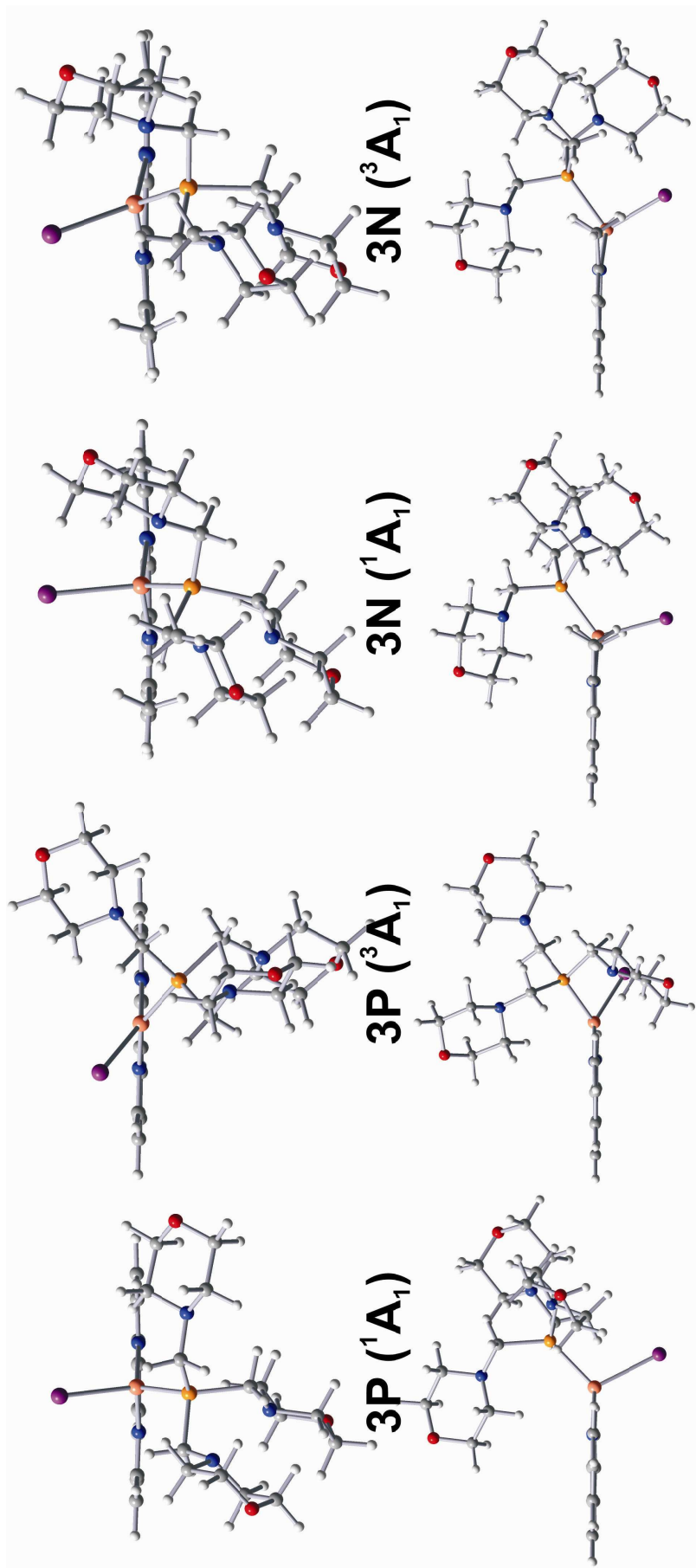
Fig. S19 Molecular structures of **3P** and **3N** in the singlet and triplet states calculated with DFT methods.

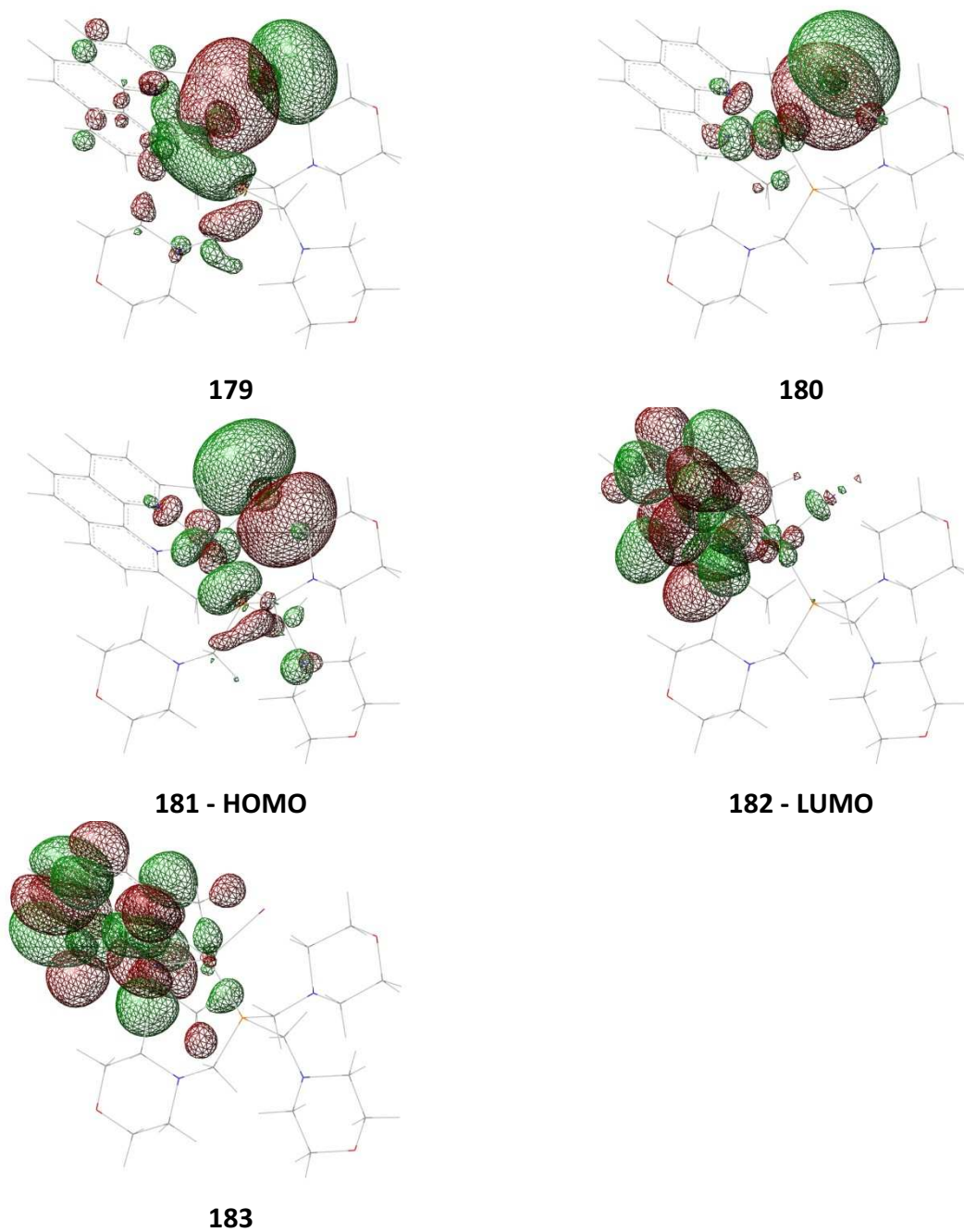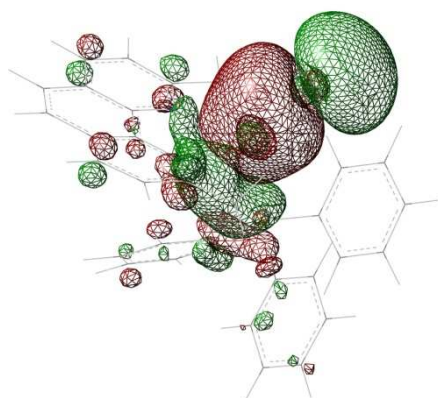| Transition: λ [nm] (oscillator strength)	Orbitals involved	%
1N		
S1: 564.17 f=0.0021		
	193->194	100.00
S2: 544.91 f=0.0005		
	192->194	100.00
S3: 523.96 f=0.0006		
	193->195	100.00
S4: 506.47 f=0.0274		
	191->194	59.27
	192->195	40.73
S5: 501.30 f=0.0353		
	191->194	37.38
	192->195	62.62
S6: 487.22 f=0.0072		
	191->195	100.00
S7: 424.01 f=0.0010		
	186->194	19.62
	187->194	5.11
	188->194	23.89
	189->194	46.39
	190->194	2.86
	192->194	2.13
S8: 392.28 f=0.0019		
	183->194	2.65
	184->194	8.16
	186->195	11.42
	187->195	3.15
	188->194	14.46
	188->195	19.07
	189->194	7.35
	189->195	31.17
	190->195	2.56
S9: 389.45 f=0.0068		
	183->194	3.95
	184->194	13.51
	186->195	5.96
	188->194	34.53
	188->195	7.81
	189->194	9.91
	189->195	19.47
	190->194	4.86
S10: 373.15 f=0.0001		
	188->194	8.34
	190->194	91.66
S11: 367.81 f=0.0010		
	183->195	3.44
	184->195	12.18
	188->195	48.82
	189->195	23.98
	190->195	11.58
S12: 360.46 f=0.0003		
	184->194	10.75
	186->194	40.24
	187->194	11.26
	189->194	37.74
S13: 359.03 f=0.0001		
	188->195	15.22
	190->195	84.78
S14: 355.69 f=0.0016		
	182->194	13.83
	184->194	42.81
	185->194	6.89
	186->194	22.90
	188->194	13.58
S15: 350.46 f=0.0003		
	184->194	4.31
	185->194	86.02
	185->195	7.04
	186->194	2.63
S16: 347.60 f=0.0011		
	193->196	100.00
S17: 345.91 f=0.0001		
	184->195	4.84
	186->195	50.23
	187->195	14.91
	189->195	26.28
	193->196	3.73
S18: 344.45 f=0.0001		
	184->194	2.59
	186->194	11.64
	187->194	85.77
S19: 339.65 f=0.0013		
	181->194	8.48
	192->196	91.52
S20: 339.15 f=0.0017		
	184->195	27.81
	185->194	4.41
	185->195	57.29
	186->195	6.10
	188->195	4.39
S21: 337.89 f=0.0002		
	183->194	2.74
	184->195	34.18
	185->194	3.08
	185->195	38.10
	186->195	11.86
	187->195	7.01
	188->195	3.03
S22: 336.00 f=0.0021		
	180->194	3.81
	181->194	21.16
	182->194	48.78
	183->194	3.11
	184->194	5.93
	186->194	2.72
	188->194	2.25
	191->196	12.24
S23: 334.47 f=0.0004		
	181->194	69.43
	182->194	16.19
	184->194	3.55
	192->196	10.83
S24: 333.31 f=0.0000		
	184->195	12.56
	186->195	10.62
	187->195	76.82
S25: 332.59 f=0.0001		
	181->194	2.68
	182->194	2.76
	183->194	77.37
	184->194	9.85
	184->195	2.78
	191->196	4.56
S26: 329.37 f=0.0208		
	182->194	8.23
	183->194	8.56
	191->196	83.22
S27: 320.20 f=0.0029		
	183->195	96.00
	184->195	4.00
S28: 315.48 f=0.0053		
	178->195	3.39
	180->194	40.96
	181->195	55.65
S29: 313.91 f=0.0042		
	180->195	10.62
	182->195	86.91
	184->195	2.47
S30: 304.93 f=0.0162		
	178->195	11.35
	180->194	37.91
	181->195	45.54
	182->194	5.19
S31: 295.57 f=0.0173		
	178->194	14.96
	179->194	31.51
	180->195	50.87
	182->195	2.66
S32: 294.68 f=0.0117		
	178->194	9.77
	179->194	71.29
	180->195	18.95
S33: 289.48 f=0.0005		
	193->197	100.00
S34: 285.39 f=0.0011		
	186->196	18.13
	187->196	4.94
	188->196	25.02
	189->196	48.56
	190->196	3.36
S35: 284.42 f=0.0003		
	179->195	93.25
	191->197	3.36
	192->197	3.39
S36: 283.32 f=0.0004		
	179->195	3.72
	192->197	96.28
S37: 279.44 f=0.0005		

```
                    178->194    4.01              193->198    2.92    S56: 236.74
                    191->197   95.99              193->199    6.41    f=0.0037
S38: 271.45                         S46: 254.78                                          172->194    4.67
f=0.0114                            f=0.0039                                             177->194   95.33
                    183->196    4.80              182->196    2.72    S57: 235.70
                    184->196   13.81              184->196   50.13    f=0.0512
                    186->196    2.38              185->196   15.10                        193->200   90.31
                    188->196   48.95              186->196   15.52                        193->201    6.26
                    189->196   20.89              188->196    9.77                        193->204    3.44
                    190->196    9.16              193->199    6.76    S58: 235.19
S39: 266.27                         S47: 253.75                       f=0.0005
f=0.0167                            f=0.0045                                              175->194    3.94
                    178->194    4.20              184->196    6.11                        176->194    3.03
                    178->195    2.29              185->196   84.58                        183->197    5.18
                    190->196    3.54              186->196    3.03                        184->197   16.24
                    191->198    2.48              193->199    6.28                        186->197    2.87
                    193->198   84.25                                                      188->197   42.61
                    193->199    3.24    S48: 253.50                                       189->197   19.68
S40: 265.55                             f=0.0331                                          190->197    6.46
f=0.0188                                          184->196    9.00
                                                  185->196    3.00    S59: 231.41
                    178->195    9.57              192->198   11.53    f=0.0033
                    188->196    9.16              192->199    3.52                        172->195    2.84
                    190->196   76.52              193->198    3.52                        175->194   19.52
                    193->198    4.75              193->199   69.43                        176->194   18.41
S41: 265.28                         S49: 250.89                                           177->195   26.17
f=0.0696                            f=0.0008                                              192->200   22.98
                    178->195   56.11              184->196    9.04                        192->201    2.94
                    180->194    6.66              186->196   10.47                        193->201    7.15
                    180->196   11.37              187->196   80.48    S60: 231.20
                    182->196    5.91                                  f=0.0243
                    188->196    5.16    S50: 247.46                                       175->194   11.22
                    190->196   14.78    f=0.0082                                          176->194    5.43
S42: 261.37                                       192->199   97.56                        177->195    9.74
f=0.3118                                          193->199    2.44                        192->200   65.30
                                        S51: 246.27                                       192->201    4.73
                    178->194   52.29    f=0.0119                                          192->204    3.58
                    178->196    4.37              177->194    3.55    T1: 572.23 f=0.0000
                    180->195   12.60              186->197   11.26                        192->194    5.09
                    181->196    8.25              187->197    3.00                        193->194   94.91
                    182->195    3.47              188->197   14.96    T2: 557.84 f=0.0000
                    186->196    3.57              189->197   28.18                        191->194   17.89
                    191->198   10.49              191->199   39.03                        192->194   74.65
                    193->198    4.96    S52: 244.84                                       192->195    2.10
S43: 258.75                             f=0.0214                                          193->194    5.36
f=0.0078                                          183->196   10.02    T3: 546.11 f=0.0000
                    184->196    2.44              186->197    8.30                        191->194   83.55
                    186->196   13.33              188->197   12.40                        192->194   16.45
                    187->196    3.70              189->197   20.66    T4: 526.64 f=0.0000
                    189->196    9.02              191->198    3.17                        191->195    3.78
                    191->198   16.30              191->199   45.45                        193->195   96.22
                    191->199    2.43    S53: 243.85                   T5: 510.08 f=0.0000
                    192->198   49.50    f=0.0076                                          180->195    3.60
                    193->199    3.28              182->196    3.83                        191->195   45.67
S44: 258.39                                       183->196   82.30                        192->194    3.27
f=0.0344                                          184->196    4.99                        192->195   42.78
                    178->194    3.72              191->199    8.88                        193->195    4.68
                    184->196    4.21    S54: 241.52                   T6: 503.65 f=0.0000
                    186->196   35.75    f=0.0025                                          180->195    2.39
                    187->196    9.69              180->196   15.91                        191->195   43.77
                    189->196   22.52              181->196    6.00                        192->195   53.84
                    191->198    3.31              182->196   72.57    T7: 435.02 f=0.0000
                    192->198   17.76              183->196    2.89                        180->195    5.16
                    193->199    3.04              184->196    2.63                        186->194   18.85
S45: 257.26                         S55: 239.51                                           187->194    4.77
f=0.0168                            f=0.0695                                              188->194   22.24
                    191->198   68.15              181->196   95.46                        189->194   40.87
                    192->198   22.52              182->196    4.54
```

190->194	2.40	186->194	31.52	184->195	7.19
191->195	2.18	187->194	8.31	185->194	4.45
192->194	3.53	189->194	33.26	185->195	47.17
T8: 429.23 f=0.0000		**T15: 359.11**		191->196	7.09
176->194	3.10	f=0.0000		192->196	31.18
178->194	10.83	188->195	13.40	**T24: 338.54**	
178->196	3.62	190->195	86.60	f=0.0000	
179->195	2.59	**T16: 355.09**		184->195	39.09
180->195	42.70	f=0.0000		186->195	14.81
181->194	3.88	178->194	14.69	188->195	6.36
182->195	18.48	180->194	6.71	191->196	28.99
183->195	4.20	180->195	2.83	192->196	10.74
186->194	2.29	181->194	11.16	**T25: 337.76**	
189->194	3.13	184->194	33.60	f=0.0000	
191->195	5.18	185->194	10.52	184->195	18.92
T9: 399.17 f=0.0000		186->194	7.72	185->194	3.89
183->194	3.37	188->194	12.77	185->195	38.36
184->194	9.14	**T17: 354.28**		186->195	5.04
186->195	12.65	f=0.0000		187->195	5.49
187->195	3.32	178->194	17.92	191->196	19.56
188->194	14.20	180->194	2.49	192->196	8.74
188->195	17.60	180->195	5.50	**T26: 334.03**	
189->194	7.68	181->194	14.05	f=0.0000	
189->195	29.88	182->194	3.51	180->194	14.62
190->195	2.18	184->194	12.29	181->194	5.25
T10: 393.14		185->194	7.81	182->194	46.27
f=0.0000		185->195	2.64	183->194	19.59
180->194	3.13	186->194	24.45	184->194	14.26
183->194	7.08	188->194	5.32	**T27: 333.34**	
184->194	12.23	189->194	4.01	f=0.0000	
186->195	6.29	**T18: 349.54**		184->195	13.31
188->194	32.43	f=0.0000		186->195	8.81
188->195	8.12	178->194	2.96	187->195	75.64
189->194	7.08	181->194	7.76	188->195	2.24
189->195	19.92	185->194	57.45	**T28: 330.04**	
190->194	3.72	185->195	3.07	f=0.0000	
T11: 374.18		187->194	4.96	178->194	7.67
f=0.0000		193->196	23.79	180->194	21.76
180->194	39.20	**T19: 348.94**		181->194	7.67
182->194	28.40	f=0.0000		182->194	2.85
183->194	3.84	181->194	2.37	183->194	57.53
184->194	2.77	185->194	18.03	188->194	2.52
185->194	3.78	189->195	2.58	**T29: 328.54**	
188->195	2.17	193->196	77.03	f=0.0000	
190->194	19.84	**T20: 346.11**		178->194	41.17
T12: 373.02		f=0.0000		180->194	7.86
f=0.0000		184->195	4.68	181->194	40.44
180->194	7.01	186->195	48.34	182->194	5.59
182->194	7.32	187->195	14.24	183->194	4.93
184->194	2.43	189->195	27.86	**T30: 324.27**	
188->194	9.41	193->196	4.88	f=0.0000	
190->194	73.82	**T21: 344.30**		178->195	52.65
T13: 368.40		f=0.0000		181->195	37.59
f=0.0000		184->194	3.14	183->195	6.51
183->195	2.59	186->194	13.06	191->196	3.25
184->195	13.17	187->194	83.80	**3N**	
186->195	2.22	**T22: 341.67**		**S1: 557.20 f=0.0021**	
188->195	48.13	f=0.0000		181->182	100.00
189->195	23.59	178->195	3.22	**S2: 539.43 f=0.0005**	
190->195	10.29	185->195	4.87	180->182	100.00
T14: 362.08		191->196	37.12	**S3: 516.16 f=0.0006**	
f=0.0000		192->196	50.91	181->183	100.00
178->194	3.21	193->196	3.89	**S4: 499.78 f=0.0252**	
181->194	9.99	**T23: 339.54**		179->182	55.85
182->194	2.94	f=0.0000		180->183	44.15
184->194	10.77	178->195	2.91	**S5: 495.06 f=0.0373**	

Column 1:

179->182 41.01
180->183 58.99
S6: 479.43 f=0.0074
179->183 100.00
S7: 419.10 f=0.0010
176->182 11.28
177->182 7.16
178->182 79.37
180->182 2.19
S8: 386.83 f=0.0013
175->182 6.21
176->183 7.99
177->182 11.13
177->183 6.99
178->183 67.68
S9: 383.07 f=0.0085
175->182 22.99
176->182 5.74
177->182 53.18
178->183 18.09
S10: 359.77
f=0.0012
175->183 19.25
176->183 6.53
177->183 71.72
178->183 2.49
S11: 352.17
f=0.0002
172->182 3.66
173->182 2.21
175->182 12.26
176->182 46.57
177->182 19.08
178->182 16.22
S12: 348.24
f=0.0022
171->182 2.29
173->182 23.93
175->182 38.37
176->182 28.44
177->182 6.96
S13: 344.55
f=0.0008
181->184 100.00
S14: 337.85
f=0.0003
175->183 5.43
176->183 60.04
177->183 10.05
178->183 13.19
180->184 11.30
S15: 337.05
f=0.0009
172->182 7.48
176->183 9.37
180->184 83.15
S16: 333.65
f=0.0014
170->182 4.23
172->182 26.61
173->182 41.68
175->182 14.30
176->182 6.12
179->184 7.07
S17: 331.75
f=0.0007

Column 2:

171->182 2.30
172->182 59.18
173->182 16.07
175->182 6.41
175->183 3.11
177->182 2.44
179->184 2.27
180->184 8.22
S18: 330.99
f=0.0003
172->182 3.74
173->183 4.32
174->182 5.39
175->183 65.42
176->183 11.33
177->183 9.80
S19: 327.27
f=0.0078
171->182 2.95
173->182 6.53
174->182 36.61
175->183 3.45
179->184 50.45
S20: 325.93
f=0.0117
174->182 55.73
179->184 44.27
S21: 314.84
f=0.0028
170->182 5.34
171->182 36.90
172->183 34.48
173->182 2.33
174->182 3.26
174->183 17.69
S22: 314.39
f=0.0024
171->182 8.62
172->183 6.97
174->183 84.41
S23: 311.96
f=0.0035
170->183 4.60
171->183 6.16
173->183 84.10
175->183 5.14
S24: 303.77
f=0.0190
166->183 4.63
167->183 5.22
170->182 2.78
171->182 23.98
172->183 59.31
173->182 4.08
S25: 295.68
f=0.0224
166->182 11.56
167->182 14.43
170->183 7.26
171->183 62.53
173->183 4.21
S26: 293.34
f=0.0069
166->182 4.92
167->182 3.90
168->182 28.12

Column 3:

S27: 287.25
f=0.0003
S28: 283.63
f=0.0003
S29: 282.91
f=0.0009
S30: 282.53
f=0.0001
S31: 281.49
f=0.0002
S32: 277.23
f=0.0003
S33: 274.80
f=0.0000
S34: 272.56
f=0.0098
S35: 269.25
f=0.0050
S36: 267.97
f=0.0207
S37: 266.89
f=0.0289
S38: 265.93

Column 4:

169->182 63.06
181->185 100.00
170->182 81.08
171->182 13.91
178->184 5.01
169->183 3.87
170->182 5.20
176->184 9.56
177->184 6.55
178->184 74.84
166->183 3.32
167->183 4.12
168->183 24.93
169->183 61.83
178->184 3.59
179->185 2.22
180->185 100.00
167->182 3.29
179->185 96.71
170->183 87.38
171->183 12.62
166->182 29.84
166->183 4.50
167->182 56.09
168->182 5.06
169->182 4.50
168->182 59.87
169->182 29.94
170->182 2.33
175->184 2.16
177->184 5.70
167->183 7.08
168->182 7.81
169->182 3.06
175->184 12.95
176->184 4.34
177->184 40.55
181->186 24.22
167->183 7.40
175->184 3.17
177->184 11.93
181->186 72.33
181->187 5.17

f=0.0385
167->183 62.52
169->183 4.15
171->182 3.18
171->184 6.26
173->184 3.60
175->184 4.52
177->184 15.78

S39: 263.55
f=0.0347
166->182 10.50
166->183 63.48
167->183 6.48
168->183 12.75
171->184 4.34
173->184 2.45

S40: 261.69
f=0.0951
166->182 12.59
167->182 4.27
168->183 52.53
169->183 25.21
179->186 5.40

S41: 261.20
f=0.1654
166->182 15.40
166->183 12.60
167->182 10.29
168->183 20.75
169->183 10.24
170->183 2.59
171->183 6.92
172->184 3.76
179->186 11.38
180->186 6.06

S42: 259.44
f=0.0629
166->182 3.90
179->186 5.46
180->186 78.34
181->186 2.84
181->187 9.47

S43: 258.21
f=0.0301
179->186 76.98
179->187 2.82
180->186 10.61
181->186 3.61
181->187 5.98

S44: 254.75
f=0.0312
176->184 3.74
177->184 3.06
180->186 12.72
181->186 5.13
181->187 75.35

S45: 254.02
f=0.0114
175->184 5.84
176->184 63.86
177->184 9.43
178->184 15.60
181->187 5.27

S46: 250.57
f=0.0003
173->184 6.80

S47: 249.20
f=0.0096
180->187 100.00

S48: 246.14
f=0.0323
178->185 8.29
179->186 5.87
179->187 85.85

S49: 243.47
f=0.0062
176->185 9.64
177->185 7.73
178->185 73.83
179->187 8.80

S50: 240.81
f=0.0026
173->184 9.88
174->184 90.12

S51: 240.52
f=0.0042
170->184 7.36
171->184 8.57
172->184 5.02
173->184 65.22
174->184 7.45
175->184 6.37

S52: 238.21
f=0.0639
171->184 3.49
172->184 94.11
173->184 2.40

S53: 235.32
f=0.0468
181->188 91.76
181->189 4.92
181->192 3.32

160->182 14.32
162->182 5.29
165->182 4.18
175->185 19.91
176->185 6.18
177->185 50.12

S54: 232.84
f=0.0008
158->182 4.32
160->183 3.64
163->182 5.16
164->182 13.13
165->182 68.05
178->185 2.60
178->186 3.10

S55: 232.74
f=0.0024
180->188 86.74
180->189 5.14
180->192 4.18
181->189 3.94

S56: 231.00
f=0.0224

S57: 229.88
f=0.0043
160->182 41.48
162->182 12.58

175->184 66.48
176->184 15.95
177->184 10.77

165->183 7.11
175->185 3.63
177->185 11.44
180->188 3.34
181->189 20.42

S58: 229.30
f=0.0005
160->182 8.57
162->182 4.18
177->185 7.07
179->188 2.83
180->188 2.97
181->188 3.11
181->189 71.26

S59: 227.48
f=0.0019
165->182 3.05
177->186 9.43
178->186 41.24
179->188 21.07
179->189 4.21
180->188 3.76
180->189 17.25

S60: 224.99
f=0.0400
171->184 3.35
177->186 4.91
178->186 27.34
179->188 29.83
180->189 34.56

T1: 565.52 f=0.0000
180->182 7.03
181->182 92.97

T2: 551.36 f=0.0000
178->182 2.24
179->182 10.79
180->182 78.90
181->182 8.07

T3: 538.46 f=0.0000
179->182 89.60
180->182 10.40

T4: 518.85 f=0.0000
179->183 3.96
181->183 96.04

T5: 502.75 f=0.0000
171->183 3.35
179->183 39.64
180->182 2.79
180->183 49.04
181->183 5.17

T6: 497.30 f=0.0000
171->183 3.24
179->183 48.58
180->183 48.18

T7: 431.20 f=0.0000
171->183 11.68
173->183 4.06
176->182 8.77
177->182 6.28
178->182 61.40
179->183 4.54
180->182 3.27

T8: 427.53 f=0.0000
162->182 3.09
166->182 5.70
167->182 4.07

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              170->183   3.54          175->182  43.86                          172->183   34.96
              171->183  36.33          176->182  31.04                          179->184    6.98
              172->182   3.26          177->182   8.87    T25: 314.13
              173->183  16.12    T16: 346.01             f=0.0000
              174->183   2.88    f=0.0000                                       173->183    9.92
              176->182   3.38                            179->184   2.16        174->183   90.08
              178->182  16.30                            181->184  97.84    T26: 311.65
              179->183   5.32    T17: 338.72                                 f=0.0000
T9: 393.80 f=0.0000              f=0.0000                                       170->183    9.41
              175->182  10.68          179->184  26.52                          171->183   17.71
              176->182   3.60          180->184  69.46                          172->183    6.30
              176->183   7.52          181->184   4.01                          173->183   57.79
              177->182  18.46    T18: 337.96                                    174->183    5.39
              177->183   5.56    f=0.0000                                       175->183    3.41
              178->183  54.18          175->183   4.87    T27: 310.09
T10: 387.97                            176->183  65.68    f=0.0000
f=0.0000                               177->183  10.27                          162->183    3.71
              171->182   8.41          178->183  16.29                          166->183   11.00
              173->182   2.46          179->184   2.89                          167->183   12.89
              174->182   3.62    T19: 336.01                                    171->183    4.49
              175->182  15.62    f=0.0000                                       171->184    6.48
              176->182   4.48                            166->183   3.03        172->183   48.04
              176->183   3.30                            167->183   2.52        173->183    4.17
              177->182  33.69                            176->183   4.25        173->184    2.87
              178->183  28.43                            179->184  58.86        179->184    6.34
T11: 371.86                            180->184  31.35    T28: 299.28
f=0.0000                         T20: 331.27             f=0.0000
              162->183   2.31    f=0.0000                                       166->182    5.93
              170->182   4.35                            170->182   2.31        167->182    5.42
              171->182  43.59          171->182   4.10                          168->182   26.10
              173->182  33.53          172->182   2.70                          169->182   62.54
              174->182   3.59          173->182  20.77    T29: 289.51
              175->182   4.18          174->182   6.84    f=0.0000
              177->182   8.46          175->182   3.14                          159->182   26.43
T12: 360.58                            175->183  46.58                          160->183    2.89
f=0.0000                               176->183   6.57                          161->182    2.88
              175->183  19.90          177->183   6.97                          162->183   12.57
              176->183   7.01    T21: 330.67                                    166->183    3.71
              177->183  70.62    f=0.0000                                       166->185    4.80
              178->183   2.47          170->182   6.61                          167->183    5.57
T13: 356.20                            171->182  14.12                          167->185    3.91
f=0.0000                               173->182  32.20                          171->184   16.94
              166->182  10.50          175->182  10.36                          172->183   10.58
              167->182  10.65          175->183  25.90                          173->184    7.26
              171->183   8.54          176->183   6.78                          180->185    2.47
              172->182  29.70          177->183   4.03    T30: 287.84
              173->183   2.87    T22: 326.89             f=0.0000
              175->182   3.95    f=0.0000                                       181->185  100.00
              176->182  19.24          166->182  20.03    4N
              177->182   7.72          167->182  18.68    S1: 569.93 f=0.0034
              178->182   6.83          172->182  46.24                          160->161  100.00
T14: 349.91                            174->182  15.05    S2: 544.49 f=0.0001
f=0.0000                         T23: 325.17                                    157->161    2.17
              166->182  12.90    f=0.0000                                       159->161   97.83
              167->182  10.24          167->182   2.91    S3: 528.83 f=0.0005
              171->183   4.60          170->182   2.23                          160->162  100.00
              172->182   8.94          171->182   8.22    S4: 501.97 f=0.0007
              173->183   2.61          172->182   5.82                          159->162  100.00
              175->182   8.79          174->182  72.88    S5: 485.72 f=0.0543
              176->182  27.08          175->183   2.90                          158->161  100.00
              177->182  13.17          176->183   2.19    S6: 467.35 f=0.0075
              178->182  11.67          177->182   2.84                          158->162  100.00
T15: 347.11                      T24: 323.53             S7: 419.35 f=0.0003
f=0.0000                         f=0.0000                                       156->161    5.25
              171->182   7.75          166->183  30.33                          157->161   91.85
              173->182   8.48          167->183  27.72                          159->161    2.90
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S8: 390.48 f=0.0139
156->161 75.61
157->161 3.69
157->162 20.69

S9: 387.22 f=0.0019
156->161 19.28
156->162 3.15
157->162 77.57

S10: 371.68 f=0.0106
160->163 100.00

S11: 365.37 f=0.0019
156->162 96.17
157->162 3.83

S12: 355.30 f=0.0084
159->163 8.51
160->164 89.39
160->165 2.11

S13: 353.80 f=0.0025
159->163 91.87
160->164 8.13

S14: 351.20 f=0.0031
155->161 3.35
160->164 2.81
160->165 93.85

S15: 343.44 f=0.0002
155->161 96.37
160->165 3.63

S16: 340.63 f=0.0095
154->161 2.16
158->163 94.18
159->165 3.66

S17: 339.84 f=0.0007
154->161 7.78
158->163 5.49
159->165 86.73

S18: 339.44 f=0.0011
159->164 100.00

S19: 334.66 f=0.0002
154->161 90.77
159->165 9.23

S20: 331.16 f=0.0085
160->166 89.81
160->167 10.19

S21: 325.58 f=0.0092
158->164 93.88
158->165 2.55
160->167 3.58

S22: 323.78 f=0.0123
158->165 40.92
160->166 9.88
160->167 49.20

S23: 321.66 f=0.0176

S24: 318.83 f=0.0003

S25: 317.54 f=0.0006
159->166 85.76
159->167 14.24

S26: 316.91 f=0.0010
148->162 3.74
153->161 44.48
154->162 51.77

S27: 310.40 f=0.0002
159->166 14.51
159->167 85.49

S28: 306.24 f=0.0087
148->162 4.74
153->161 20.36
154->162 28.69
158->166 36.75
158->167 4.78
160->168 4.68

S29: 304.88 f=0.0161
148->162 3.17
153->161 15.28
154->162 21.31
158->166 60.23

S30: 302.92 f=0.0008
158->166 3.23
160->168 94.60
160->169 2.17

S31: 298.64 f=0.0067
158->166 4.26
158->167 51.81
160->169 43.93

S32: 297.49 f=0.0237
157->163 5.66
158->167 38.82
160->168 2.78
160->169 52.74

S33: 296.51 f=0.0269
148->161 21.79
149->161 3.52
153->162 74.69

S34: 293.75 f=0.0228
149->161 2.33
150->161 76.11
151->161 7.85
157->163 13.70

S35: 291.52 f=0.0025
157->163 10.77
159->168 85.23
159->169 4.00

S36: 291.17
158->164 6.49
158->165 54.39
160->167 39.12

S37: 290.02 f=0.0086
155->162 100.00

S38: 286.94 f=0.0012
148->162 3.74
153->161 44.48
154->162 51.77

S39: 285.85 f=0.0003
159->166 14.51
159->167 85.49

S40: 284.50 f=0.0118
148->162 4.74
153->161 20.36
154->162 28.69
158->166 36.75
158->167 4.78
160->168 4.68

S41: 283.73 f=0.0020
148->162 3.17
153->161 15.28
154->162 21.31
158->166 60.23

S42: 283.13 f=0.0010
158->166 3.23
160->168 94.60
160->169 2.17

S43: 282.62 f=0.0004
158->166 4.26
158->167 51.81
160->169 43.93

S44: 281.30 f=0.0025
157->163 5.66
158->167 38.82
160->168 2.78
160->169 52.74

S45: 280.23 f=0.0071
148->161 21.79
149->161 3.52
153->162 74.69

S46: 276.57 f=0.0056
149->161 2.33
150->161 76.11
151->161 7.85
157->163 13.70

S47: 275.77 f=0.0032
157->163 10.77
159->168 85.23
159->169 4.00

S48: 275.39 f=0.0024

f=0.0006
160->170 100.00

150->161 9.52
151->161 3.24
152->161 2.30
157->163 68.38
159->168 13.75
160->170 2.81

159->168 4.63
159->169 95.37

147->161 3.01
151->161 7.75
152->161 69.80
156->163 19.44

152->161 9.16
156->163 68.22
157->165 11.84
158->168 4.15
159->170 6.62

152->161 4.64
156->163 5.18
156->165 4.65
157->165 85.54

156->163 4.22
157->164 3.08
159->170 92.70

149->162 2.94
150->162 87.61
151->162 6.72
152->162 2.72

157->164 16.35
158->168 83.65

156->163 3.02
157->164 83.70
158->168 13.28

147->162 2.56
151->162 9.38
152->162 88.05

158->169 100.00

147->161 3.58
149->161 2.87
150->161 6.61

151->161	65.44	157->166	86.85	156->162	5.02
152->161	13.94	157->167	10.90	157->161	12.62
156->164	2.73	**S57: 263.92**		158->162	9.33
156->165	2.47	**f=0.0506**		**T9: 399.75 f=0.0000**	
158->169	2.37	146->161	54.10	153->161	4.19
S49: 273.41		148->161	8.13	156->161	79.69
f=0.0003		148->162	29.32	157->161	3.09
148->161	2.34	149->162	4.40	157->162	13.03
149->161	3.25	153->165	4.05	**T10: 391.86**	
156->164	8.08			**f=0.0000**	
158->170	86.33	**S58: 261.91**		153->161	3.76
S50: 273.29		**f=0.0176**		156->161	10.73
f=0.0099		146->161	24.64	156->162	4.57
151->161	2.82	147->161	7.52	157->162	80.95
156->164	81.46	147->162	14.07		
156->165	5.41	148->162	24.53	**T11: 382.61**	
158->170	10.30	149->161	4.34	**f=0.0000**	
S51: 271.86		149->162	22.32	147->163	2.44
f=0.0131		153->165	2.57	156->163	3.84
147->161	3.35	**S59: 260.67**		158->163	10.09
148->161	2.34	**f=0.1506**		160->163	83.64
148->162	2.36	145->161	2.59	**T12: 368.21**	
149->161	19.34	146->161	14.79	**f=0.0000**	
150->161	2.43	147->162	8.45	145->164	2.35
151->161	6.55	148->161	25.01	152->164	2.41
156->164	4.90	153->162	6.84	153->161	28.14
156->165	55.74	154->165	3.30	156->164	3.39
157->165	2.99	157->166	8.87	158->164	6.36
S52: 270.98		157->167	30.15	160->164	57.35
f=0.0110		**S60: 260.51**		**T13: 368.02**	
147->161	8.08	**f=0.0782**		**f=0.0000**	
148->161	5.77	146->161	5.81	153->161	73.48
149->161	49.81	147->162	4.12	156->161	4.68
150->161	2.72	148->161	11.80	160->164	21.84
156->164	2.88	153->162	3.31	**T14: 365.87**	
156->165	30.74	156->166	3.27	**f=0.0000**	
S53: 267.56		157->166	5.65	148->161	4.53
f=0.0005		157->167	66.04	156->162	90.83
147->162	3.60	**T1: 579.74 f=0.0000**		157->162	4.64
149->162	3.88	160->161	100.00	**T15: 354.53**	
150->162	5.64	**T2: 554.05 f=0.0000**		**f=0.0000**	
151->162	76.33	157->161	3.83	159->163	93.16
152->162	10.55	159->161	93.61	160->165	6.84
S54: 266.24		160->161	2.55	**T16: 353.83**	
f=0.0043		**T3: 530.96 f=0.0000**		**f=0.0000**	
145->161	2.19	160->162	100.00	147->163	2.36
146->161	2.78	**T4: 520.01 f=0.0000**		148->161	3.74
147->161	68.33	158->161	93.68	153->162	2.56
148->161	2.55	159->162	6.32	154->161	4.04
149->161	13.14	**T5: 505.06 f=0.0000**		158->163	12.03
149->162	5.91	158->161	6.94	159->163	10.68
151->161	2.27	159->162	93.06	160->163	2.39
151->162	2.83	**T6: 489.10 f=0.0000**		160->165	62.19
S55: 265.48		153->162	14.70	**T17: 352.81**	
f=0.0566		158->162	85.30	**f=0.0000**	
146->161	5.64	**T7: 428.62 f=0.0000**		141->170	2.13
147->161	4.09	153->162	10.13	148->161	32.57
148->161	2.50	156->161	3.40	149->161	4.89
148->162	17.95	157->161	78.25	153->162	19.39
149->162	48.16	158->162	4.25	154->161	30.27
150->162	3.94	159->161	3.97	156->162	2.13
153->161	6.37	**T8: 426.35 f=0.0000**		160->165	8.62
153->165	11.34	148->161	9.35	**T18: 350.14**	
S56: 265.08		148->165	2.45	**f=0.0000**	
f=0.0051		150->162	2.86	145->163	2.27
		153->162	55.09	146->166	3.13
157->165	2.26	154->161	3.28	147->163	4.41

Col 1		Col 2		Col 3		Col 4	
	158->163 42.03		145->163 5.99	S6: 549.58 f=0.0470			
	160->163 14.08		146->166 5.50			183->186 24.55	
	160->165 28.52		146->167 4.58			183->187 75.45	
	160->167 5.56		147->163 3.18	S7: 451.28 f=0.0011			
T19: 341.86			151->169 2.64			176->186 4.16	
f=0.0000			156->163 3.67			178->186 19.44	
	145->164 5.66		158->163 21.78			178->187 3.09	
	149->166 2.79		158->164 16.02			179->186 14.37	
	149->168 5.02		160->166 23.22			179->187 2.34	
	152->164 4.75		160->167 13.40			181->186 17.92	
	152->167 3.46	T27: 326.19				181->187 2.89	
	158->163 10.86	f=0.0000				182->186 31.24	
	158->164 10.53		148->161 34.14			182->187 4.56	
	158->167 2.72		149->161 5.26	S8: 425.50 f=0.0011			
	159->164 3.55		154->161 58.34			176->187 2.41	
	160->164 28.60		158->164 2.26			178->186 2.21	
	160->166 10.63	T28: 324.33				178->187 17.30	
	160->167 11.43	f=0.0000				179->187 13.35	
T20: 341.41			141->161 2.56			181->186 3.15	
f=0.0000			148->162 35.31			181->187 15.43	
	155->161 100.00		149->162 5.37			182->186 6.45	
T21: 340.21			154->162 43.58			182->187 39.70	
f=0.0000			155->162 2.57	S9: 410.61 f=0.0069			
	159->164 4.49		158->165 10.61			175->186 9.61	
	159->165 93.29	T29: 322.51				176->186 18.76	
	159->166 2.22	f=0.0000				180->186 9.37	
T22: 339.66			145->163 4.15			181->186 36.27	
f=0.0000			146->166 7.25			181->187 2.49	
	151->169 3.49		146->167 4.58			182->186 23.50	
	159->164 90.38		147->163 10.55	S10: 402.27			
	159->165 6.13		156->163 2.73	f=0.0014			
T23: 338.87			158->163 6.43			175->186 5.25	
f=0.0000			158->164 3.47			176->186 8.02	
	145->164 2.53		158->166 3.21			176->187 2.73	
	145->167 2.33		160->167 57.64			178->186 9.96	
	147->163 6.11	T30: 320.94				179->186 21.34	
	147->164 3.31	f=0.0000				180->186 8.38	
	151->164 3.35		145->164 4.71			181->186 4.65	
	151->166 3.57		147->168 2.60			182->186 39.67	
	151->169 21.64		149->166 6.07	S11: 396.70			
	152->163 12.58		149->168 4.55	f=0.0011			
	152->164 7.95		149->169 2.55			175->187 2.54	
	152->165 2.22		152->164 4.34			176->187 3.09	
	152->167 6.83		152->167 3.79			180->187 2.52	
	152->168 4.66		156->164 2.82			181->187 50.10	
	152->169 2.48		158->164 57.34			182->187 41.75	
	158->163 2.23		160->167 11.24	S12: 388.89			
	158->164 2.44	**1P**		f=0.0000			
	159->164 11.18	S1: 630.85 f=0.0064				175->187 5.97	
	160->167 4.58		183->186 3.29			176->187 11.89	
T24: 332.62			185->186 87.38			178->187 12.43	
f=0.0000			185->187 9.33			179->187 24.67	
	145->164 2.37	S2: 610.42 f=0.0006				180->186 6.26	
	158->163 2.56		184->186 77.77			180->187 21.14	
	158->164 14.03		184->187 12.90			181->187 2.70	
	160->164 5.26		185->187 9.34			182->187 14.95	
	160->166 72.90	S3: 607.73 f=0.0014		S13: 383.30			
	160->167 2.89		184->186 8.04	f=0.0003			
T25: 332.06			185->186 8.91			176->186 16.33	
f=0.0000			185->187 83.05			176->187 4.68	
	148->162 16.33	S4: 581.15 f=0.0006				178->186 18.93	
	149->162 2.40		184->186 14.47			179->186 8.09	
	153->165 6.46		184->187 85.53			180->186 11.95	
	158->165 74.81	S5: 555.05 f=0.0257				181->186 36.52	
T26: 330.29			183->186 70.61			182->186 3.50	
f=0.0000			183->187 29.39	S14: 381.19			

f=0.0010
176->186 10.87
179->186 3.70
180->186 45.53
185->188 39.89

S15: 380.76
f=0.0045
176->186 9.41
180->186 20.42
181->187 3.44
185->188 66.74

S16: 373.73
f=0.0001
176->186 7.38
176->187 25.39
178->187 17.73
179->187 3.18
180->186 3.52
180->187 16.51
181->187 24.00
182->187 2.29

S17: 373.04
f=0.0001
177->186 75.90
177->187 24.10

S18: 370.82
f=0.0005
176->187 8.82
179->187 2.71
180->187 27.49
184->188 60.98

S19: 370.42
f=0.0002
176->186 2.98
176->187 19.08
179->187 6.53
180->187 33.55
184->188 37.86

S20: 368.93
f=0.0001
177->186 24.45
177->187 75.55

S21: 360.96
f=0.0000
176->186 4.73
178->186 43.44
178->187 5.04
179->186 41.78
179->187 5.01

S22: 360.11
f=0.0069
174->186 7.53
183->188 92.47

S23: 356.87
f=0.0000
176->187 8.13
178->186 5.29
178->187 42.06
179->186 4.37
179->187 40.16

S24: 355.29
f=0.0010
174->186 28.56
174->187 4.02
175->186 43.63
175->187 4.05
176->186 14.05
176->187 2.43
183->188 3.27

S25: 352.44
f=0.0016
173->186 72.12
173->187 11.50
174->186 9.68
175->186 4.10
183->188 2.60

S26: 349.19
f=0.0057
173->186 16.39
174->186 39.44
174->187 6.14
175->186 31.95
181->186 2.60
183->188 3.48

S27: 346.66
f=0.0001
175->186 5.31
175->187 84.59
176->187 10.09

S28: 333.49
f=0.0020
173->186 2.69
173->187 21.98
174->186 10.70
174->187 64.63

S29: 332.31
f=0.0066
172->186 2.30
173->186 8.70
173->187 66.13
174->187 22.86

S30: 309.38
f=0.0002
185->189 100.00

S31: 308.59
f=0.0114
170->187 2.23
172->186 82.68
172->187 12.71
173->187 2.38

S32: 303.03
f=0.0011
171->186 16.33
172->186 12.20
172->187 71.47

S33: 301.88
f=0.0003
172->187 4.49
176->188 3.16
178->188 16.90
179->188 12.58
181->188 16.12
182->188 34.65
184->189 12.11

S34: 301.49
f=0.0003
178->188 2.61
181->188 2.78
182->188 5.43
184->189 89.18

S35: 300.42
f=0.0012
170->187 17.76
171->186 54.87
171->187 17.22
172->187 10.14

S36: 296.28
f=0.0002
171->187 7.27
183->189 92.73

S37: 287.06
f=0.0202
170->186 27.55
170->187 3.92
171->186 10.14
171->187 47.21
172->187 2.21
183->189 8.97

S38: 285.85
f=0.0019
175->188 3.21
176->188 5.97
180->188 3.54
181->188 47.88
182->188 39.41

S39: 281.63
f=0.0016
175->188 7.70
176->188 14.96
178->188 12.34
179->188 26.46
180->188 21.38
182->188 17.15

S40: 274.46
f=0.0026
183->190 2.78
185->190 97.22

S41: 273.73
f=0.0008
176->188 19.11
178->188 18.62
179->188 6.30
180->188 24.32
181->188 29.01
182->188 2.64

S42: 272.02
f=0.0001
175->188 2.74
176->188 38.50
179->188 6.29
180->188 52.46

S43: 269.90
f=0.0002
177->188 100.00

S44: 264.59
f=0.0178
183->190 36.82
184->190 63.18

S45: 263.41
f=0.0003
176->188 8.19
178->188 47.33
179->188 44.48

S46: 262.26
f=0.0498
170->186 5.58
170->187 16.06
171->186 4.12

Column 1		Column 2		Column 3	
171->188	4.74	176->189	13.00	170->186	4.98
183->190	49.90	178->189	10.21	171->186	4.66
184->190	19.60	179->189	22.79	171->187	19.54
S47: 261.42		180->189	14.25	172->187	3.32
f=0.0521		182->189	23.31	178->187	14.03
170->186	5.97	185->193	4.98	179->187	11.68
170->187	35.89	**S58: 239.96**		181->186	2.21
171->186	8.00	**f=0.0096**		181->187	7.03
171->187	2.38	169->186	10.04	182->186	4.60
171->188	10.53	169->187	82.32	182->187	27.95
183->190	16.83	185->193	7.63	**T9: 428.74 f=0.0000**	
184->190	20.39	**S59: 239.85**		170->186	9.11
S48: 258.59		**f=0.1045**		170->187	2.47
f=0.0035		169->187	4.43	170->188	2.37
174->188	3.19	179->189	2.64	171->186	7.62
175->188	85.25	182->189	2.68	171->187	35.93
176->188	11.56	185->192	6.25	172->186	2.02
S49: 255.91		185->193	75.45	172->187	6.54
f=0.1272		185->194	8.55	173->186	2.30
170->186	21.66	**S60: 239.05**		174->187	1.95
170->187	5.00	**f=0.0078**		176->186	2.71
170->188	2.77	183->191	97.28	176->187	1.95
171->187	5.86	185->191	2.72	178->187	4.13
173->188	64.71	**T1: 652.43 f=0.0000**		179->187	2.83
S50: 255.01		183->186	4.41	181->186	3.62
f=0.0044		184->186	3.37	181->187	8.56
176->189	3.82	185->186	84.14	182->187	5.88
178->189	21.16	185->187	8.08	**T10: 413.87**	
179->189	15.94	**T2: 623.39 f=0.0000**		**f=0.0000**	
181->189	19.22	183->186	3.12	175->186	10.60
182->189	39.86	183->187	2.07	176->186	19.58
S51: 252.34		184->186	69.44	179->186	3.32
f=0.0034		184->187	18.27	180->186	10.12
174->188	96.66	185->186	3.65	181->186	27.11
175->188	3.34	185->187	3.45	181->187	3.49
S52: 248.68		**T3: 615.66 f=0.0000**		182->186	25.78
f=0.0230		183->187	6.30	**T11: 402.42**	
183->191	3.51	185->186	9.53	**f=0.0000**	
185->191	96.49	185->187	84.17	175->186	4.66
S53: 247.88		**T4: 602.99 f=0.0000**		176->186	7.90
f=0.2471		183->186	84.48	178->186	9.54
170->186	24.40	183->187	6.42	179->186	20.69
170->187	6.34	184->186	9.10	180->186	8.11
170->188	6.52	**T5: 584.24 f=0.0000**		181->186	4.96
171->187	8.87	183->186	6.41	182->186	41.78
173->188	53.86	183->187	4.65	182->187	2.36
S54: 244.97		184->186	17.94	**T12: 396.92**	
f=0.0013		184->187	68.88	**f=0.0000**	
169->186	86.36	185->187	2.12	175->187	2.78
169->187	10.41	**T6: 568.86 f=0.0000**		176->187	3.54
184->191	3.24	183->186	4.76	180->187	3.18
S55: 243.71		183->187	80.75	181->187	47.11
f=0.0001		184->187	10.81	182->187	43.39
169->186	2.52	185->187	3.68	**T13: 389.66**	
184->191	97.48	**T7: 465.12 f=0.0000**		**f=0.0000**	
S56: 243.13		176->186	5.58	175->187	5.53
f=0.0029		178->186	19.45	176->186	2.33
175->189	5.86	178->187	3.86	176->187	10.87
176->189	9.62	179->186	13.93	178->187	11.85
180->189	5.89	179->187	3.13	179->187	23.36
181->189	47.41	181->186	17.96	180->186	5.44
182->189	31.22	181->187	2.86	180->187	20.38
S57: 240.33		182->186	26.11	181->187	3.20
f=0.0086		182->187	4.60	182->187	17.04
169->187	5.20	184->186	2.52	**T14: 385.09**	
175->189	6.26	**T8: 433.75 f=0.0000**		**f=0.0000**	

176->186	2.27			179->187	5.06	173->187	33.04
178->186	2.20	T24: 358.48				174->187	16.99
181->186	8.53	f=0.0000				**3P**	
183->188	5.64			171->186	28.68	S1: 628.66 f=0.0074	
185->188	81.36			172->186	6.80	171->174	2.49
T15: 383.54				173->186	5.18	173->174	91.34
f=0.0000				173->187	9.24	173->175	6.17
176->186	13.11			174->186	34.28	S2: 607.87 f=0.0007	
176->187	5.04			174->187	4.84	172->174	86.23
178->186	15.95			183->188	10.97	172->175	9.56
179->186	7.07	T25: 357.12				173->175	4.21
180->186	10.97	f=0.0000				S3: 603.90 f=0.0014	
181->186	32.11			170->186	6.46	172->174	3.35
182->186	3.68			171->187	10.55	173->174	6.28
185->188	12.06			172->187	2.84	173->175	90.37
T16: 381.15				173->186	41.84	S4: 577.03 f=0.0004	
f=0.0000				173->187	2.19	172->174	10.28
176->186	19.15			174->186	4.38	172->175	89.72
176->187	2.94			174->187	2.27	S5: 545.92 f=0.0388	
178->187	2.45			175->186	5.69	171->174	81.66
179->186	5.58			176->186	5.20	171->175	18.34
180->186	66.33			178->186	2.86	S6: 541.21 f=0.0349	
181->187	3.54			178->187	4.91	171->174	14.53
T17: 374.20				179->186	2.65	171->175	85.47
f=0.0000				179->187	5.72	S7: 447.25 f=0.0019	
176->186	5.71			183->188	2.45	167->174	3.16
176->187	27.68	T26: 356.78				168->174	24.15
178->187	16.25	f=0.0000				168->175	2.56
179->187	2.60			173->186	11.74	169->174	30.61
180->186	3.84			176->187	9.01	169->175	3.23
180->187	13.61			178->186	2.93	170->174	33.04
181->186	2.24			178->187	38.10	170->175	3.25
181->187	25.59			179->186	2.56	S8: 420.98 f=0.0007	
182->187	2.48			179->187	35.65	168->175	24.09
T18: 373.40		T27: 354.00				169->174	3.45
f=0.0000		f=0.0000				169->175	27.16
177->186	73.99			171->186	2.33	170->174	4.54
177->187	26.01			173->186	5.34	170->175	40.77
T19: 372.24				174->186	8.68	S9: 404.96 f=0.0094	
f=0.0000				175->186	64.23	166->174	6.51
180->187	2.21			175->187	4.70	167->174	34.33
183->188	8.79			176->186	11.35	167->175	2.43
184->188	84.94			179->186	3.38	168->174	25.01
185->188	4.07	T28: 346.78				169->174	24.83
T20: 370.66		f=0.0000				170->174	6.89
f=0.0000				174->187	2.20	S10: 397.70	
176->187	26.19			175->186	9.31	f=0.0005	
179->187	10.00			175->187	78.66	167->174	3.07
180->187	63.80			176->187	9.84	168->174	22.76
T21: 368.97		T29: 346.01				169->174	17.88
f=0.0000		f=0.0000				170->174	56.29
177->186	26.58			171->186	23.00	S11: 388.88	
177->187	73.42			171->187	6.73	f=0.0007	
T22: 366.78				172->186	7.01	166->175	2.28
f=0.0000				173->187	5.50	167->175	6.98
171->186	4.38			174->186	41.72	169->175	50.98
177->187	2.53			174->187	2.92	170->175	39.76
183->188	73.56			175->186	7.07	S12: 385.14	
184->188	13.84			175->187	6.05	f=0.0002	
185->188	5.69	T30: 335.82				166->175	2.64
T23: 361.02		f=0.0000				167->175	18.93
f=0.0000				170->186	11.23	168->174	3.27
176->186	4.32			170->187	11.37	168->175	57.67
178->186	44.46			171->186	2.31	170->175	17.49
178->187	5.07			171->187	3.07	S13: 380.26	
179->186	41.09			173->186	22.00	f=0.0054	

173->176 100.00

S14: 374.26
f=0.0002
164->174   6.56
167->174   40.96
167->175   6.24
168->174   19.33
169->174   21.06
172->176   5.84

S15: 369.62
f=0.0003
167->174   3.02
172->176   96.98

S16: 364.26
f=0.0001
167->174   7.38
167->175   63.24
168->175   13.37
169->175   16.01

S17: 356.69
f=0.0061
165->174   15.38
171->176   84.62

S18: 352.63
f=0.0041
165->174   69.10
165->175   6.70
166->174   5.33
167->174   2.96
171->176   15.90

S19: 350.34
f=0.0002
164->174   74.92
164->175   5.93
166->174   14.13
167->174   5.01

S20: 346.82
f=0.0025
164->174   14.09
165->174   4.82
166->174   74.97
166->175   2.62
168->174   3.50

S21: 341.44
f=0.0000
166->174   3.75
166->175   92.77
167->175   3.48

S22: 332.47
f=0.0012
165->174   8.62
165->175   91.38

S23: 330.81
f=0.0062
162->174   2.47
164->174   6.94
164->175   90.58

S24: 308.91
f=0.0004
173->177 100.00

S25: 308.07
f=0.0115
158->175   3.25
160->174   5.96
161->174   6.85
162->174   73.32
162->175   7.67
164->175   2.94

S26: 302.15
f=0.0008
158->174   2.90
158->175   5.38
159->174   24.37
160->174   7.78
160->175   3.80
161->174   5.04
161->175   2.75
162->174   6.93
162->175   38.92
172->177   2.12

S27: 300.99
f=0.0001
162->175   3.00
172->177   97.00

S28: 300.38
f=0.0019
158->175   12.63
159->174   18.88
159->175   12.15
160->174   16.15
161->175   5.46
162->175   32.29
172->177   2.45

S29: 300.04
f=0.0006
167->176   2.83
168->176   24.82
169->176   31.42
170->176   40.93

S30: 294.26
f=0.0008
159->175   6.23
160->175   4.81
171->177   88.96

S31: 293.78
f=0.0002
163->174 100.00

S32: 287.86
f=0.0045
158->174   5.09
159->175   4.87
160->174   4.54
163->175   81.49
171->177   4.01

S33: 287.16
f=0.0136
158->174   21.49
159->175   10.73
160->174   3.70
160->175   34.93
163->175   17.92
171->177   11.24

S34: 286.00
f=0.0013
159->174   35.21
159->175   3.15
160->174   44.50
160->175   5.89
161->174   3.63
162->174   5.34
163->175   2.28

S35: 282.86
f=0.0007
159->174   4.81
159->175   44.38
160->174   4.26
160->175   34.62
161->175   2.91
162->175   5.82
169->176   3.19

S36: 282.35
f=0.0018
159->175   2.97
160->175   2.11
161->174   2.96
166->176   2.85
167->176   12.62
168->176   3.11
169->176   44.88
170->176   28.50

S37: 280.71
f=0.0002
160->174   2.84
161->174   46.76
161->175   4.52
162->174   8.26
167->176   4.05
168->176   15.48
169->176   2.39
170->176   15.70

S38: 280.01
f=0.0006
161->174   26.39
161->175   3.88
162->174   2.23
167->176   14.16
168->176   39.87
170->176   13.46

S39: 277.35
f=0.0001
160->175   5.17
161->174   8.37
161->175   77.39
162->175   9.08

S40: 276.81
f=0.0026
173->178 100.00

S41: 268.72
f=0.0005
167->176   63.79
168->176   16.69
169->176   19.52

S42: 266.30
f=0.0185
171->178   18.25
172->178   81.75

S43: 263.13
f=0.0119
171->178   83.74
172->178   16.26

S44: 261.65
f=0.0862
158->174   6.74
158->175   55.72
159->174   8.17
159->176   9.38
160->174   4.74
160->176   6.53

162->176	2.59		154->174	2.62	**T5: 579.56 f=0.0000**		
171->178	2.53		157->174	70.58		171->174	8.85
172->178	3.60		157->175	4.80		171->175	2.18
S45: 256.02			167->177	4.86		172->174	11.56
f=0.0255			168->177	2.44		172->175	77.41
158->174	3.90		169->177	9.57	**T6: 559.69 f=0.0000**		
164->176	11.98		171->179	5.12		171->174	2.80
166->176	79.81	**S55: 239.22**				171->175	87.36
167->176	4.30	**f=0.0021**				172->175	6.36
S46: 255.56			167->177	10.69		173->175	3.48
f=0.1222			168->177	38.95	**T7: 461.46 f=0.0000**		
158->174	20.70		169->177	6.42		167->174	3.84
158->175	3.21		170->177	43.94		168->174	23.66
158->176	2.59	**S56: 237.51**				168->175	3.91
159->175	3.44	**f=0.0183**				169->174	30.25
160->175	2.45		157->174	5.92		169->175	3.47
164->176	35.12		171->179	88.56		170->174	28.39
165->176	16.19		171->181	3.26		170->175	3.51
166->176	16.29		173->179	2.26		172->174	2.98
S47: 253.80		**S57: 236.75**			**T8: 431.71 f=0.0000**		
f=0.0030		**f=0.0592**				152->174	2.12
164->176	2.94		157->175	3.28		152->176	2.22
167->177	2.48		172->179	3.77		158->174	9.58
168->177	25.87		172->180	9.69		158->176	2.40
169->177	30.21		172->181	75.74		159->174	3.18
170->177	38.51		172->182	3.58		159->175	22.34
S48: 252.17			172->183	3.94		160->174	3.21
f=0.0040		**S58: 235.68**				160->175	16.03
164->176	9.51	**f=0.0129**				162->175	5.79
165->176	86.13		153->174	2.94		168->175	13.80
166->176	4.35		154->175	2.22		169->175	5.47
S49: 248.25			157->174	5.53		170->175	13.87
f=0.0365			157->175	77.21	**T9: 425.51 f=0.0000**		
164->176	2.78		172->181	3.43		158->174	5.61
171->179	2.41		173->180	8.67		159->175	13.18
173->179	94.80	**S59: 234.38**				160->175	8.82
S50: 247.65		**f=0.0025**				162->175	3.89
f=0.2129			157->175	8.73		167->174	4.43
158->174	21.51		173->180	82.95		167->175	3.23
158->175	3.84		173->181	8.32		168->175	10.92
158->176	5.62	**S60: 233.10**				169->174	6.36
159->175	4.59	**f=0.0033**				169->175	21.53
160->175	3.55		159->176	12.58		170->174	2.43
164->176	51.14		161->176	8.75		170->175	19.62
172->181	2.94		162->176	72.10	**T10: 408.60**		
173->179	6.80		170->178	6.57	**f=0.0000**		
S51: 243.37		**T1: 648.83 f=0.0000**				166->174	6.69
f=0.0032			171->174	3.27		167->174	34.41
172->179	96.95		172->174	3.70		168->174	26.17
172->181	3.05		173->174	88.52		169->174	19.86
S52: 241.57			173->175	4.51		169->175	2.75
f=0.1052		**T2: 620.83 f=0.0000**				170->174	10.13
173->180	9.92		172->174	79.12	**T11: 397.80**		
173->181	84.10		172->175	12.50	**f=0.0000**		
173->182	3.71		173->174	3.07		167->174	3.76
173->183	2.28		173->175	5.31		168->174	23.43
S53: 240.97		**T3: 611.14 f=0.0000**				169->174	15.10
f=0.0028			171->175	5.34		170->174	57.72
157->174	11.98		172->175	2.55	**T12: 389.12**		
166->177	4.56		173->174	5.88	**f=0.0000**		
167->177	20.78		173->175	86.22		166->175	2.29
168->177	11.02	**T4: 591.36 f=0.0000**				167->175	7.11
169->177	35.01		171->174	85.81		169->175	48.07
170->177	16.64		171->175	4.53		170->175	42.53
S54: 240.40			172->174	6.36	**T13: 385.67**		
f=0.0010			172->175	3.30	**f=0.0000**		

166->175	2.59	f=0.0000		f=0.0000	
167->175	18.87	159->174	3.32	162->175	4.68
168->174	3.07	160->174	5.49	168->176	21.06
168->175	56.27	164->174	4.39	169->176	23.93
170->175	19.20	165->174	27.07	170->176	30.20
T14: 383.82		165->175	3.44	172->177	20.13
f=0.0000		166->174	48.21	**4P**	
171->176	5.46	166->175	2.40	**S1: 635.48 f=0.0029**	
173->176	94.54	167->174	5.69	152->153	100.00
T15: 374.84		**T22: 346.36**		**S2: 608.33 f=0.0002**	
f=0.0000		f=0.0000		151->153	7.72
164->174	7.12	159->174	6.62	152->154	92.28
167->174	37.34	160->174	7.83	**S3: 602.57 f=0.0001**	
167->175	6.24	164->174	8.72	151->153	91.83
168->174	17.34	165->174	24.70	152->154	8.17
169->174	23.14	165->175	3.03	**S4: 574.44 f=0.0000**	
172->176	8.82	166->174	49.10	151->154	100.00
T16: 370.85		**T23: 341.50**		**S5: 523.54 f=0.0090**	
f=0.0000		f=0.0000		150->153	11.59
167->174	5.25	166->174	3.58	150->154	88.41
171->176	4.90	166->175	92.98	**S6: 520.99 f=0.0682**	
172->176	87.01	167->175	3.44	150->153	87.52
173->176	2.84	**T24: 334.85**		150->154	12.48
T17: 364.69		f=0.0000		**S7: 436.31 f=0.0002**	
f=0.0000		158->174	26.91	148->153	9.07
164->175	2.56	158->175	11.74	149->153	88.71
167->174	6.32	164->174	16.13	149->154	2.22
167->175	58.73	164->175	5.16	**S8: 412.21 f=0.0006**	
168->174	2.51	165->174	6.88	148->153	15.33
168->175	11.40	165->175	33.18	148->154	4.31
169->174	3.08	**T25: 333.21**		149->154	80.35
169->175	15.40	f=0.0000		**S9: 407.30 f=0.0098**	
T18: 364.09		158->174	32.73	148->153	73.60
f=0.0000		159->174	4.67	148->154	4.09
152->175	2.45	160->174	3.32	149->153	11.29
159->174	5.25	164->175	54.49	149->154	11.02
160->174	5.34	165->175	4.79	**S10: 389.99**	
162->174	3.20	**T26: 332.20**		f=0.0004	
164->175	2.46	f=0.0000		148->154	92.76
171->176	69.25	158->174	7.34	149->154	7.24
172->176	7.10	158->175	2.99	**S11: 381.52**	
173->176	4.95	159->175	2.64	f=0.0044	
T19: 356.63		160->175	4.00	152->155	97.66
f=0.0000		164->174	10.21	152->156	2.34
158->174	3.39	164->175	18.27	**S12: 371.06**	
159->174	18.37	165->174	2.68	f=0.0118	
160->174	12.06	165->175	51.88	152->155	2.27
162->174	7.01	**T27: 318.90**		152->156	90.57
164->174	30.64	f=0.0000		152->157	7.16
164->175	9.21	152->175	2.12	**S13: 368.38**	
165->174	3.19	158->174	10.11	f=0.0003	
167->175	2.20	158->175	78.44	151->155	95.27
171->176	13.94	159->176	3.27	151->156	4.73
T20: 355.22		160->176	2.31	**S14: 362.99**	
f=0.0000		164->175	3.74	f=0.0078	
158->174	9.20	**T28: 313.10**		152->156	7.00
159->174	2.30	f=0.0000		152->157	93.00
159->175	8.21	159->174	27.03	**S15: 354.02**	
160->174	2.77	161->174	9.55	f=0.0018	
160->175	6.33	162->174	59.60	147->153	11.49
162->175	3.12	162->175	3.83	151->155	4.22
164->174	23.00	**T29: 309.96**		151->156	79.57
165->174	35.80	f=0.0000		151->157	4.72
165->175	2.89	171->177	3.23	**S16: 353.70**	
171->176	6.39	173->177	96.77	f=0.0015	
T21: 349.58		**T30: 302.66**		147->153	85.20

	150->155 2.90	S31: 304.25			150->159 5.54
	151->156 11.90	f=0.0065			151->160 9.63
S17: 347.95			137->154 5.91		151->161 7.39
f=0.0013			143->153 29.98	S40: 293.36	
	146->153 4.52		144->153 2.37	f=0.0160	
	150->155 24.10		145->153 4.05		145->154 15.18
	151->156 3.44		150->158 9.42		150->159 27.49
	151->157 67.93		152->160 26.30		151->160 29.21
S18: 347.22			152->161 21.97		151->161 25.43
f=0.0132		S32: 301.66			151->162 2.69
	147->153 2.80	f=0.0083			
	150->155 71.04		141->153 9.70	S41: 291.05	
	151->156 2.50		142->153 2.81	f=0.0029	
	151->157 23.65		144->153 2.61		151->162 100.00
S19: 345.17			145->153 6.80	S42: 289.84	
f=0.0003			152->162 78.08	f=0.0037	
	146->153 95.21	S33: 301.02			137->153 6.82
	151->157 4.79	f=0.0057			140->154 3.60
S20: 337.76			137->154 4.62		141->154 21.35
f=0.0174			141->153 22.79		143->154 6.51
	150->156 100.00		142->153 7.11		145->154 8.61
S21: 334.19			143->153 7.21		150->160 19.28
f=0.0007			144->153 7.03	S43: 287.81	150->161 33.83
	147->154 100.00		145->153 20.37	f=0.0010	
S22: 333.47			151->161 6.37		141->153 2.80
f=0.0034			152->162 24.51		144->153 80.78
	152->158 96.00	S34: 299.87			145->153 16.41
	152->159 4.00	f=0.0013			
S23: 329.68			151->160 46.67	S44: 284.98	
f=0.0123			151->161 53.33	f=0.0070	
	146->154 4.04	S35: 298.17			137->153 12.88
	150->157 95.96	f=0.0039			141->154 7.78
S24: 327.35			137->153 2.54		142->154 6.93
f=0.0063			141->154 14.40		143->154 2.80
	143->153 3.70		142->154 4.92		144->154 23.94
	146->154 92.63		143->154 67.42		145->154 4.94
	150->157 3.68		144->154 2.39		150->160 25.56
S25: 320.34			145->154 8.32	S45: 284.56	150->161 15.18
f=0.0008		S36: 296.04		f=0.0037	
	151->158 95.13	f=0.0035			141->154 5.03
	151->159 4.87		137->154 7.08		142->153 25.83
S26: 319.42			140->153 7.34		142->154 4.14
f=0.0170			141->153 31.27		144->154 10.19
	152->158 3.37		145->153 39.89		148->155 20.30
	152->159 96.63		145->154 5.07		149->155 6.11
S27: 309.14			149->155 9.35		149->156 22.21
f=0.0001		S37: 295.29			150->160 6.19
	152->160 48.84	f=0.0001			
	152->161 51.16		145->153 5.50	S46: 283.95	
S28: 307.64			148->155 7.91	f=0.0039	
f=0.0003			149->155 80.68		141->153 4.09
	151->158 4.55		149->156 5.91		141->154 3.70
	151->159 95.45	S38: 294.23			142->153 46.44
S29: 306.67		f=0.0086			142->154 6.85
f=0.0009			150->159 67.69		148->155 15.26
	150->158 69.14		151->160 19.11		149->155 4.01
	152->160 13.95		151->161 13.21		149->156 13.01
	152->161 16.91	S39: 293.53			150->161 6.64
S30: 305.49		f=0.0046		S47: 283.76	
f=0.0084			141->154 4.48	f=0.0034	
	137->154 4.25		142->154 3.17		137->153 5.10
	143->153 42.43		143->154 5.77		141->154 8.32
	145->153 3.10		144->154 7.80		142->153 4.52
	150->158 23.65		145->153 2.26		142->154 2.82
	152->160 13.44		145->154 51.24		143->154 4.63
	152->161 13.12		149->155 2.72		144->154 53.15
					145->154 7.18

	148->155 2.94	138->154 6.62		152->155 23.08
	149->156 4.47	140->153 2.98		152->156 71.33
	150->161 6.86	S60: 264.71	T14: 373.03	
S48: 282.61		f=0.0013	f=0.0000	
f=0.0031		138->153 6.28		148->157 3.94
	148->155 34.93	138->154 90.83		150->157 5.68
	149->156 3.92	140->154 2.89		152->157 90.39
	150->160 33.37	T1: 652.70 f=0.0000	T15: 369.66	
	150->161 27.78	152->153 100.00	f=0.0000	
S49: 281.58		T2: 619.63 f=0.0000		151->155 94.68
f=0.0050		149->153 3.01		151->156 5.32
	148->155 20.26	151->153 82.06	T16: 363.83	
	148->156 3.14	152->154 14.93	f=0.0000	
	149->156 46.38	T3: 608.51 f=0.0000		134->154 3.53
	149->157 2.39	151->153 14.36		141->153 9.95
	150->160 17.20	152->154 85.64		143->153 12.05
	150->161 10.62	T4: 584.14 f=0.0000		144->153 4.61
S50: 280.59		150->153 76.20		145->153 2.39
f=0.0008		151->154 23.80		146->154 3.63
	140->153 5.51	T5: 574.81 f=0.0000		147->153 45.55
	141->154 8.59	150->153 25.49		150->155 18.28
	142->153 13.72	151->154 74.51	T17: 357.91	
	142->154 72.18	T6: 547.01 f=0.0000	f=0.0000	
S51: 278.79		143->154 2.95		143->153 2.36
f=0.0250		150->154 97.05		147->153 41.37
	148->156 86.35	T7: 455.89 f=0.0000		150->155 53.38
	149->157 7.17	148->153 10.62		150->156 2.90
	150->162 6.48	149->153 82.03	T18: 356.80	
S52: 277.68		149->154 3.69	f=0.0000	
f=0.0039		151->153 3.66		137->153 10.33
	148->156 11.33	T8: 428.14 f=0.0000		141->154 6.19
	149->157 27.38	133->161 1.78		143->154 3.95
	150->162 61.29	134->153 2.69		146->153 65.41
S53: 277.03		134->155 2.18		151->155 4.54
f=0.0063		137->153 14.52		151->156 9.58
	149->156 2.33	137->155 2.76	T19: 355.53	
	149->157 63.50	140->154 4.25	f=0.0000	
	150->162 34.17	141->154 31.72		146->153 9.39
S54: 275.42		143->154 21.68		151->155 3.09
f=0.0005		144->154 5.19		151->156 83.82
	138->153 2.71	145->154 3.73		151->157 3.69
	140->153 78.78	146->153 4.40	T20: 350.82	
	140->154 3.98	147->154 1.95	f=0.0000	
	141->153 12.04	150->154 3.16		139->156 3.48
	142->154 2.50	T9: 423.05 f=0.0000		139->159 3.03
S55: 273.58		148->153 49.10		141->153 13.81
f=0.0105		148->154 2.17		143->153 12.62
	139->153 53.26	149->154 48.74		147->153 8.91
	140->153 2.31	T10: 414.16		150->155 19.20
	148->157 44.43	f=0.0000		150->156 25.94
S56: 273.23		148->153 38.09		152->156 9.75
f=0.0127		148->154 7.71		152->159 3.26
	139->153 44.96	149->153 13.62	T21: 348.91	
	148->157 55.04	149->154 40.58	f=0.0000	
S57: 272.39		T11: 391.27		141->153 19.98
f=0.0001		f=0.0000		143->153 14.25
	138->154 2.93	148->154 91.87		147->153 7.08
	140->153 2.44	149->154 8.13		150->155 7.87
	140->154 84.26	T12: 385.06		150->156 34.57
	141->154 10.37	f=0.0000		151->157 10.69
S58: 270.09		150->156 3.99		152->156 5.55
f=0.0000		152->155 80.09	T22: 348.42	
	139->154 100.00	152->156 15.93	f=0.0000	
S59: 267.77		T13: 381.15		150->156 4.09
f=0.0002		f=0.0000		151->156 5.54
	138->153 90.40	150->156 5.59		151->157 90.38

T23: 343.56
f=0.0000

138->157	4.45
138->159	3.57
140->158	2.56
140->159	2.90
142->158	4.65
142->160	4.04
142->162	2.69
145->157	10.13
148->157	8.43
150->156	3.86
150->157	29.46
152->157	15.92
152->158	7.34

T24: 338.94
f=0.0000

138->157	4.81
140->156	3.66
140->157	7.00
144->157	2.46
144->158	3.58
144->162	27.35
145->156	11.07
145->157	5.37
145->159	14.58
145->160	3.18
148->159	2.78
150->156	3.07

T25: 335.65
f=0.0000

144->162	2.82
147->154	2.91
150->156	4.57
150->157	17.64
152->158	72.07

T26: 335.37
f=0.0000

137->153	24.50
146->153	7.62
147->154	65.31
152->158	2.58

T27: 333.23
f=0.0000

137->153	45.99
137->154	2.42
141->154	5.03
143->154	4.79
146->153	13.42
147->154	28.35

T28: 331.15
f=0.0000

137->153	2.75
137->154	8.61
141->153	4.07
143->153	3.59

152->158	3.53
152->159	7.56

146->154	80.98

T29: 330.17
f=0.0000

138->156	4.43
139->156	4.43
139->159	5.17
140->158	5.00
142->160	3.27
145->157	4.09
150->155	2.46
150->156	11.03
150->157	28.54
152->158	23.14
152->159	8.46

T30: 326.11
f=0.0000

138->157	5.84
138->158	2.62
139->156	5.88
139->159	5.50
140->160	5.61
142->158	13.73
145->157	2.88
145->159	2.57
148->156	4.19
148->157	4.01
150->156	15.66
150->157	31.52

DFT optimised geometries :

1N

Cu	-0.93219500	-0.76730900	0.15993200
I	-0.33609400	-2.48817200	2.13441300
C	-1.38885000	1.67297400	2.48010600
H	-1.51454800	2.36371500	3.31751400
H	-0.84228200	2.18285300	1.67856400
H	-0.79030100	0.81520100	2.80715200
C	-1.13192500	-3.00184800	-2.34086700
H	-0.48815700	-2.14766400	-2.56969300
H	-0.66956100	-3.53475900	-1.50282000
H	-1.16585700	-3.66680800	-3.20727200
N	-2.69048200	0.30199200	0.96352600
N	-2.58192500	-1.58887900	-1.00655000
C	-2.50295900	-2.53411500	-1.94586600
C	-3.66310100	-3.09383900	-2.52834900
C	-4.90850500	-2.67216500	-2.11643300
C	-5.01316400	-1.68843200	-1.11041400
C	-6.27268500	-1.21812100	-0.61126000
C	-6.32616300	-0.28994100	0.38370300
C	-5.12453200	0.24605300	0.95374600
C	-5.12823500	1.18899200	2.00354700
C	-3.93175300	1.65013700	2.50800900
C	-2.71161300	1.18751700	1.96194800
C	-3.85883400	-0.17624700	0.46944800
C	-3.80164500	-1.17134800	-0.58149800
H	-3.55815800	-3.85630500	-3.29299200
H	-5.81125900	-3.09316800	-2.55101300
H	-7.18408700	-1.62813100	-1.03733800
H	-7.28144600	0.05546900	0.76910500
H	-6.07487900	1.53696200	2.40847100
H	6.04202700	-3.00007800	-1.93382300
P	0.99069000	0.33737400	-0.60315400
C	6.62844000	4.13361100	0.66646200
C	4.22675500	3.87925900	0.73928100

C	5.62243600	1.94565500	0.43860500
C	3.08591300	2.98133100	1.21444100
C	4.48700900	1.04712700	0.92128700
C	2.05159300	0.79210700	0.88147300
C	-0.89748400	5.22050400	-1.04952600
C	0.17836500	4.25346800	-1.53756500
C	5.17510000	-2.79793600	-1.29292100
C	0.90510300	1.95106600	-1.55915700
C	-3.24108000	5.78984000	-1.21010900
C	4.28097800	-1.76218500	-1.97288600
C	2.26850100	-0.45349700	-1.74906200
C	5.29173600	-5.07171000	-0.49154800
C	-2.53373700	3.47788000	-1.20248000
C	-1.45636600	2.50509100	-1.67452300
C	3.24920900	-3.79244400	-0.27313700
C	2.35207100	-2.76359100	-0.95312300
H	6.54520200	5.09425600	1.18581700
H	7.57466200	3.66947200	0.96369800
H	4.16471900	4.84753500	1.25021300
H	6.67674500	4.33792600	-0.42130400
H	6.58389500	1.50410900	0.72578400
H	3.11544000	2.91666000	2.31854000
H	4.59562600	0.88772200	2.01006700
H	4.10811200	4.06886500	-0.34765500
H	2.12549400	3.42686200	0.93358100
H	5.59656200	1.99843900	-0.66905600
H	4.53934300	0.07148600	0.43094400
H	1.37808200	1.23974400	1.61985200
H	1.14420600	4.53216700	-1.10223400
H	-0.65235800	6.23415300	-1.38797600
H	2.36383600	-0.16963200	1.30040500
H	-0.89759800	5.23096800	0.05922700
H	5.55808200	-2.37416600	-0.34207700
H	1.88327700	2.42074900	-1.40681200

Atom	x	y	z
H	0.26613800	4.34270100	-2.63693300
H	4.83560600	-0.82371400	-2.08871800
H	-2.97796800	6.79308400	-1.56158200
H	-3.91044500	2.36774200	3.32138800
H	-3.40662300	5.84479400	-0.11615600
H	2.94153200	0.35891100	-2.04623900
H	5.68414800	-4.80163500	0.50814500
H	3.50091400	-3.43348600	0.74272900
H	6.14653100	-5.26762400	-1.14813700
H	0.82943900	1.69897800	-2.63470600
H	-2.65677700	3.38245100	-0.10578100
H	4.01695900	-2.12548100	-2.98468500
H	-4.18839800	5.50445500	-1.67958400
H	1.73092100	-0.77928700	-2.66199200
H	4.72277300	-6.00138500	-0.38829300
H	-1.43776700	2.50213500	-2.78212000
H	1.48156800	-2.57887200	-0.31784700
H	-1.70147000	1.49491000	-1.33684400
H	-3.48988500	3.20460300	-1.66405700
H	2.69517100	-4.73037700	-0.15890000
H	1.99997300	-3.17597800	-1.91896100
N	5.51941900	3.27254600	1.04259600
N	3.19300700	1.65721500	0.59894600
N	-0.14201600	2.87700100	-1.13732400
N	-2.20134100	4.84702700	-1.58874300
N	3.08151100	-1.50846200	-1.16623700
N	4.44691800	-4.04247200	-1.07624200

3N

Atom	x	y	z
Cu	-0.78787100	-0.60902700	0.17407100
I	-0.31942600	-2.32661400	2.17395300
C	-1.15089100	-2.89302900	-2.26786600
H	-1.23972700	-3.61639100	-3.08189000
H	-0.43143200	-2.12070000	-2.55580100
H	-0.74305800	-3.39783300	-1.38561500
C	-1.06908300	1.89911700	2.45308200
H	-0.45555900	2.35063200	1.66499900
H	-0.56173700	0.99224700	2.80057100
H	-1.15243000	2.60505100	3.28298500
N	-2.45623300	0.63237000	0.91905400
N	-2.48443700	-1.30387700	-1.01174100
C	-2.47661200	-2.27591600	-1.92702100
C	-3.67061600	-2.72605500	-2.53532500
C	-4.87685000	-2.16636400	-2.17467600
C	-4.90871800	-1.15347800	-1.19304800
C	-6.12728100	-0.54416700	-0.74539300
C	-6.11465300	0.40672700	0.22911600
C	-4.88186800	0.82767700	0.82853000
C	-4.82094200	1.78872300	1.85994400
C	-3.59973500	2.13437800	2.39644200
C	-2.41748600	1.53674100	1.90047200
C	-3.65230800	0.26633000	0.39465200
C	-3.66644000	-0.75235700	-0.63512400
H	-3.62297400	-3.51449800	-3.27897800
H	-5.80495800	-2.50139100	-2.63002800
H	-7.06270800	-0.86694000	-1.19369900
H	-7.04000200	0.85833800	0.57553400
H	-5.73845600	2.24210200	2.22547000
H	-3.53010000	2.86383200	3.19640500
P	1.22260700	0.32310100	-0.61232900
C	-1.05987500	2.60900900	-1.76221500
C	-2.07098000	3.66758300	-1.33225300
C	2.45105700	-0.57583600	-1.73229500
C	4.34274800	-2.05695700	-1.93254200
C	2.34119300	-2.86617400	-0.87968700
C	1.26390600	1.92346500	-1.59583100
C	5.11945600	-3.17664700	-1.23988900
C	3.17129900	-3.95747400	-0.21292600

Atom	x	y	z
C	0.66468000	4.26749300	-1.62757500
C	-0.38850000	5.28268000	-1.18868200
C	2.31366700	0.71297400	0.86973900
C	4.76190100	0.82411900	0.93554900
C	5.94442400	1.66962500	0.47138400
C	3.47541700	2.84295300	1.17184800
C	4.69540200	3.63794200	0.70969300
H	-1.02356400	2.57662100	-2.86922600
H	1.90328300	-0.87240800	-2.64873100
H	-3.03873800	3.48478100	-1.80828000
H	4.04278400	-2.39884200	-2.94208100
H	1.93072000	-3.25779800	-1.83100400
H	-1.37649700	1.62576800	-1.40398500
H	1.19338700	1.65840300	-2.66850800
H	3.18871700	0.17928800	-2.02798700
H	0.78779000	4.33106000	-2.72562400
H	4.99159700	-1.18117800	-2.05562700
H	5.94991200	-3.50868500	-1.87077300
H	1.50526700	-2.60350300	-0.22441300
H	2.57686900	-4.86622300	-0.09050600
H	-2.20591600	3.62949800	-0.23961200
H	2.26616000	2.33535700	-1.43268800
H	-0.12974800	6.28255700	-1.54948000
H	5.53232400	-2.79977500	-0.28883200
H	3.49470000	-3.61627700	0.78250900
H	1.62894200	4.51537000	-1.16888300
H	-0.43535000	5.30773400	-0.08717300
H	5.93800900	1.73778200	-0.62954900
H	2.56971000	-0.26715600	1.28399500
H	4.63636100	3.79854300	-0.38039900
H	4.77622600	-0.15657700	0.45079300
H	1.67659000	1.20019400	1.61528400
H	2.55751100	3.35268600	0.85722400
H	6.88991500	1.22058300	0.78916600
H	4.72956900	4.61339200	1.20427200
H	4.84130700	0.66570600	2.02718500
H	3.47101900	2.79863400	2.27756900
N	3.17458600	-1.68176400	-1.12513800
N	0.26597100	2.91616700	-1.20937200
N	3.50862900	1.50165200	0.58249200
O	-1.66361700	4.97083400	-1.72881300
O	4.30125500	-4.30923900	-1.00734700
O	5.90480300	2.97284000	1.04079500

4N

Atom	x	y	z
Cu	0.38550100	-0.74837900	-0.18790800
I	0.13850900	-3.25825800	-0.99841300
C	0.88324200	-1.88592400	2.95800700
H	0.62025900	-2.64601700	2.21384000
H	1.07876500	-2.36920100	3.91839200
H	0.01376700	-1.23036700	3.06997300
C	0.60647000	0.41631800	-3.35445300
H	-0.24751600	0.97123000	-2.95058300
H	0.38291400	-0.65096600	-3.25335200
H	0.70958600	0.66632700	-4.41321500
N	2.01832200	-0.56953600	1.26297100
N	1.91570800	0.35304700	-1.31357300
C	1.85588100	0.74496900	-2.58736900
C	2.93241600	1.43296200	-3.19476500
C	4.07150300	1.70177700	-2.46788400
C	4.16036400	1.27372400	-1.12583900
C	5.32578200	1.48399100	-0.31734100
C	5.38400200	1.01054900	0.95829300
C	4.27997100	0.29400200	1.52764300
C	4.31288200	-0.25571000	2.82725400
C	3.22656400	-0.96170000	3.29517600
C	2.07656200	-1.10827200	2.48371300
C	3.09476700	0.09630900	0.77192100

C	3.03679500	0.59198200	-0.58920900
H	2.84906500	1.73856200	-4.23238700
H	4.90863500	2.22828200	-2.91865100
H	6.16764000	2.01712900	-0.75022600
H	6.27380100	1.15687900	1.56433400
H	5.20133200	-0.12899700	3.44030800
H	3.23784500	-1.41055200	4.28273900
P	-1.56804300	0.52750400	0.17205300
C	-5.24106700	-0.47250500	-2.49846800
C	-5.39724100	0.39914300	-1.41638900
C	-3.99511900	-1.04210500	-2.75804000
C	-4.30707800	0.70488000	-0.60336800
C	-2.89876600	-0.73531500	-1.94748800
C	-3.18948700	-0.94733100	3.64166700
C	-3.04260100	0.15050300	-0.87042700
C	-2.63239900	-0.81071600	2.37084100
C	-3.40021100	0.17922600	4.44153500
C	-2.28901200	0.46010800	1.87515500
C	-3.05426700	1.44199300	3.96076000
C	-2.00137700	3.15017400	-0.94124200
C	-2.50406500	1.58464100	2.68375900
C	-1.23748600	2.32654200	-0.10153500
C	-1.64970200	4.48917300	-1.13359300
C	-0.10636400	2.87491700	0.53050600
C	-0.53835700	5.02693900	-0.48501500
C	0.23231600	4.21518800	0.35164500
H	-6.09333100	-0.71529700	-3.12703600
H	-6.36961400	0.83357100	-1.20161200
H	-3.87251300	-1.73882100	-3.58204900
H	-3.45486100	-1.93489100	4.00812700
H	-4.44004500	1.36839600	0.24628300
H	-2.46278200	-1.69292600	1.75845900
H	-1.94206400	-1.21705700	-2.12451300
H	-3.83007500	0.07150300	5.43327200
H	-2.87201400	2.74966300	-1.44882500
H	-2.25083700	5.11149900	-1.79067700
H	-3.21602000	2.32269400	4.57624900
H	-2.24564900	2.57380600	2.32037900
H	0.51255300	2.24456400	1.16340900
H	-0.26999000	6.06899800	-0.63334400
H	1.10353900	4.62294500	0.85664400
1P			
Cu	0.00000000	0.00000000	0.00000000
I	0.00000000	0.00000000	2.66160038
N	-1.66465876	-1.10148241	-0.85824769
N	-1.37469632	1.59206225	-0.61486234
C	-1.23439041	2.90186623	-0.44807774
C	-2.24871576	3.82761063	-0.75339174
C	-3.45162023	3.36201970	-1.24743050
C	-3.63847534	1.97394402	-1.42406823
C	-4.86001120	1.40435639	-1.91803847
C	-5.00098041	0.05636596	-2.05376130
C	-3.93430776	-0.83853818	-1.70320625
C	-4.04465915	-2.24200791	-1.80545044
C	-2.97721028	-3.03489772	-1.43234121
C	-1.80392830	-2.41923616	-0.96090323
C	-2.70788159	-0.31121903	-1.22000993
C	-2.55572614	1.12083182	-1.08424324
H	-0.28150051	3.23440241	-0.04687626
H	-2.07551216	4.88684586	-0.59608837
H	-4.25773963	4.04742828	-1.49469762
H	-5.67576520	2.07351809	-2.17700136
H	-5.93072143	-0.36713841	-2.42321323
H	-4.96847720	-2.68211199	-2.17087281
H	-3.02887583	-4.11668953	-1.49324634
H	-0.95170559	-3.01766732	-0.65395505
P	2.22320199	0.00000000	-0.65501645

C	2.97153986	1.60771362	-0.03428806
H	2.48401715	2.38101053	-0.63876216
H	2.62140349	1.74174696	0.99802791
N	4.42641139	1.71727350	-0.15173048
C	4.87229646	2.92105745	-0.85751626
H	4.61608648	3.84062821	-0.29798274
H	4.36768760	2.96822024	-1.82833323
C	6.38421782	2.87691019	-1.07119096
H	6.62597270	2.03515663	-1.75188935
H	6.70938380	3.80209160	-1.56174770
N	7.07955908	2.75471482	0.20671106
C	6.62989867	1.56323054	0.92276664
H	7.13253545	1.52704853	1.89620103
H	6.89313120	0.63462695	0.37664787
C	5.11868547	1.60317197	1.13559462
H	4.79674021	0.68569338	1.63683941
H	4.86858777	2.45006989	1.80105124
C	8.52442772	2.78293973	0.04788536
H	8.91584036	1.93924590	-0.55373003
H	9.00557017	2.74690695	1.03082935
H	8.82561350	3.71472995	-0.44239548
C	2.88292004	-0.04000703	-2.40700025
H	3.93493826	0.26047317	-2.34099393
H	2.85302356	-1.08801915	-2.75339373
N	2.18187838	0.88550179	-3.29372723
C	2.99303238	1.27217543	-4.45086556
H	3.22546817	0.40353288	-5.09622107
H	3.94334035	1.68603517	-4.09489567
C	2.26141910	2.32557337	-5.28106085
H	2.15297997	3.24779581	-4.67500627
H	2.86424283	2.57808180	-6.16154075
N	0.96734828	1.81862398	-5.72861456
C	0.15660091	1.41036828	-4.58366216
H	-0.78341356	0.98428671	-4.95412240
H	-0.10000148	2.27268745	-3.93588028
C	0.89026645	0.36423175	-3.74850468
H	0.28639296	0.10446505	-2.87483519
H	1.02472167	-0.55282822	-4.35500218
C	0.27300212	2.77060419	-6.57947993
H	-0.66479360	2.33242043	-6.93720317
H	0.89047759	3.00752736	-7.45240744
H	0.03011344	3.72222584	-6.06662268
C	3.33657556	-1.29583789	0.11046936
H	4.35996695	-1.06244914	-0.20118500
H	3.28490545	-1.18670657	1.20562811
N	2.97961075	-2.64171861	-0.33770179
C	4.13901693	-3.51853936	-0.51827925
H	4.67091972	-3.69992311	0.43476747
H	4.84161700	-3.04012907	-1.20978698
C	3.69286199	-4.85915528	-1.09968991
H	3.28600956	-4.68990099	-2.11714549
H	4.56174821	-5.52092650	-1.19627674
N	2.71330683	-5.49718206	-0.22488213
C	1.56160716	-4.62268000	-0.01869995
H	0.87530471	-5.10628033	0.68631970
H	1.00792914	-4.45470458	-0.96666751
C	2.00238652	-3.27793077	0.55112986
H	2.42913969	-3.43685723	1.55856373
H	1.14249451	-2.61224105	0.67190773
C	2.32517903	-6.81275789	-0.70477430
H	3.20973054	-7.45290253	-0.78971770
3P			
Cu	-0.83506700	-0.55315500	-0.63284900
I	-0.50525200	-2.15951400	-2.71506600
N	-2.19873900	1.06837000	-1.20845200
N	-2.58208700	-0.92090600	0.60715100
C	-2.77247000	-1.91246700	1.47119800

Atom	X	Y	Z
C	-3.96968000	-2.09095500	2.18714100
C	-5.00641500	-1.20033000	1.98784300
C	-4.84362800	-0.14156000	1.06851800
C	-5.87656600	0.81554600	0.78799700
C	-5.68734900	1.80531200	-0.12865400
C	-4.44713000	1.92539200	-0.84170800
C	-4.21280200	2.91568000	-1.82049300
C	-2.99717100	2.94873700	-2.47585100
C	-2.01576100	1.99904200	-2.13757700
C	-3.39489200	1.01091700	-0.57360700
C	-3.59751500	-0.04462700	0.39505200
H	-1.94293700	-2.60067500	1.60086500
H	-4.06345300	-2.92092600	2.87915100
H	-5.94636000	-1.30701400	2.52227000
H	-6.82054300	0.72771800	1.31835600
H	-6.47815500	2.51917400	-0.34120200
H	-4.99360600	3.63432300	-2.05396700
H	-2.78945600	3.68775200	-3.24222700
H	-1.05471800	1.98682700	-2.64342400
P	1.30784800	-0.03507500	0.11010600
C	-0.30817200	2.02304100	2.22101000
C	0.76006800	-4.12466800	2.37782400
C	2.80317300	-3.63211000	3.41330000
C	1.18558500	-3.37317000	1.12052100
C	3.28022800	-2.87293500	2.17606200
C	2.49025100	-1.46939000	0.33618400
C	1.80689600	0.97518300	1.60620300
C	2.13928600	0.89925400	-1.29270800
C	4.46558200	0.59790900	-2.01825600
C	5.90588700	0.91245200	-1.61969500
C	-1.03600500	3.36219300	2.29226700
C	1.75150000	3.16902400	2.63735700
C	3.79272100	2.68715000	-1.03160800
C	0.97598200	4.48379300	2.69652700
C	5.25081100	2.94591100	-0.65896700
H	0.12338200	-4.97596300	2.11909200
H	3.64436800	-4.12230400	3.91263600
H	0.19488300	-3.44587200	3.04004100
H	2.34015900	-2.92070600	4.11755700
H	1.64558500	-4.08447600	0.40995900
H	3.85428000	-3.56261200	1.52819400
H	0.31616200	-2.93974700	0.61567900
H	3.95175400	-2.06236300	2.48300100
H	2.52124500	-2.03132300	-0.61137900
H	3.48329000	-1.03882200	0.50380200
H	1.71754200	0.31391100	2.48650600
H	-0.31552100	1.55349600	3.22457800
H	-0.83077300	1.35251300	1.53286300
H	4.30604300	-0.48542000	-1.99562700
H	2.86905100	1.21072800	1.47259400
H	6.12070900	0.45851900	-0.63794100
H	2.00216800	0.27366300	-2.18333300
H	1.85162500	2.76188600	3.66197300
H	6.60672400	0.50577700	-2.35439200
H	-2.03790200	3.23296700	2.71238100
H	4.29314900	0.94062800	-3.05549700
H	1.53539100	1.80093300	-1.45089900
H	2.76162500	3.35602300	2.25381500
H	-1.13065500	3.78145400	1.27680800
H	5.43615700	2.58163500	0.36566200
H	3.12899300	3.13982400	-0.28684000
H	1.44086700	5.17303100	3.40779300
H	3.58075700	3.16628800	-2.00673200
H	0.97869900	4.95261900	1.69835600
H	5.47520400	4.01617500	-0.69551800

Atom	X	Y	Z
N	2.12340900	-2.30318300	1.47946100
N	1.06516300	2.22649100	1.74613500
N	3.54465700	1.24354800	-1.07686700
O	1.88113000	-4.65675400	3.07277300
O	-0.35789500	4.28062900	3.13963800
O	6.13683300	2.31438600	-1.57149400
4P			
Cu	-0.43629100	-0.62959200	-0.13661400
I	-0.37325600	-3.25819400	0.01410100
N	-2.05404600	0.01684300	-1.44413500
N	-1.94451600	0.13242500	1.27511000
C	-1.88473400	0.15972200	2.60182800
C	-2.97910500	0.51707600	3.41089300
C	-4.17480000	0.85397400	2.80758800
C	-4.27371700	0.82785800	1.39930300
C	-5.48023200	1.15443400	0.69323600
C	-5.53369800	1.10128600	-0.66685200
C	-4.38564400	0.71609800	-1.43807900
C	-4.39984900	0.63058200	-2.84723900
C	-3.25574100	0.24084200	-3.51532700
C	-2.10156200	-0.05935100	-2.76922800
C	-3.17209800	0.39484900	-0.77517000
C	-3.11482200	0.45343600	0.66975600
H	-0.93157000	-0.11406700	3.04496500
H	-2.87081000	0.52126900	4.49023100
H	-5.04142700	1.13384000	3.40043600
H	-6.35575000	1.44048600	1.26944100
H	-6.45244500	1.34452700	-1.19321900
H	-5.31134100	0.86732900	-3.38932500
H	-3.23343800	0.15939700	-4.59677300
H	-1.18908600	-0.37785600	-3.26489300
P	1.60438700	0.48138500	-0.08549300
C	1.59801100	2.19581600	-0.77639300
C	0.46937400	2.98973500	-0.50580700
C	0.37511100	4.28826700	-1.00399100
C	1.39860500	4.80853800	-1.80045600
C	2.51527800	4.02394100	-2.08932900
C	2.61807300	2.72726400	-1.57884200
C	2.15726000	0.70274900	1.66319500
C	2.66002100	1.90552200	2.17913100
C	3.04590600	1.99175200	3.51946800
C	2.93779200	0.87952000	4.35508000
C	2.43782900	-0.32319700	3.84815000
C	2.04337500	-0.41275900	2.51299400
C	3.03970900	-0.34928300	-0.88399500
C	2.78146700	-1.34032000	-1.84212400
C	3.83637300	-1.99239100	-2.48392500
C	5.15597500	-1.66852800	-2.16804800
C	5.42272000	-0.69543200	-1.20102500
C	4.37144100	-0.04166700	-0.55875900
H	-0.33976200	2.57998300	0.09309200
H	-0.50110700	4.89031300	-0.77969600
H	1.32189800	5.81657500	-2.19802400
H	3.31211300	4.41919400	-2.71327800
H	3.49237900	2.12869700	-1.81121800
H	2.74742600	2.77712200	1.53809000
H	3.43346100	2.92970300	3.90786100
H	3.24030100	0.94873800	5.39622900
H	2.35151700	-1.19385300	4.49217300
H	1.64643100	-1.34831900	2.12448200
H	1.75614300	-1.62862900	-2.05312100
H	3.62304900	-2.76609000	-3.21553900
H	5.97612500	-2.18214600	-2.66189500
H	6.44913100	-0.45170900	-0.94121300
H	4.58597700	0.70026600	0.20499500