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Unexpected reversible pyrazine based methylation in a Ru(II) complex bearing a pyrazin-2'-yl-1,2,4-triazolato ligand and its effect on acid/base and photophysical properties

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Electronic Supplementary Information

Unexpected Reversible Pyrazine based Methylation in a Ru(II) complex bearing a pyrazine-yl-1,2,4-triazolato ligand and its effect on acid/base and photophysical properties

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Phenyltriazole complex 1a

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1. S.I.Gorelsky, AOMix program, http://www.sg-chem.net/
2. S.I.Gorelsky, A.B.P.Lever, J.Organomet.Chem. 635, 187-196 (2001)
*****
This file was created on Wed Nov 7 09:08:00 2012
Calculations from Gaussian
%chk=CorrectOneaOpt.chk
Molecule: C32H24N9Ru(1+)
Details: # rb3lyp/lanl2dz SCF=Tight Pop=Full IOp(3/33=1) Geom=Check Guess=Read
Source file: CorrectOneaAOMix.log
Population analysis: MPA
439 orbitals( 439 canonical) 147 alpha + 147 beta electrons
Number of fragments: 4
Fragment 1 ( 24 atoms, 160 orbitals): Phenyl Triazole
Fragment 2 ( 1 atoms, 9 orbitals): Pyrazine Nitrogen
Fragment 3 ( 40 atoms, 248 orbitals): Bipy
Fragment 4 ( 1 atoms, 22 orbitals): Ru Atom

COMPOSITIONS OF MOLECULAR ORBITALS (GROSS CONTRIBUTIONS, %)
AND OVERLAP POPULATIONS (OP) BETWEEN FRAGMENTS
```

Alpha MO:	1	2	3	4	5	6	7	8	9	10
Energy(eV):	-394.61	-394.53	-394.45	-394.42	-394.34	-393.39	-393.23	-392.62	-391.85	-282.50
Symmetry:	na	na	na	na	na	na	na	na	na	na
=====										
FRAG# 1:	0.00	0.00	0.00	0.00	99.98	99.98	0.09	100.01	100.00	0.00
FRAG# 2:	0.00	0.00	0.00	0.00	0.00	0.00	99.91	0.00	0.00	0.00
FRAG# 3:	99.98	99.98	99.98	99.98	0.00	0.00	0.00	0.00	0.00	99.97
FRAG# 4:	0.02	0.02	0.02	0.02	0.02	0.02	0.00	0.00	0.00	0.03
OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.000	0.000

OP(1 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(1 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(3 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Alpha MO:	11	12	13	14	15	16	17	18	19	20
Energy(eV):	-282.44	-282.30	-282.26	-282.06	-281.96	-281.86	-281.85	-281.82	-281.74	-281.44
Symmetry:	na	na	na	na	na	na	na	na	na	na
=====										
FRAG# 1:	0.00	0.00	0.00	0.00	99.98	0.00	0.00	0.00	100.00	0.00
FRAG# 2:	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FRAG# 3:	99.98	99.97	99.98	100.00	0.00	99.99	99.99	99.99	0.00	100.00
FRAG# 4:	0.02	0.03	0.02	0.00	0.02	0.01	0.01	0.01	0.01	0.00
OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(1 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(1 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(3 & 4)	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Alpha MO:	21	22	23	24	25	26	27	28	29	30
Energy(eV):	-281.40	-281.34	-281.33	-281.32	-281.32	-281.29	-281.22	-281.18	-281.18	-281.13
Symmetry:	na	na	na	na	na	na	na	na	na	na
=====										
FRAG# 1:	0.00	99.98	0.00	99.97	0.00	0.00	0.00	0.00	0.00	0.00
FRAG# 2:	0.00	0.01	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00
FRAG# 3:	100.00	0.00	100.00	0.00	100.00	100.00	100.00	100.00	100.00	100.00
FRAG# 4:	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(1 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(1 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(3 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Alpha MO:	31	32	33	34	35	36	37	38	39	40
Energy(eV):	-281.12	-281.07	-281.05	-281.02	-280.68	-279.34	-278.93	-278.92	-278.91	-278.88
Symmetry:	na	na	na	na	na	na	na	na	na	na
=====										
FRAG# 1:	0.00	0.00	99.97	0.00	100.00	100.00	100.00	100.00	100.00	100.00
FRAG# 2:	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FRAG# 3:	100.00	100.00	0.00	100.00	0.00	0.00	0.00	0.00	0.00	0.00
FRAG# 4:	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(1 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(1 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(3 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Alpha MO:	41	42	43	44	45	46	47	48	49	50
Energy(eV):	-278.84	-81.31	-50.90	-50.85	-50.58	-30.98	-30.16	-29.97	-29.92	-29.45
Symmetry:	na	na	na	na	na	na	na	na	na	na
=====										
FRAG# 1:	100.00	0.17	0.01	-0.30	-0.11	99.29	2.60	7.39	73.78	0.06
FRAG# 2:	0.00	0.00	0.00	0.00	0.00	0.22	0.24	1.39	15.63	0.00
FRAG# 3:	0.00	0.41	-0.42	-0.12	-0.05	0.46	98.10	91.52	11.27	99.16
FRAG# 4:	0.00	99.42	100.41	100.42	100.16	0.03	-0.93	-0.30	-0.67	0.78
OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	0.002	0.002	0.010	0.114	0.000
OP(1 & 3)	0.000	0.000	0.000	0.000	0.000	0.003	0.004	0.004	0.001	0.001
OP(1 & 4)	0.000	0.003	0.000	-0.007	-0.002	-0.003	-0.003	0.002	-0.014	0.000
OP(2 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.001	0.000
OP(3 & 4)	0.000	0.007	-0.009	-0.003	-0.002	-0.002	-0.025	-0.019	-0.005	0.011

Alpha MO:	51	52	53	54	55	56	57	58	59	60
Energy(eV):	-29.30	-27.93	-26.18	-25.70	-25.51	-25.48	-25.45	-25.31	-25.30	-25.21
Symmetry:	na	na	na	na	na	na	na	na	na	na
=====										
FRAG# 1:	0.02	56.73	98.29	0.31	0.20	0.25	0.03	0.02	0.43	98.24

FRAG#	2:	0.00	42.12	0.09	0.00	0.00	0.00	0.00	0.00	0.00	0.60
FRAG#	3:	99.11	0.18	0.47	98.56	98.77	99.57	99.54	100.01	99.06	0.88
FRAG#	4:	0.87	0.97	1.15	1.12	1.03	0.18	0.43	-0.03	0.51	0.27
OP (1 & 2)		0.000	0.206	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.006
OP (1 & 3)		0.000	0.002	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP (1 & 4)		0.000	0.015	0.015	0.000	-0.001	0.000	0.000	0.000	0.000	0.003
OP (2 & 3)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP (2 & 4)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP (3 & 4)		0.013	0.000	0.000	0.012	0.012	0.001	0.006	-0.002	0.007	0.000

[illegible]

FRAG#	1:	99.36	0.17	0.01	97.30	98.29	99.90	0.09	0.17	0.81	15.35
FRAG#	2:	0.63	0.00	0.00	2.36	1.03	0.08	0.00	0.02	0.07	1.35
FRAG#	3:	0.04	100.00	100.14	0.18	0.09	0.02	98.83	98.54	98.31	82.56
FRAG#	4:	-0.02	-0.17	-0.15	0.16	0.60	0.01	1.08	1.27	0.81	0.75
OP(1 & 2)		0.006	0.000	0.000	0.020	0.008	0.000	0.000	0.000	0.000	-0.003
OP(1 & 3)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.001	0.001
OP(1 & 4)		-0.001	0.000	0.000	0.000	0.008	0.000	-0.002	-0.002	0.000	0.001
OP(2 & 3)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(3 & 4)		0.000	-0.004	-0.003	0.000	-0.001	0.000	0.014	0.015	0.009	0.000

[illegible]

FRAG#	1:	74.70	91.42	0.17	0.16	0.05	-0.01	96.75	94.74	2.42	1.28
FRAG#	2:	6.68	7.78	0.00	0.00	0.01	0.00	1.48	2.63	0.07	0.01
FRAG#	3:	17.95	0.28	99.70	99.60	98.32	98.25	0.88	1.44	95.12	98.07
FRAG#	4:	0.68	0.52	0.13	0.24	1.62	1.76	0.90	1.18	2.40	0.64
OP(1 & 2)		-0.016	0.049	0.000	0.000	0.000	0.000	0.009	-0.014	0.000	0.000
OP(1 & 3)		-0.004	0.000	0.000	0.000	0.000	-0.001	0.000	0.000	-0.002	0.003
OP(1 & 4)		0.002	0.006	0.000	0.000	-0.001	-0.001	0.011	0.012	-0.002	0.000
OP(2 & 3)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(3 & 4)		-0.001	-0.002	0.001	0.002	0.018	0.019	-0.001	0.000	0.028	0.000

[illegible]

FRAG#	1:	97.39	93.00	0.44	0.21	1.87	0.30	89.91	68.47	23.28	0.56
FRAG#	2:	1.48	5.58	0.00	0.01	0.04	0.02	3.00	5.81	1.93	0.02
FRAG#	3:	0.65	0.44	98.47	98.63	97.46	97.92	4.91	25.32	74.65	99.28
FRAG#	4:	0.48	0.97	1.08	1.15	0.64	1.76	2.18	0.40	0.14	0.14
OP(1 & 2)	-0.002	0.043	0.000	0.000	0.000	0.000	0.000	0.025	0.043	0.015	0.000
OP(1 & 3)	0.001	0.000	-0.001	0.001	0.001	0.001	-0.001	0.000	0.000	0.000	0.001
OP(1 & 4)	0.004	0.008	-0.004	-0.001	0.001	-0.007	0.022	0.000	-0.002	-0.001	0.000
OP(2 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(3 & 4)	-0.001	-0.003	-0.001	0.002	-0.002	-0.002	-0.009	-0.004	-0.007	-0.002	0.000

[illegible][illegible]

FRAG#	1:	93.74	98.50	10.61	20.86	15.43	98.54	86.60	1.06	0.89	61.53
FRAG#	2:	0.41	0.02	1.45	0.51	0.23	0.00	0.10	0.20	0.15	19.93
FRAG#	3:	1.28	0.62	15.50	13.34	12.26	0.21	1.53	94.44	93.85	15.04
FRAG#	4:	4.57	0.86	72.44	65.28	72.08	1.25	11.77	4.29	5.12	3.49
OP(1 & 2)		-0.001	-0.002	-0.003	-0.001	0.000	0.000	0.000	-0.002	-0.002	-0.256
OP(1 & 3)		0.001	-0.006	0.003	0.006	0.003	0.000	-0.001	-0.004	-0.005	-0.007
OP(1 & 4)		0.003	0.005	-0.034	-0.051	-0.030	-0.002	-0.030	-0.002	-0.005	-0.025
OP(2 & 3)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.001
OP(3 & 4)		-0.005	-0.005	-0.075	-0.067	-0.073	-0.001	-0.014	-0.037	-0.046	-0.004
=====											
Alpha MO:		151	152	153	154	155	156	157	158	159	160
		LUMO+3	LUMO+4	LUMO+5	LUMO+6	LUMO+7	LUMO+8	LUMO+9	LUMO+10	LUMO+11	LUMO+12
Energy(eV):		-4.51	-4.26	-4.21	-4.06	-3.84	-2.99	-2.75	-2.47	-2.43	-2.20
Symmetry:		na	na	na	na	na	na	na	na	na	na
=====											
FRAG#	1:	11.31	0.26	1.60	3.71	89.94	0.46	0.36	96.85	9.57	13.38
FRAG#	2:	2.43	0.02	0.00	0.07	1.82	0.03	0.01	0.07	0.02	0.00
FRAG#	3:	83.34	97.81	95.53	94.03	7.64	98.88	99.27	0.74	24.15	18.97
FRAG#	4:	2.93	1.91	2.87	2.18	0.60	0.63	0.36	2.35	66.27	67.65
OP(1 & 2)		-0.035	0.000	0.000	-0.001	-0.029	-0.001	0.000	-0.001	-0.012	-0.001
OP(1 & 3)		0.006	0.001	0.001	0.002	-0.009	0.002	-0.002	-0.001	-0.215	-0.238
OP(1 & 4)		-0.010	-0.002	-0.002	-0.002	0.002	-0.002	0.000	-0.011	-0.562	-0.522
OP(2 & 3)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)		0.000	0.000	0.000	0.000	-0.001	0.000	0.000	0.000	0.002	-0.004
OP(3 & 4)		-0.019	-0.019	-0.026	-0.023	-0.007	-0.015	-0.009	-0.040	-1.296	-1.408
=====											
Alpha MO:		161	162	163	164	165	166	167	168	169	170
		LUMO+13	LUMO+14	LUMO+15	LUMO+16	LUMO+17	LUMO+18	LUMO+19	LUMO+20	LUMO+21	LUMO+22
Energy(eV):		-1.82	-1.66	-1.64	-1.60	-1.13	-0.56	-0.47	-0.34	0.09	0.12
Symmetry:		na	na	na	na	na	na	na	na	na	na
=====											
FRAG#	1:	2.28	0.23	76.34	12.94	87.10	0.53	-9.51	0.41	86.37	12.08
FRAG#	2:	0.31	0.09	0.48	-0.08	10.42	-0.01	-0.30	0.00	1.21	0.15
FRAG#	3:	-7.88	-8.96	-1.06	-3.17	1.00	98.51	-1.73	98.81	12.24	84.28
FRAG#	4:	105.29	108.65	24.24	90.30	1.48	0.97	111.54	0.78	0.18	3.49
OP(1 & 2)		-0.011	-0.003	-0.016	0.004	-0.417	-0.001	-0.062	0.000	-0.090	-0.013
OP(1 & 3)		0.140	0.087	0.048	0.192	0.004	0.009	1.281	0.004	0.006	0.141
OP(1 & 4)		-0.607	-0.771	-0.409	-1.320	-0.017	-0.042	-4.476	-0.028	-0.008	-0.364
OP(2 & 3)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)		0.005	-0.006	-0.010	-0.028	-0.005	-0.002	-0.044	0.000	-0.002	0.001
OP(3 & 4)		-2.836	-3.153	-0.435	-2.067	-0.045	-0.065	-10.8	-0.075	-0.047	-0.967
=====											
Alpha MO:		171	172	173	174	175	176	177	178	179	180
		LUMO+23	LUMO+24	LUMO+25	LUMO+26	LUMO+27	LUMO+28	LUMO+29	LUMO+30	LUMO+31	LUMO+32
Energy(eV):		0.32	0.57	0.65	0.72	0.80	0.84	0.94	1.03	1.05	1.14
Symmetry:		na	na	na	na	na	na	na	na	na	na
=====											
FRAG#	1:	2.01	8.32	18.45	7.54	7.52	15.04	4.74	35.42	58.38	21.69
FRAG#	2:	0.01	0.12	-0.36	-0.12	0.21	0.12	-0.05	-0.41	3.14	0.73
FRAG#	3:	94.64	89.76	80.33	91.48	92.94	83.43	94.60	66.17	37.71	76.28
FRAG#	4:	3.34	1.80	1.57	1.10	-0.67	1.41	0.71	-1.18	0.77	1.29
OP(1 & 2)		-0.009	-0.010	-0.223	-0.097	-0.078	-0.152	-0.037	-0.550	-0.264	-0.166
OP(1 & 3)		0.186	0.039	0.013	0.092	-0.014	-0.056	0.001	-0.049	0.021	0.048
OP(1 & 4)		-0.436	-0.176	-0.092	-0.190	-0.018	-0.527	-0.114	-0.415	-0.037	-0.093
OP(2 & 3)		0.000	0.000	-0.001	-0.001	0.000	-0.001	0.000	-0.001	0.000	-0.002
OP(2 & 4)		0.002	0.001	0.010	0.011	0.007	0.021	-0.005	0.016	-0.003	0.013
OP(3 & 4)		-1.589	-0.536	-0.234	-1.048	-0.764	-0.229	-0.066	-0.337	-0.113	-0.305
=====											
Alpha MO:		181	182	183	184	185	186	187	188	189	190
		LUMO+33	LUMO+34	LUMO+35	LUMO+36	LUMO+37	LUMO+38	LUMO+39	LUMO+40	LUMO+41	LUMO+42
Energy(eV):		1.26	1.31	1.42	1.45	1.55	1.76	1.90	2.00	2.30	2.34
Symmetry:		na	na	na	na	na	na	na	na	na	na
=====											
FRAG#	1:	16.06	1.40	3.86	1.35	18.20	39.21	52.00	81.36	4.93	24.78
FRAG#	2:	-0.10	-0.04	0.09	0.00	0.16	-0.20	0.05	-0.85	-0.27	0.09
FRAG#	3:	83.29	99.52	94.16	98.49	82.85	59.94	48.40	17.09	92.79	57.75
FRAG#	4:	0.75	-0.88	1.88	0.16	-1.21	1.05	-0.45	2.40	2.55	17.38
OP(1 & 2)		-0.503	-0.038	-0.007	-0.001	-0.038	-1.576	-0.236	-0.352	-0.212	-0.059
OP(1 & 3)		-0.061	0.003	-0.078	0.006	0.018	0.080	0.088	0.012	-0.030	0.073
OP(1 & 4)		-0.191	-0.005	-0.091	-0.039	-0.386	-0.074	-0.955	-0.231	0.001	-0.525

OP(2 & 3)	-0.003	0.000	0.000	0.000	0.000	0.006	0.000	-0.003	0.000	0.000
OP(2 & 4)	0.061	-0.002	0.001	0.000	0.003	-0.016	0.006	0.008	-0.003	-0.026
OP(3 & 4)	-0.320	-0.584	-0.013	-0.092	-1.030	-0.299	-0.947	-0.142	-0.153	-0.531

[illegible]

FRAG#	1:	89.00	45.10	35.82	19.36	86.34	82.29	61.38	31.40	46.88	7.37
FRAG#	2:	-0.03	-0.28	-1.10	-0.71	0.00	-0.80	-0.22	-0.20	-0.93	0.05
FRAG#	3:	10.83	46.38	65.37	72.06	14.08	16.15	34.30	64.94	59.13	92.40
FRAG#	4:	0.20	8.80	-0.09	9.28	-0.42	2.36	4.54	3.85	-5.07	0.19
OP (1 & 2)		-0.433	-0.160	-0.603	-0.278	-0.001	-0.186	-0.065	-0.096	-0.443	-0.010
OP (1 & 3)		0.024	-0.009	0.124	0.182	0.035	0.024	0.016	0.394	0.472	0.028
OP (1 & 4)		-0.119	-0.238	-0.405	-0.770	-0.074	-0.094	-0.295	-1.389	-0.905	-0.105
OP (2 & 3)		0.001	-0.001	0.001	0.001	0.000	0.000	0.000	0.000	0.002	0.000
OP (2 & 4)		-0.017	-0.011	0.058	-0.053	0.000	-0.013	-0.003	0.003	-0.024	0.001
OP (3 & 4)		-0.105	-0.242	-0.740	-1.117	-0.257	-0.115	-0.070	-1.894	-2.465	-0.300

[illegible]

FRAG#	1:	19.40	48.90	62.57	14.59	70.02	16.74	17.85	10.46	71.09	32.87
FRAG#	2:	-1.17	-1.83	-0.95	-0.48	-1.24	-0.23	-0.19	-0.21	0.42	-1.02
FRAG#	3:	78.39	50.01	34.69	88.39	28.52	76.09	76.31	87.12	27.52	63.07
FRAG#	4:	3.37	2.93	3.70	-2.50	2.70	7.40	6.03	2.64	0.97	5.07
OP (1 & 2)		-0.498	-0.877	-0.608	-0.189	-0.541	-0.193	-0.100	-0.088	-0.167	-0.652
OP (1 & 3)		0.027	0.033	0.014	0.030	0.011	0.147	0.005	-0.010	-0.042	-0.036
OP (1 & 4)		0.005	-0.139	-0.071	-0.187	-0.054	-0.462	-0.259	-0.035	-0.019	-0.046
OP (2 & 3)		-0.001	0.000	0.000	0.000	0.000	-0.001	0.000	0.000	0.000	-0.001
OP (2 & 4)		-0.032	-0.001	-0.031	-0.003	0.001	0.005	-0.010	-0.004	0.006	-0.009
OP (3 & 4)		-0.223	-0.733	-0.178	-0.636	-0.193	-1.055	-0.217	-0.141	-0.351	-0.607

[illegible]

FRAG#	1:	48.57	8.59	17.69	57.58	19.90	16.29	37.40	35.11	30.12	55.98
FRAG#	2:	0.10	-0.28	-0.22	-0.93	0.02	-0.24	-2.72	-1.35	-0.60	3.25
FRAG#	3:	48.24	86.61	80.62	42.66	69.59	65.65	45.77	64.39	69.45	23.44
FRAG#	4:	3.09	5.08	1.91	0.69	10.49	18.29	19.55	1.85	1.04	17.33
OP(1 & 2)		-0.258	-0.125	-0.155	-0.116	-0.182	-0.057	-0.255	-0.362	-0.148	-0.540
OP(1 & 3)		0.014	-0.053	0.003	0.054	-0.072	-0.422	-0.063	0.166	0.014	0.340
OP(1 & 4)		-0.104	-0.291	-0.134	-0.301	-0.483	-1.038	-0.222	-0.609	-0.116	-1.495
OP(2 & 3)		0.000	0.000	0.000	0.000	-0.002	-0.001	0.000	-0.001	0.000	0.001
OP(2 & 4)		-0.011	0.002	0.010	-0.009	0.023	0.020	-0.015	0.007	0.010	0.033
OP(3 & 4)		-0.178	-0.366	-0.084	-0.502	-1.277	-1.802	-2.466	-0.536	-0.619	-1.566

[illegible]

FRAG#	1:	44.71	41.46	85.35	21.03	26.85	17.04	20.26	21.37	31.50	69.99
FRAG#	2:	-0.03	-1.14	-0.72	-0.67	-1.00	-0.18	-0.69	-1.54	-5.11	-10.83
FRAG#	3:	54.84	56.45	15.24	75.80	71.87	83.40	80.71	69.96	69.34	37.36
FRAG#	4:	0.48	3.23	0.13	3.85	2.28	-0.26	-0.28	10.21	4.26	3.49
OP (1 & 2)		-0.032	-0.128	-0.169	-0.169	-0.145	-0.051	-0.176	-0.128	-0.539	-1.126
OP (1 & 3)		-0.151	-0.023	0.091	0.091	-0.027	0.138	0.040	0.023	0.040	-0.119
OP (1 & 4)		-0.298	-0.229	-0.250	-0.393	-0.169	-0.604	-0.941	-0.256	-0.060	-0.496
OP (2 & 3)		0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000
OP (2 & 4)		0.004	-0.006	0.003	-0.003	0.002	0.005	0.006	0.009	-0.001	-0.002
OP (3 & 4)		-0.235	-0.410	-0.398	-0.364	-0.390	-0.598	-0.279	-2.113	-0.816	-0.064

[illegible]

FRAG#	1:	48.41	37.34	64.31	39.42	30.81	13.32	31.01	33.99	56.87	58.31
FRAG#	2:	0.23	-2.48	-4.93	-3.14	-2.30	-0.72	-0.25	-1.79	-0.51	-0.22
FRAG#	3:	48.39	56.18	35.24	60.54	68.15	72.54	56.45	64.02	36.94	40.49
FRAG#	4:	2.96	8.96	5.38	3.19	3.35	14.86	12.79	3.78	6.69	1.42
OP(1 & 2)		-0.074	-0.306	-0.599	-0.628	-0.296	-0.191	-0.076	-0.264	-0.094	-0.070
OP(1 & 3)		0.149	0.141	0.176	-0.116	0.091	0.083	0.060	-0.019	0.054	0.116
OP(1 & 4)		-0.577	-0.566	-1.118	-0.421	-0.521	-0.190	-0.397	-0.268	-0.733	-0.667
OP(2 & 3)		0.000	0.000	-0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)		0.008	-0.005	0.011	-0.008	0.003	0.002	0.015	-0.011	0.007	0.010
OP(3 & 4)		-1.147	-1.325	-0.652	-1.244	-0.557	-2.446	-2.192	-0.547	-0.631	-0.396
Alpha MO:		241	242	243	244	245	246	247	248	249	250
Energy(eV):		6.79	6.84	6.90	7.04	7.14	7.27	7.35	7.45	7.52	7.56
Symmetry:		na	na	na	na	na	na	na	na	na	na
FRAG#	1:	65.41	33.06	36.93	57.55	55.59	34.09	43.58	16.47	27.34	19.39
FRAG#	2:	-0.36	0.09	-1.56	-0.16	-1.64	-0.25	-1.03	-0.03	0.61	-0.15
FRAG#	3:	34.18	56.46	61.96	38.64	38.98	64.20	54.86	81.18	67.41	78.21
FRAG#	4:	0.78	10.39	2.67	3.98	7.08	1.96	2.60	2.39	4.63	2.55
OP(1 & 2)		-0.064	-0.067	-0.347	-0.164	-0.256	-0.072	-0.106	-0.015	-0.080	-0.156
OP(1 & 3)		-0.003	0.291	0.053	-0.021	0.091	0.021	-0.065	0.025	0.016	0.079
OP(1 & 4)		-0.115	-1.741	-0.382	-0.070	-0.847	-0.284	-0.381	-0.169	-0.191	-0.176
OP(2 & 3)		0.000	0.000	0.000	-0.001	0.000	-0.001	0.001	0.000	0.001	-0.002
OP(2 & 4)		0.002	0.001	-0.003	-0.001	0.009	0.009	-0.012	-0.001	-0.017	0.024
OP(3 & 4)		-0.042	-1.740	-1.079	-0.233	-0.415	-0.480	-0.216	-1.200	-0.410	-0.905
Alpha MO:		251	252	253	254	255	256	257	258	259	260
Energy(eV):		7.64	7.69	7.74	7.78	7.84	7.87	7.95	7.99	8.05	8.20
Symmetry:		na	na	na	na	na	na	na	na	na	na
FRAG#	1:	5.74	51.17	18.18	10.64	23.44	27.70	32.95	41.21	12.90	26.41
FRAG#	2:	-0.05	-0.95	-0.14	0.46	-0.40	-0.20	-0.12	0.66	0.03	-0.20
FRAG#	3:	85.69	46.96	80.55	85.00	71.09	71.22	64.01	58.85	83.47	73.17
FRAG#	4:	8.62	2.81	1.42	3.89	5.87	1.28	3.15	-0.71	3.60	0.62
OP(1 & 2)		-0.023	-0.219	-0.013	-0.214	-0.328	-0.035	-0.268	-0.230	-0.028	-0.542
OP(1 & 3)		-0.070	0.006	-0.015	-0.290	-0.006	-0.004	-0.002	0.028	0.051	0.024
OP(1 & 4)		-1.686	-0.013	-0.054	-0.773	-0.697	-0.100	-0.171	-0.148	-0.186	-0.076
OP(2 & 3)		0.000	0.002	0.000	-0.001	0.000	0.000	0.004	0.000	0.001	-0.001
OP(2 & 4)		-0.013	-0.020	0.003	0.007	0.006	0.002	-0.005	0.015	-0.002	-0.006
OP(3 & 4)		-0.763	-0.368	-0.337	-1.166	-0.645	-0.052	-0.468	-0.270	-1.917	-0.559
Alpha MO:		261	262	263	264	265	266	267	268	269	270
Energy(eV):		8.25	8.30	8.33	8.41	8.47	8.56	8.68	8.76	8.78	9.03
Symmetry:		na	na	na	na	na	na	na	na	na	na
FRAG#	1:	35.81	47.12	25.36	77.10	49.27	43.30	28.15	34.51	23.96	27.69
FRAG#	2:	0.39	-1.21	-0.59	-0.10	-0.34	1.13	0.81	0.43	-0.02	-0.05
FRAG#	3:	63.51	53.56	73.76	22.35	50.38	54.93	68.76	54.63	73.20	70.80
FRAG#	4:	0.30	0.54	1.48	0.64	0.69	0.63	2.27	10.43	2.87	1.56
OP(1 & 2)		-0.135	-0.213	-0.211	-0.038	-0.134	-0.081	-0.194	-0.157	-0.052	-0.070
OP(1 & 3)		0.028	0.021	0.014	0.011	0.058	0.136	0.024	0.042	-0.013	-0.014
OP(1 & 4)		-0.315	-0.144	-0.017	-0.040	-0.118	-0.442	-0.099	-0.077	-0.046	-0.243
OP(2 & 3)		-0.001	0.004	0.002	0.000	-0.001	-0.002	0.000	0.000	-0.001	-0.001
OP(2 & 4)		0.010	-0.037	-0.007	-0.002	0.007	0.031	-0.007	0.000	0.001	0.010
OP(3 & 4)		-0.958	-0.136	-0.093	-0.075	-0.175	-2.118	-0.501	-0.110	-0.156	-0.813
Alpha MO:		271	272	273	274	275	276	277	278	279	280
Energy(eV):		9.10	9.25	9.31	9.35	9.41	9.52	9.62	9.75	9.81	9.91
Symmetry:		na	na	na	na	na	na	na	na	na	na
FRAG#	1:	65.16	19.59	26.73	60.28	40.44	53.89	37.28	14.22	53.20	59.66
FRAG#	2:	1.40	0.66	-0.46	0.57	0.26	-1.09	0.22	-0.95	0.86	0.24
FRAG#	3:	32.10	78.29	71.82	37.20	57.94	46.46	62.22	87.65	44.64	37.01
FRAG#	4:	1.33	1.47	1.91	1.95	1.36	0.74	0.27	-0.92	1.30	3.09
OP(1 & 2)		-0.359	-0.151	-0.096	-0.355	-0.840	-0.240	-0.012	-0.279	-0.002	-0.037
OP(1 & 3)		-0.051	0.077	-0.008	-0.054	-0.017	-0.051	0.014	0.022	-0.107	0.080
OP(1 & 4)		-0.238	-0.408	-0.066	-0.335	-0.032	-0.057	-0.246	-0.071	-0.194	-0.324
OP(2 & 3)		0.000	0.000	-0.001	-0.002	0.000	-0.002	0.000	0.000	0.000	0.000
OP(2 & 4)		0.000	0.007	0.001	-0.005	-0.013	0.024	0.000	0.016	-0.003	-0.004
OP(3 & 4)		-0.543	-0.420	-0.118	-1.317	-0.209	-0.769	-0.610	-0.391	-0.305	-1.804

Alpha MO:	281	282	283	284	285	286	287	288	289	290
Energy(eV):	9.94	10.01	10.07	10.12	10.21	10.36	10.48	10.56	10.62	10.66
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	46.53	31.43	68.03	53.24	62.54	41.04	46.17	42.61	34.41	50.41
FRAG# 2:	0.07	-0.16	0.01	1.43	0.17	-0.85	0.82	1.65	-0.28	0.94
FRAG# 3:	47.45	69.27	28.37	42.79	35.51	53.45	43.46	56.48	45.86	49.07
FRAG# 4:	5.95	-0.54	3.58	2.54	1.78	6.35	9.55	-0.74	20.01	-0.41
OP(1 & 2)	-0.169	-0.207	-0.015	-0.435	-0.091	-0.813	-0.103	-0.835	-0.074	-1.297
OP(1 & 3)	0.060	0.049	0.008	-0.094	-0.147	0.078	0.131	-0.064	0.148	-0.088
OP(1 & 4)	-0.278	-0.108	-0.093	-0.176	-0.550	-0.609	-0.720	-0.254	-3.470	-0.209
OP(2 & 3)	0.000	-0.001	0.000	0.000	-0.001	0.000	0.001	-0.001	0.000	0.002
OP(2 & 4)	-0.011	0.000	0.000	0.000	-0.018	0.006	-0.010	0.011	0.011	0.008
OP(3 & 4)	-0.863	-0.519	-0.582	-0.924	-0.188	-1.678	-1.712	-0.255	-2.826	-0.381
Alpha MO:	291	292	293	294	295	296	297	298	299	300
Energy(eV):	10.81	10.89	11.00	11.25	11.35	11.54	11.56	11.60	11.81	12.03
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	78.59	60.22	32.65	81.23	35.29	22.71	53.27	55.89	40.02	50.34
FRAG# 2:	0.77	0.69	0.53	-1.27	1.38	0.84	2.13	1.67	1.16	3.84
FRAG# 3:	16.26	37.80	59.29	21.21	58.56	67.09	36.53	30.04	53.68	29.73
FRAG# 4:	4.38	1.30	7.53	-1.18	4.76	9.35	8.07	12.40	5.14	16.09
OP(1 & 2)	-0.409	-0.102	-0.009	-1.710	-1.525	-0.069	-1.555	-1.131	-0.313	-0.571
OP(1 & 3)	0.049	-0.041	0.241	-0.279	0.021	0.700	0.158	0.144	0.066	0.432
OP(1 & 4)	-0.692	-0.161	-1.395	-0.356	-0.376	-1.634	-0.968	-0.810	-0.179	-1.151
OP(2 & 3)	-0.001	-0.001	0.000	-0.005	0.001	0.000	-0.004	-0.005	0.001	0.008
OP(2 & 4)	-0.004	0.007	0.000	0.148	0.011	0.005	0.089	0.100	-0.012	-0.028
OP(3 & 4)	-0.744	-0.137	-2.488	-0.917	-1.645	-8.539	-1.656	-2.027	-2.051	-5.667
Alpha MO:	301	302	303	304	305	306	307	308	309	310
Energy(eV):	12.06	12.22	12.27	12.35	12.54	12.68	12.77	12.78	12.84	13.16
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	58.87	54.13	34.98	37.33	49.42	41.11	40.79	55.35	36.90	12.82
FRAG# 2:	0.21	2.19	0.53	2.34	1.80	1.16	0.72	0.35	3.25	1.73
FRAG# 3:	33.22	38.09	63.09	57.91	43.20	55.39	46.95	40.74	56.99	82.98
FRAG# 4:	7.70	5.59	1.40	2.42	5.57	2.35	11.54	3.55	2.86	2.46
OP(1 & 2)	-0.329	-0.354	-0.200	-0.299	-0.224	-0.498	-0.239	-0.246	-0.388	-0.117
OP(1 & 3)	0.155	0.309	0.094	0.184	-0.011	0.029	-0.145	0.092	-0.383	-0.109
OP(1 & 4)	-0.561	-1.176	-1.055	-1.264	-0.251	-0.554	-0.245	-0.741	-0.902	-0.084
OP(2 & 3)	0.001	0.001	0.000	-0.004	-0.004	-0.001	-0.001	0.000	0.003	0.000
OP(2 & 4)	0.009	0.019	0.058	0.062	0.034	0.009	0.006	-0.002	0.017	-0.001
OP(3 & 4)	-3.333	-4.387	-2.938	-2.169	-2.832	-2.080	-0.165	-1.429	-0.566	-2.079
Alpha MO:	311	312	313	314	315	316	317	318	319	320
Energy(eV):	13.32	13.42	13.55	13.59	13.76	13.91	13.94	14.07	14.13	14.22
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	52.14	24.43	23.61	20.83	27.01	18.72	20.09	38.94	30.41	39.70
FRAG# 2:	2.96	1.72	1.73	1.88	6.42	2.98	4.12	1.45	12.30	0.50
FRAG# 3:	41.66	72.02	69.63	70.13	66.05	70.69	69.96	59.01	56.18	57.99
FRAG# 4:	3.24	1.83	5.03	7.15	0.52	7.61	5.83	0.59	1.11	1.81
OP(1 & 2)	-0.146	-0.611	-0.169	-0.207	-2.441	-0.769	-0.071	-0.080	-1.360	-0.442
OP(1 & 3)	-0.096	-0.237	-0.181	-0.058	-0.129	0.028	-0.122	-0.022	-0.281	-0.066
OP(1 & 4)	-0.328	-0.057	-0.115	-0.246	-0.238	-0.236	-0.673	-0.367	-1.350	-0.337
OP(2 & 3)	-0.005	-0.004	-0.001	0.000	-0.008	-0.002	-0.001	-0.001	0.011	0.007
OP(2 & 4)	0.001	0.031	0.005	-0.019	0.114	0.002	0.013	0.005	0.067	-0.008
OP(3 & 4)	-1.832	-1.206	-1.043	-0.522	-0.744	-1.083	-0.527	-1.064	-0.319	-1.681
Alpha MO:	321	322	323	324	325	326	327	328	329	330
Energy(eV):	14.60	14.63	14.79	14.91	15.04	15.09	15.27	15.44	15.56	15.71
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	27.87	34.13	5.71	36.21	38.97	26.79	43.45	22.29	33.49	48.21
FRAG# 2:	1.10	1.36	1.16	5.67	2.89	1.03	1.99	56.35	16.98	8.09
FRAG# 3:	69.03	65.91	93.29	57.46	55.08	70.02	54.07	19.75	47.96	43.27
FRAG# 4:	2.00	-1.40	-0.16	0.65	3.05	2.15	0.48	1.60	1.56	0.43
OP(1 & 2)	-0.256	-0.580	-0.193	-0.946	-0.711	-0.447	-0.053	-1.675	-0.598	-0.327
OP(1 & 3)	0.139	0.220	0.294	-0.003	-0.208	0.528	0.048	-0.130	-0.015	0.144

OP(1 & 4)	-0.471	-0.797	-0.703	-0.211	-1.131	-1.146	-0.277	-0.138	-0.301	-0.852
OP(2 & 3)	0.002	0.011	0.000	-0.007	0.007	-0.001	0.000	-0.003	-0.004	-0.002
OP(2 & 4)	-0.012	-0.061	-0.027	0.064	-0.082	-0.001	0.006	0.007	-0.014	0.024
OP(3 & 4)	-1.934	-2.619	-2.487	-1.530	-1.323	-5.404	-1.308	-0.123	-0.160	-0.676
Alpha MO:	331	332	333	334	335	336	337	338	339	340
Energy(eV):	15.81	15.97	16.15	16.23	16.54	16.64	17.01	17.17	17.31	17.36
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	34.52	14.55	63.19	13.56	20.48	70.41	62.44	39.36	68.80	70.43
FRAG# 2:	5.14	9.03	6.56	4.61	4.81	5.15	2.79	4.94	1.14	1.17
FRAG# 3:	61.69	77.71	31.53	81.12	73.94	23.98	27.47	58.06	30.19	28.33
FRAG# 4:	-1.35	-1.29	-1.28	0.70	0.77	0.46	7.30	-2.36	-0.13	0.08
OP(1 & 2)	-0.722	-0.497	-0.337	-0.263	-0.341	-0.424	-0.380	-0.340	-0.115	-0.146
OP(1 & 3)	-0.018	0.023	-0.083	-0.052	-0.299	-0.018	-0.144	0.418	-0.099	0.314
OP(1 & 4)	-0.638	-0.562	-0.214	-0.024	-0.125	-0.643	-1.225	-1.768	-0.134	-1.432
OP(2 & 3)	0.009	0.005	0.002	0.004	0.004	-0.004	0.003	-0.003	-0.001	0.001
OP(2 & 4)	-0.058	0.036	0.012	0.000	0.003	-0.016	-0.022	0.035	-0.004	-0.016
OP(3 & 4)	-0.395	-1.491	-0.645	-1.509	-0.475	-0.821	-2.096	-2.852	-0.359	-1.834
Alpha MO:	341	342	343	344	345	346	347	348	349	350
Energy(eV):	17.61	17.80	17.89	17.95	18.04	18.20	18.46	18.74	18.84	19.20
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	64.07	40.47	34.38	38.12	62.43	50.77	44.70	28.61	28.30	41.15
FRAG# 2:	1.77	4.41	1.19	2.54	1.29	8.09	0.51	0.65	2.02	4.03
FRAG# 3:	32.88	55.97	61.76	55.63	34.40	30.46	54.94	60.12	56.61	44.97
FRAG# 4:	1.28	-0.85	2.66	3.71	1.88	10.68	-0.15	10.62	13.07	9.84
OP(1 & 2)	-0.441	-0.388	-0.143	-0.238	-0.083	-1.226	-0.349	-0.152	-0.141	-0.467
OP(1 & 3)	-0.144	-0.247	-0.026	0.004	-0.031	0.551	-0.204	0.831	-0.110	0.384
OP(1 & 4)	-0.162	-0.584	-0.753	-0.291	-0.322	-2.318	-0.178	-3.206	-0.347	-1.859
OP(2 & 3)	-0.001	0.001	0.002	0.000	0.003	-0.002	0.000	-0.003	0.002	-0.001
OP(2 & 4)	0.008	0.017	-0.022	0.000	-0.008	-0.040	0.001	0.053	-0.005	0.006
OP(3 & 4)	-0.645	-0.516	-1.443	-0.840	-0.305	-2.647	-0.404	-4.082	-2.926	-3.470
Alpha MO:	351	352	353	354	355	356	357	358	359	360
Energy(eV):	19.26	19.43	19.77	20.05	20.11	20.64	21.17	21.39	22.02	22.33
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	56.95	52.98	33.68	65.15	11.07	60.00	35.39	25.84	57.19	-2.17
FRAG# 2:	8.02	3.06	3.17	4.20	1.28	3.66	12.66	1.71	1.43	81.63
FRAG# 3:	30.65	38.65	61.57	22.13	70.22	42.13	44.00	44.60	26.20	21.42
FRAG# 4:	4.37	5.31	1.59	8.53	17.43	-5.79	7.95	27.84	15.17	-0.87
OP(1 & 2)	-1.198	-0.326	-0.349	-1.275	-0.124	-0.579	-2.510	-0.443	-0.192	-25.8
OP(1 & 3)	-0.700	0.299	-0.166	0.383	0.602	1.956	0.044	0.134	-0.492	0.209
OP(1 & 4)	-0.547	-1.656	-0.201	-3.027	-1.147	-5.414	-1.545	-0.933	-0.784	-3.089
OP(2 & 3)	-0.003	-0.002	0.004	-0.003	-0.009	-0.003	-0.002	-0.005	0.001	-0.018
OP(2 & 4)	0.039	0.018	0.003	0.042	0.011	0.023	0.003	0.008	0.001	0.109
OP(3 & 4)	-2.219	-1.656	-1.585	-1.124	-8.758	-12.5	-4.050	-2.334	-4.218	-1.271
Alpha MO:	361	362	363	364	365	366	367	368	369	370
Energy(eV):	22.55	22.95	23.35	24.25	24.62	24.74	24.87	25.38	25.41	25.57
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	40.81	40.57	37.54	1.83	38.20	49.74	24.00	7.24	48.07	9.11
FRAG# 2:	8.01	21.81	16.68	0.61	0.97	8.26	3.99	0.53	2.01	0.28
FRAG# 3:	40.26	43.13	52.90	52.03	43.33	32.14	47.78	96.20	48.38	101.83
FRAG# 4:	10.92	-5.50	-7.11	45.53	17.50	9.86	24.23	-3.98	1.53	-11.22
OP(1 & 2)	-3.370	-8.766	-6.893	-0.229	-1.412	-3.777	-1.019	-0.293	-0.972	-0.154
OP(1 & 3)	-0.013	2.884	-0.937	-5.488	-5.876	-0.939	1.072	-0.390	-0.298	1.872
OP(1 & 4)	-2.119	-15.1	-0.600	-5.605	-15.8	-3.003	-9.825	-5.661	-14.5	-3.959
OP(2 & 3)	0.006	0.004	0.005	-0.001	-0.004	0.002	0.005	-0.001	-0.001	0.001
OP(2 & 4)	0.026	-0.042	-0.035	-0.015	0.069	-0.030	-0.054	0.019	0.021	0.003
OP(3 & 4)	-9.381	-15.0	-15.4	-31.1	-15.5	-12.8	-11.6	-13.8	-27.7	-13.2
Alpha MO:	371	372	373	374	375	376	377	378	379	380
Energy(eV):	25.86	26.01	26.18	26.32	26.84	27.05	27.10	27.56	27.88	28.01
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	17.42	25.73	6.68	10.53	29.15	7.81	8.06	32.52	20.69	40.77
FRAG# 2:	0.22	0.01	0.02	0.08	0.29	0.07	0.96	4.67	0.03	0.79

FRAG#	3:	82.30	66.09	95.17	87.74	64.27	85.38	86.75	61.21	83.61	59.56
FRAG#	4:	0.06	8.17	-1.87	1.65	6.28	6.74	4.24	1.60	-4.34	-1.12
OP (1 & 2)		-0.053	-0.100	-0.028	-0.034	-0.190	-0.049	-0.165	-0.710	-0.015	-0.233
OP (1 & 3)		-0.059	-0.751	-0.261	0.362	-5.202	1.266	0.750	1.834	0.868	-0.099
OP (1 & 4)		-0.830	-5.315	-2.427	-4.922	-8.729	-6.787	-2.409	-8.409	-2.595	-0.958
OP (2 & 3)		0.002	0.000	-0.001	0.000	0.001	0.001	-0.001	0.000	-0.001	-0.001
OP (2 & 4)		-0.019	0.011	0.013	0.010	-0.009	-0.012	0.004	0.034	0.003	0.008
OP (3 & 4)		-13.2	-5.396	-4.628	-5.184	-17.3	-7.395	-18.4	-14.0	-5.883	-1.465
Alpha MO:		381	382	383	384	385	386	387	388	389	390
Energy(eV):		28.03	28.19	28.30	28.44	28.67	28.78	28.81	28.93	28.99	29.22
Symmetry:		na	na	na	na	na	na	na	na	na	na
FRAG#	1:	66.37	21.99	16.43	28.01	27.77	38.93	26.70	23.70	21.13	41.14
FRAG#	2:	0.10	0.79	1.93	2.81	0.34	0.38	0.28	0.41	0.71	0.19
FRAG#	3:	34.62	79.34	76.15	76.61	69.30	58.68	68.96	72.93	77.25	58.24
FRAG#	4:	-1.09	-2.13	5.48	-7.43	2.58	2.02	4.06	2.96	0.91	0.42
OP (1 & 2)		-0.166	-1.003	-0.682	-1.227	-0.060	-0.118	-0.123	-0.039	-0.163	-0.091
OP (1 & 3)		0.006	0.513	1.611	-0.870	0.324	-0.748	-0.006	-0.008	-0.241	1.086
OP (1 & 4)		-1.546	-2.460	-8.280	0.404	-2.113	-0.508	-0.559	-0.555	-1.343	-4.737
OP (2 & 3)		0.001	-0.003	0.001	0.008	0.001	0.000	0.002	-0.001	0.000	0.000
OP (2 & 4)		-0.024	0.062	0.012	-0.029	-0.007	-0.018	-0.011	0.000	-0.003	0.029
OP (3 & 4)		-0.492	-3.283	-4.066	-4.398	-6.124	-4.664	-3.410	-1.462	-0.570	-6.636
Alpha MO:		391	392	393	394	395	396	397	398	399	400
Energy(eV):		29.49	29.57	29.78	30.22	30.36	30.49	30.52	30.63	30.72	31.39
Symmetry:		na	na	na	na	na	na	na	na	na	na
FRAG#	1:	52.54	44.65	60.93	56.95	26.09	24.74	57.31	19.48	3.04	41.28
FRAG#	2:	2.20	0.28	0.56	0.07	0.49	0.21	0.38	0.09	-0.03	0.33
FRAG#	3:	44.70	52.47	44.58	41.32	58.83	55.42	41.21	76.65	95.95	57.11
FRAG#	4:	0.56	2.60	-6.07	1.66	14.59	19.63	1.10	3.78	1.02	1.28
OP (1 & 2)		-0.734	-0.359	-0.447	-0.028	-0.076	-0.042	-0.225	-0.069	-0.024	-0.076
OP (1 & 3)		-0.095	-1.035	0.291	0.453	-1.215	-0.387	-0.129	-1.715	-0.442	-3.076
OP (1 & 4)		-3.323	-5.437	-6.163	-4.260	-2.030	-2.081	-0.558	-2.462	-0.509	-40.5
OP (2 & 3)		0.000	-0.002	-0.002	0.001	0.000	0.000	0.000	0.004	0.000	-0.001
OP (2 & 4)		-0.010	0.057	0.077	-0.004	-0.002	0.005	-0.010	-0.017	0.005	0.004
OP (3 & 4)		-1.288	-5.339	-7.406	-3.081	-11.8	-6.549	-4.336	-23.9	-14.9	-21.4
Alpha MO:		401	402	403	404	405	406	407	408	409	410
Energy(eV):		31.73	31.92	32.04	32.13	32.27	32.93	33.36	33.53	34.41	34.65
Symmetry:		na	na	na	na	na	na	na	na	na	na
FRAG#	1:	22.89	78.94	47.19	19.20	50.48	89.76	60.77	95.15	30.63	28.40
FRAG#	2:	0.42	0.08	0.54	0.11	0.56	0.40	3.23	0.05	6.11	0.60
FRAG#	3:	75.05	21.35	52.34	82.92	49.43	10.48	37.96	5.37	64.96	70.57
FRAG#	4:	1.64	-0.37	-0.07	-2.25	-0.47	-0.63	-1.98	-0.58	-1.70	0.42
OP (1 & 2)		-0.055	-0.081	-0.094	-0.149	-0.025	-0.158	-0.746	-0.035	-0.331	-0.999
OP (1 & 3)		-3.039	-0.045	0.481	-0.222	2.812	0.257	-0.568	-0.115	-0.668	-0.847
OP (1 & 4)		-20.6	-0.429	-4.130	-0.185	-6.151	-1.918	-11.7	-0.607	-1.863	-0.042
OP (2 & 3)		-0.001	-0.001	-0.004	-0.004	0.000	0.005	-0.008	0.000	0.001	0.007
OP (2 & 4)		0.019	-0.003	0.025	-0.002	0.005	-0.025	0.191	0.002	0.042	0.008
OP (3 & 4)		-22.5	-7.036	-38.1	-2.119	-21.4	-3.305	-4.062	-0.106	-15.3	-3.295
Alpha MO:		411	412	413	414	415	416	417	418	419	420
Energy(eV):		34.77	35.22	35.78	36.08	36.25	36.44	36.58	37.10	37.81	38.69
Symmetry:		na	na	na	na	na	na	na	na	na	na
FRAG#	1:	23.73	40.16	26.26	44.12	10.75	13.43	41.73	11.71	89.81	82.32
FRAG#	2:	2.86	0.22	1.86	0.02	1.54	1.35	0.33	0.15	-4.33	0.55
FRAG#	3:	73.32	60.58	66.16	54.25	86.84	81.58	57.76	85.55	13.86	17.17
FRAG#	4:	0.09	-0.96	5.71	1.61	0.86	3.64	0.18	2.59	0.66	-0.06
OP (1 & 2)		-0.155	-0.130	-0.248	-0.206	-0.222	-0.873	-0.337	-0.077	-5.049	-1.207
OP (1 & 3)		-0.090	0.392	2.376	1.873	-0.488	0.343	-0.210	0.798	0.336	-0.077
OP (1 & 4)		-5.773	-2.279	-5.431	-3.829	-3.297	-13.3	-0.297	-2.804	-1.570	-0.574
OP (2 & 3)		0.004	0.002	0.000	0.001	0.001	-0.006	0.001	0.002	-0.003	-0.002
OP (2 & 4)		0.048	0.025	-0.001	-0.007	0.022	0.199	-0.004	0.005	-0.005	-0.006
OP (3 & 4)		-3.516	-5.667	-67.2	-27.9	-1.918	-26.3	-2.192	-22.0	-2.159	-1.246
Alpha MO:		421	422	423	424	425	426	427	428	429	430
Energy(eV):		39.60	39.89	40.03	40.32	40.40	41.29	42.59	43.17	43.42	43.49

Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	65.84	19.27	5.06	18.83	21.21	63.22	32.13	15.65	38.63	67.01
FRAG# 2:	0.03	0.02	0.01	0.64	0.03	4.54	40.36	12.24	0.62	1.97
FRAG# 3:	34.10	80.78	95.36	80.07	79.41	33.84	36.95	79.16	64.31	32.63
FRAG# 4:	0.03	-0.05	-0.43	0.46	-0.65	-1.60	-9.45	-7.06	-3.56	-1.62
OP (1 & 2)	-1.112	-0.194	-0.017	-0.863	-0.109	-3.437	-17.5	-5.549	-0.328	-1.039
OP (1 & 3)	-0.932	-0.037	0.016	-0.138	0.146	-0.511	-2.063	1.607	0.469	-0.146
OP (1 & 4)	-8.854	-0.668	-0.278	-1.954	-0.652	-2.959	-9.817	-7.679	-1.038	-0.459
OP (2 & 3)	0.000	-0.001	0.000	0.002	0.000	0.001	0.007	0.047	-0.006	-0.002
OP (2 & 4)	0.005	-0.006	0.000	-0.007	-0.003	-0.128	-0.147	-0.200	0.017	0.035
OP (3 & 4)	-4.348	-1.362	-1.602	-0.477	-3.400	-7.838	-9.141	-19.2	-6.750	-3.249

Alpha MO:	431	432	433	434	435	436	437	438	439
Energy (eV):	44.80	46.81	47.39	48.11	48.92	50.08	51.28	52.16	338.04
Symmetry:	na	na	na	na	na	na	na	na	na

FRAG# 1:	89.45	17.50	14.05	43.90	79.49	15.13	30.41	78.45	13.09
FRAG# 2:	2.47	16.51	12.25	18.63	1.07	1.14	-0.02	0.44	0.00
FRAG# 3:	9.50	76.91	95.19	43.56	19.88	91.40	88.47	26.39	19.02
FRAG# 4:	-1.42	-10.93	-21.49	-6.10	-0.44	-7.68	-18.86	-5.27	67.88
OP (1 & 2)	-2.101	-9.670	-7.037	-10.4	-0.616	-0.744	-0.252	-1.648	-0.995
OP (1 & 3)	-0.073	1.101	1.335	-0.126	0.082	-1.279	-5.120	-1.844	3.447
OP (1 & 4)	-2.697	-7.677	-3.540	-1.118	-2.682	-3.859	-25.0	-2.020	-11.8
OP (2 & 3)	-0.002	-0.009	0.010	-0.016	0.000	0.001	-0.001	0.003	-0.009
OP (2 & 4)	-0.097	0.280	0.094	0.300	-0.068	0.078	0.052	-0.009	0.199
OP (3 & 4)	-5.797	-3.645	-24.7	-4.977	-6.801	-21.0	-23.4	-12.8	-13.5

Alpha-spin HOMO-LUMO gap: 2.277 eV (18361.3 cm-1)

The sum of energies of the occupied orbitals:
alpha-spin MOs: -14499.837 eV

--- COMPOSITIONS OF ALPHA-SPIN MOLECULAR ORBITALS ---

Orbital	E (eV)	Fragments			
		1	2	3	4
439	338.04	13.1	0.0	19.0	67.9
438	52.16	78.5	0.4	26.4	-5.3
437	51.28	30.4	0.0	88.5	-18.9
436	50.08	15.1	1.1	91.4	-7.7
435	48.92	79.5	1.1	19.9	-0.4
434	48.11	43.9	18.6	43.6	-6.1
433	47.39	14.1	12.2	95.2	-21.5
432	46.81	17.5	16.5	76.9	-10.9
431	44.80	89.5	2.5	9.5	-1.4
430	43.49	67.0	2.0	32.6	-1.6
429	43.42	38.6	0.6	64.3	-3.6
428	43.17	15.7	12.2	79.2	-7.1
427	42.59	32.1	40.4	37.0	-9.4
426	41.29	63.2	4.5	33.8	-1.6
425	40.40	21.2	0.0	79.4	-0.6
424	40.32	18.8	0.6	80.1	0.5
423	40.03	5.1	0.0	95.4	-0.4
422	39.89	19.3	0.0	80.8	-0.1
421	39.60	65.8	0.0	34.1	0.0
420	38.69	82.3	0.5	17.2	-0.1
419	37.81	89.8	-4.3	13.9	0.7
418	37.10	11.7	0.1	85.5	2.6
417	36.58	41.7	0.3	57.8	0.2
416	36.44	13.4	1.3	81.6	3.6
415	36.25	10.7	1.5	86.8	0.9
414	36.08	44.1	0.0	54.3	1.6
413	35.78	26.3	1.9	66.2	5.7
412	35.22	40.2	0.2	60.6	-1.0
411	34.77	23.7	2.9	73.3	0.1
410	34.65	28.4	0.6	70.6	0.4
409	34.41	30.6	6.1	65.0	-1.7
408	33.53	95.2	0.1	5.4	-0.6
407	33.36	60.8	3.2	38.0	-2.0
406	32.93	89.8	0.4	10.5	-0.6
405	32.27	50.5	0.6	49.4	-0.5

404	32.13	19.2	0.1	82.9	-2.2
403	32.04	47.2	0.5	52.3	-0.1
402	31.92	78.9	0.1	21.3	-0.4
401	31.73	22.9	0.4	75.0	1.6
400	31.39	41.3	0.3	57.1	1.3
399	30.72	3.0	0.0	96.0	1.0
398	30.63	19.5	0.1	76.6	3.8
397	30.52	57.3	0.4	41.2	1.1
396	30.49	24.7	0.2	55.4	19.6
395	30.36	26.1	0.5	58.8	14.6
394	30.22	56.9	0.1	41.3	1.7
393	29.78	60.9	0.6	44.6	-6.1
392	29.57	44.6	0.3	52.5	2.6
391	29.49	52.5	2.2	44.7	0.6
390	29.22	41.1	0.2	58.2	0.4
389	28.99	21.1	0.7	77.3	0.9
388	28.93	23.7	0.4	72.9	3.0
387	28.81	26.7	0.3	69.0	4.1
386	28.78	38.9	0.4	58.7	2.0
385	28.67	27.8	0.3	69.3	2.6
384	28.44	28.0	2.8	76.6	-7.4
383	28.30	16.4	1.9	76.2	5.5
382	28.19	22.0	0.8	79.3	-2.1
381	28.03	66.4	0.1	34.6	-1.1
380	28.01	40.8	0.8	59.6	-1.1
379	27.88	20.7	0.0	83.6	-4.3
378	27.56	32.5	4.7	61.2	1.6
377	27.10	8.1	1.0	86.7	4.2
376	27.05	7.8	0.1	85.4	6.7
375	26.84	29.2	0.3	64.3	6.3
374	26.32	10.5	0.1	87.7	1.6
373	26.18	6.7	0.0	95.2	-1.9
372	26.01	25.7	0.0	66.1	8.2
371	25.86	17.4	0.2	82.3	0.1
370	25.57	9.1	0.3	101.8	-11.2
369	25.41	48.1	2.0	48.4	1.5
368	25.38	7.2	0.5	96.2	-4.0
367	24.87	24.0	4.0	47.8	24.2
366	24.74	49.7	8.3	32.1	9.9
365	24.62	38.2	1.0	43.3	17.5
364	24.25	1.8	0.6	52.0	45.5
363	23.35	37.5	16.7	52.9	-7.1
362	22.95	40.6	21.8	43.1	-5.5
361	22.55	40.8	8.0	40.3	10.9
360	22.33	-2.2	81.6	21.4	-0.9
359	22.02	57.2	1.4	26.2	15.2
358	21.39	25.8	1.7	44.6	27.8
357	21.17	35.4	12.7	44.0	7.9
356	20.64	60.0	3.7	42.1	-5.8
355	20.11	11.1	1.3	70.2	17.4
354	20.05	65.2	4.2	22.1	8.5
353	19.77	33.7	3.2	61.6	1.6
352	19.43	53.0	3.1	38.7	5.3
351	19.26	57.0	8.0	30.7	4.4
350	19.20	41.2	4.0	45.0	9.8
349	18.84	28.3	2.0	56.6	13.1
348	18.74	28.6	0.7	60.1	10.6
347	18.46	44.7	0.5	54.9	-0.1
346	18.20	50.8	8.1	30.5	10.7
345	18.04	62.4	1.3	34.4	1.9
344	17.95	38.1	2.5	55.6	3.7
343	17.89	34.4	1.2	61.8	2.7
342	17.80	40.5	4.4	56.0	-0.8
341	17.61	64.1	1.8	32.9	1.3
340	17.36	70.4	1.2	28.3	0.1
339	17.31	68.8	1.1	30.2	-0.1
338	17.17	39.4	4.9	58.1	-2.4
337	17.01	62.4	2.8	27.5	7.3
336	16.64	70.4	5.1	24.0	0.5
335	16.54	20.5	4.8	73.9	0.8
334	16.23	13.6	4.6	81.1	0.7

333	16.15	63.2	6.6	31.5	-1.3
332	15.97	14.5	9.0	77.7	-1.3
331	15.81	34.5	5.1	61.7	-1.4
330	15.71	48.2	8.1	43.3	0.4
329	15.56	33.5	17.0	48.0	1.6
328	15.44	22.3	56.4	19.8	1.6
327	15.27	43.5	2.0	54.1	0.5
326	15.09	26.8	1.0	70.0	2.2
325	15.04	39.0	2.9	55.1	3.0
324	14.91	36.2	5.7	57.5	0.6
323	14.79	5.7	1.2	93.3	-0.2
322	14.63	34.1	1.4	65.9	-1.4
321	14.60	27.9	1.1	69.0	2.0
320	14.22	39.7	0.5	58.0	1.8
319	14.13	30.4	12.3	56.2	1.1
318	14.07	38.9	1.5	59.0	0.6
317	13.94	20.1	4.1	70.0	5.8
316	13.91	18.7	3.0	70.7	7.6
315	13.76	27.0	6.4	66.1	0.5
314	13.59	20.8	1.9	70.1	7.2
313	13.55	23.6	1.7	69.6	5.0
312	13.42	24.4	1.7	72.0	1.8
311	13.32	52.1	3.0	41.7	3.2
310	13.16	12.8	1.7	83.0	2.5
309	12.84	36.9	3.3	57.0	2.9
308	12.78	55.4	0.3	40.7	3.6
307	12.77	40.8	0.7	46.9	11.5
306	12.68	41.1	1.2	55.4	2.3
305	12.54	49.4	1.8	43.2	5.6
304	12.35	37.3	2.3	57.9	2.4
303	12.27	35.0	0.5	63.1	1.4
302	12.22	54.1	2.2	38.1	5.6
301	12.06	58.9	0.2	33.2	7.7
300	12.03	50.3	3.8	29.7	16.1
299	11.81	40.0	1.2	53.7	5.1
298	11.60	55.9	1.7	30.0	12.4
297	11.56	53.3	2.1	36.5	8.1
296	11.54	22.7	0.8	67.1	9.4
295	11.35	35.3	1.4	58.6	4.8
294	11.25	81.2	-1.3	21.2	-1.2
293	11.00	32.7	0.5	59.3	7.5
292	10.89	60.2	0.7	37.8	1.3
291	10.81	78.6	0.8	16.3	4.4
290	10.66	50.4	0.9	49.1	-0.4
289	10.62	34.4	-0.3	45.9	20.0
288	10.56	42.6	1.6	56.5	-0.7
287	10.48	46.2	0.8	43.5	9.6
286	10.36	41.0	-0.8	53.5	6.4
285	10.21	62.5	0.2	35.5	1.8
284	10.12	53.2	1.4	42.8	2.5
283	10.07	68.0	0.0	28.4	3.6
282	10.01	31.4	-0.2	69.3	-0.5
281	9.94	46.5	0.1	47.5	6.0
280	9.91	59.7	0.2	37.0	3.1
279	9.81	53.2	0.9	44.6	1.3
278	9.75	14.2	-0.9	87.6	-0.9
277	9.62	37.3	0.2	62.2	0.3
276	9.52	53.9	-1.1	46.5	0.7
275	9.41	40.4	0.3	57.9	1.4
274	9.35	60.3	0.6	37.2	2.0
273	9.31	26.7	-0.5	71.8	1.9
272	9.25	19.6	0.7	78.3	1.5
271	9.10	65.2	1.4	32.1	1.3
270	9.03	27.7	-0.1	70.8	1.6
269	8.78	24.0	0.0	73.2	2.9
268	8.76	34.5	0.4	54.6	10.4
267	8.68	28.2	0.8	68.8	2.3
266	8.56	43.3	1.1	54.9	0.6
265	8.47	49.3	-0.3	50.4	0.7
264	8.41	77.1	-0.1	22.4	0.6
263	8.33	25.4	-0.6	73.8	1.5

262	8.30	47.1	-1.2	53.6	0.5
261	8.25	35.8	0.4	63.5	0.3
260	8.20	26.4	-0.2	73.2	0.6
259	8.05	12.9	0.0	83.5	3.6
258	7.99	41.2	0.7	58.8	-0.7
257	7.95	33.0	-0.1	64.0	3.2
256	7.87	27.7	-0.2	71.2	1.3
255	7.84	23.4	-0.4	71.1	5.9
254	7.78	10.6	0.5	85.0	3.9
253	7.74	18.2	-0.1	80.5	1.4
252	7.69	51.2	-1.0	47.0	2.8
251	7.64	5.7	0.0	85.7	8.6
250	7.56	19.4	-0.2	78.2	2.5
249	7.52	27.3	0.6	67.4	4.6
248	7.45	16.5	0.0	81.2	2.4
247	7.35	43.6	-1.0	54.9	2.6
246	7.27	34.1	-0.2	64.2	2.0
245	7.14	55.6	-1.6	39.0	7.1
244	7.04	57.5	-0.2	38.6	4.0
243	6.90	36.9	-1.6	62.0	2.7
242	6.84	33.1	0.1	56.5	10.4
241	6.79	65.4	-0.4	34.2	0.8
240	6.72	58.3	-0.2	40.5	1.4
239	6.69	56.9	-0.5	36.9	6.7
238	6.62	34.0	-1.8	64.0	3.8
237	6.49	31.0	-0.3	56.4	12.8
236	6.41	13.3	-0.7	72.5	14.9
235	6.35	30.8	-2.3	68.1	3.3
234	6.24	39.4	-3.1	60.5	3.2
233	6.17	64.3	-4.9	35.2	5.4
232	5.99	37.3	-2.5	56.2	9.0
231	5.93	48.4	0.2	48.4	3.0
230	5.84	70.0	-10.8	37.4	3.5
229	5.79	31.5	-5.1	69.3	4.3
228	5.73	21.4	-1.5	70.0	10.2
227	5.58	20.3	-0.7	80.7	-0.3
226	5.53	17.0	-0.2	83.4	-0.3
225	5.48	26.8	-1.0	71.9	2.3
224	5.42	21.0	-0.7	75.8	3.8
223	5.37	85.4	-0.7	15.2	0.1
222	5.27	41.5	-1.1	56.5	3.2
221	5.14	44.7	0.0	54.8	0.5
220	5.03	56.0	3.2	23.4	17.3
219	4.90	30.1	-0.6	69.4	1.0
218	4.78	35.1	-1.3	64.4	1.9
217	4.66	37.4	-2.7	45.8	19.6
216	4.47	16.3	-0.2	65.7	18.3
215	4.44	19.9	0.0	69.6	10.5
214	4.29	57.6	-0.9	42.7	0.7
213	4.19	17.7	-0.2	80.6	1.9
212	4.11	8.6	-0.3	86.6	5.1
211	4.08	48.6	0.1	48.2	3.1
210	3.96	32.9	-1.0	63.1	5.1
209	3.90	71.1	0.4	27.5	1.0
208	3.83	10.5	-0.2	87.1	2.6
207	3.75	17.8	-0.2	76.3	6.0
206	3.73	16.7	-0.2	76.1	7.4
205	3.53	70.0	-1.2	28.5	2.7
204	3.44	14.6	-0.5	88.4	-2.5
203	3.40	62.6	-0.9	34.7	3.7
202	3.33	48.9	-1.8	50.0	2.9
201	3.28	19.4	-1.2	78.4	3.4
200	3.18	7.4	0.0	92.4	0.2
199	3.11	46.9	-0.9	59.1	-5.1
198	3.01	31.4	-0.2	64.9	3.9
197	2.99	61.4	-0.2	34.3	4.5
196	2.90	82.3	-0.8	16.1	2.4
195	2.88	86.3	0.0	14.1	-0.4
194	2.71	19.4	-0.7	72.1	9.3
193	2.68	35.8	-1.1	65.4	-0.1
192	2.53	45.1	-0.3	46.4	8.8

191	2.36	89.0	0.0	10.8	0.2
190	2.34	24.8	0.1	57.8	17.4
189	2.30	4.9	-0.3	92.8	2.5
188	2.00	81.4	-0.9	17.1	2.4
187	1.90	52.0	0.0	48.4	-0.5
186	1.76	39.2	-0.2	59.9	1.1
185	1.55	18.2	0.2	82.8	-1.2
184	1.45	1.3	0.0	98.5	0.2
183	1.42	3.9	0.1	94.2	1.9
182	1.31	1.4	0.0	99.5	-0.9
181	1.26	16.1	-0.1	83.3	0.8
180	1.14	21.7	0.7	76.3	1.3
179	1.05	58.4	3.1	37.7	0.8
178	1.03	35.4	-0.4	66.2	-1.2
177	0.94	4.7	0.0	94.6	0.7
176	0.84	15.0	0.1	83.4	1.4
175	0.80	7.5	0.2	92.9	-0.7
174	0.72	7.5	-0.1	91.5	1.1
173	0.65	18.5	-0.4	80.3	1.6
172	0.57	8.3	0.1	89.8	1.8
171	0.32	2.0	0.0	94.6	3.3
170	0.12	12.1	0.1	84.3	3.5
169	0.09	86.4	1.2	12.2	0.2
168	-0.34	0.4	0.0	98.8	0.8
167	-0.47	-9.5	-0.3	-1.7	111.5
166	-0.56	0.5	0.0	98.5	1.0
165	-1.13	87.1	10.4	1.0	1.5
164	-1.60	12.9	-0.1	-3.2	90.3
163	-1.64	76.3	0.5	-1.1	24.2
162	-1.66	0.2	0.1	-9.0	108.6
161	-1.82	2.3	0.3	-7.9	105.3
160	-2.20	13.4	0.0	19.0	67.6
159	-2.43	9.6	0.0	24.1	66.3
158	-2.47	96.8	0.1	0.7	2.3
157	-2.75	0.4	0.0	99.3	0.4
156	-2.99	0.5	0.0	98.9	0.6
155	-3.84	89.9	1.8	7.6	0.6
154	-4.06	3.7	0.1	94.0	2.2
153	-4.21	1.6	0.0	95.5	2.9
152	-4.26	0.3	0.0	97.8	1.9
151	-4.51	11.3	2.4	83.3	2.9
150	-4.66	61.5	19.9	15.0	3.5
149	-5.10	0.9	0.1	93.8	5.1
148	-5.33	1.1	0.2	94.4	4.3
----- E(gap)= 2.277 eV					
147	-7.60	86.6	0.1	1.5	11.8
146	-8.31	98.5	0.0	0.2	1.3
145	-8.45	15.4	0.2	12.3	72.1
144	-8.55	20.9	0.5	13.3	65.3
143	-8.64	10.6	1.4	15.5	72.4
142	-9.15	98.5	0.0	0.6	0.9
141	-9.17	93.7	0.4	1.3	4.6
140	-9.57	36.8	59.6	1.5	2.1
139	-9.98	6.8	0.0	92.8	0.4
138	-10.10	80.9	6.0	9.4	3.6
137	-10.18	59.6	1.3	32.5	6.5
136	-10.20	21.2	0.1	75.5	3.2
135	-10.84	99.9	0.0	0.0	0.1
134	-10.91	97.6	0.0	2.2	0.2
133	-11.08	99.1	0.0	0.7	0.2
132	-11.30	2.4	0.0	96.6	1.0
131	-11.42	13.6	0.1	84.9	1.4
130	-11.49	12.5	5.4	81.1	1.1
129	-11.53	26.0	0.2	73.3	0.6
128	-11.67	49.0	0.9	48.0	2.1
127	-11.70	13.0	0.1	86.6	0.3
126	-11.72	3.9	0.4	93.2	2.5
125	-11.86	5.9	0.5	88.9	4.8
124	-12.00	22.4	3.3	75.5	-1.2
123	-12.10	37.8	0.8	62.9	-1.5
122	-12.15	49.2	30.1	16.5	4.2

121	-12.86	2.9	1.3	86.8	9.0
120	-12.91	98.7	0.0	1.1	0.2
119	-12.94	74.9	0.2	19.7	5.3
118	-13.18	51.9	5.4	33.2	9.5
117	-13.23	81.0	1.6	14.2	3.2
116	-13.45	0.5	0.1	99.1	0.4
115	-13.56	3.9	0.1	95.6	0.4
114	-13.67	74.1	6.3	19.1	0.4
113	-13.73	40.3	0.2	57.5	2.1
112	-13.74	45.1	2.6	51.1	1.2
111	-13.90	29.1	0.5	67.4	3.0
110	-13.98	55.7	3.2	41.1	0.1
109	-14.13	16.7	2.3	80.4	0.6
108	-14.21	94.5	1.4	3.8	0.2
107	-14.37	11.3	0.1	87.0	1.6
106	-14.55	14.4	1.7	83.3	0.6
105	-14.81	4.6	0.5	88.9	6.0
104	-14.88	33.6	1.4	63.4	1.6
103	-15.00	29.7	1.4	65.0	4.0
102	-15.06	67.3	0.4	29.8	2.5
101	-15.20	21.5	0.1	74.4	4.0
100	-15.23	14.8	0.5	84.0	0.7
99	-15.30	6.9	0.1	91.7	1.2
98	-15.50	18.1	0.4	80.1	1.3
97	-15.56	7.3	0.1	91.7	0.8
96	-15.68	70.4	0.9	27.9	0.8
95	-15.77	11.6	0.2	87.0	1.1
94	-15.87	3.9	0.1	95.0	1.0
93	-16.22	89.8	1.5	7.6	1.1
92	-16.23	3.5	0.1	95.9	0.5
91	-16.38	0.1	0.0	99.3	0.6
90	-16.57	0.6	0.0	99.3	0.1
89	-16.72	23.3	1.9	74.6	0.1
88	-16.74	68.5	5.8	25.3	0.4
87	-16.97	89.9	3.0	4.9	2.2
86	-17.19	0.3	0.0	97.9	1.8
85	-17.20	1.9	0.0	97.5	0.6
84	-17.32	0.2	0.0	98.6	1.1
83	-17.35	0.4	0.0	98.5	1.1
82	-17.51	93.0	5.6	0.4	1.0
81	-17.80	97.4	1.5	0.7	0.5
80	-18.28	1.3	0.0	98.1	0.6
79	-18.51	2.4	0.1	95.1	2.4
78	-18.64	94.7	2.6	1.4	1.2
77	-18.99	96.7	1.5	0.9	0.9
76	-20.00	0.0	0.0	98.2	1.8
75	-20.15	0.0	0.0	98.3	1.6
74	-20.34	0.2	0.0	99.6	0.2
73	-20.48	0.2	0.0	99.7	0.1
72	-20.92	91.4	7.8	0.3	0.5
71	-21.17	74.7	6.7	17.9	0.7
70	-21.20	15.3	1.3	82.6	0.7
69	-21.35	0.8	0.1	98.3	0.8
68	-21.49	0.2	0.0	98.5	1.3
67	-21.64	0.1	0.0	98.8	1.1
66	-21.77	99.9	0.1	0.0	0.0
65	-22.03	98.3	1.0	0.1	0.6
64	-23.63	97.3	2.4	0.2	0.2
63	-23.82	0.0	0.0	100.1	-0.1
62	-23.98	0.2	0.0	100.0	-0.2
61	-24.65	99.4	0.6	0.0	0.0
60	-25.21	98.2	0.6	0.9	0.3
59	-25.30	0.4	0.0	99.1	0.5
58	-25.31	0.0	0.0	100.0	0.0
57	-25.45	0.0	0.0	99.5	0.4
56	-25.48	0.2	0.0	99.6	0.2
55	-25.51	0.2	0.0	98.8	1.0
54	-25.70	0.3	0.0	98.6	1.1
53	-26.18	98.3	0.1	0.5	1.2
52	-27.93	56.7	42.1	0.2	1.0
51	-29.30	0.0	0.0	99.1	0.9

50	-29.45	0.1	0.0	99.2	0.8
49	-29.92	73.8	15.6	11.3	-0.7
48	-29.97	7.4	1.4	91.5	-0.3
47	-30.16	2.6	0.2	98.1	-0.9
46	-30.98	99.3	0.2	0.5	0.0
45	-50.58	-0.1	0.0	-0.1	100.2
44	-50.85	-0.3	0.0	-0.1	100.4
43	-50.90	0.0	0.0	-0.4	100.4
42	-81.31	0.2	0.0	0.4	99.4
41	-278.84	100.0	0.0	0.0	0.0
40	-278.88	100.0	0.0	0.0	0.0
39	-278.91	100.0	0.0	0.0	0.0
38	-278.92	100.0	0.0	0.0	0.0
37	-278.93	100.0	0.0	0.0	0.0
36	-279.34	100.0	0.0	0.0	0.0
35	-280.68	100.0	0.0	0.0	0.0
34	-281.02	0.0	0.0	100.0	0.0
33	-281.05	100.0	0.0	0.0	0.0
32	-281.07	0.0	0.0	100.0	0.0
31	-281.12	0.0	0.0	100.0	0.0
30	-281.13	0.0	0.0	100.0	0.0
29	-281.18	0.0	0.0	100.0	0.0
28	-281.18	0.0	0.0	100.0	0.0
27	-281.22	0.0	0.0	100.0	0.0
26	-281.29	0.0	0.0	100.0	0.0
25	-281.32	0.0	0.0	100.0	0.0
24	-281.32	100.0	0.0	0.0	0.0
23	-281.33	0.0	0.0	100.0	0.0
22	-281.34	100.0	0.0	0.0	0.0
21	-281.40	0.0	0.0	100.0	0.0
20	-281.44	0.0	0.0	100.0	0.0
19	-281.74	100.0	0.0	0.0	0.0
18	-281.82	0.0	0.0	100.0	0.0
17	-281.85	0.0	0.0	100.0	0.0
16	-281.86	0.0	0.0	100.0	0.0
15	-281.96	100.0	0.0	0.0	0.0
14	-282.06	0.0	0.0	100.0	0.0
13	-282.26	0.0	0.0	100.0	0.0
12	-282.30	0.0	0.0	100.0	0.0
11	-282.44	0.0	0.0	100.0	0.0
10	-282.50	0.0	0.0	100.0	0.0
9	-391.85	100.0	0.0	0.0	0.0
8	-392.62	100.0	0.0	0.0	0.0
7	-393.23	0.1	99.9	0.0	0.0
6	-393.39	100.0	0.0	0.0	0.0
5	-394.34	100.0	0.0	0.0	0.0
4	-394.42	0.0	0.0	100.0	0.0
3	-394.45	0.0	0.0	100.0	0.0
2	-394.53	0.0	0.0	100.0	0.0
1	-394.61	0.0	0.0	100.0	0.0

----- Density-of-States Calculations -----
Using Gaussian functions with the half-widths 0.50 eV
The data window: from -17.0 to 4.7 eV

----- Density-of-States Calculations -----
Using Gaussian functions with the half-widths 0.50 eV
The data window: from -17.0 to 4.7 eV

DFT data for hydrogentriazole complex – non phenyl analogue of 1a

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Use of the AOMix program should be acknowledged in publications as:

1. S.I.Gorelsky, AOMix program, <http://www.sg-chem.net/>
2. S.I.Gorelsky, A.B.P.Lever, J.Organomet.Chem. 635, 187-196 (2001)

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Calculations from Gaussian

```
%chk=CorrectHydrogenOpt.chk
```

Molecule: C₂₆H₂₀N₉Ru (1+)

```
Details: # rb31vp/lanl2dz SCF=Tight Pop=Full IOp(3/33=1) Geom=Check Guess=Read
```

Source file: CorrectHydrogenAOMix.log

Population analysis: MPA

```
377 orbitals( 377 canonical) 127 alpha + 127 beta electrons
```

Number of fragments: 4

Fragment 1 (14 atoms, 98 orbitals): Hydrogen Triazole

Fragment 2 (1 atoms, 9 orbitals): Pyrazine Nitrogen

Fragment 3 (40 atoms, 248 orbitals): Bipv

Fragment 4 (1 atoms, 22 orbitals): Ru Atom

COMPOSITIONS OF MOLECULAR ORBITALS (GROSS CONTRIBUTIONS, %)

AND OVERLAP POPULATIONS (OP) BETWEEN FRAGMENTS

[illegible][illegible][illegible][illegible][illegible][illegible]

OP(3 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Alpha MO:	31	32	33	34	35	36	37	38	39	40
Energy(eV):	-281.14	-281.10	-281.10	-281.03	-280.49	-81.34	-50.93	-50.88	-50.61	-31.03
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	0.00	99.97	0.00	0.00	100.00	0.14	0.01	-0.26	-0.10	99.93
FRAG# 2:	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.22
FRAG# 3:	100.00	0.00	100.00	100.00	0.00	0.40	-0.42	-0.12	-0.06	0.47
FRAG# 4:	0.00	0.03	0.00	0.00	0.00	99.46	100.41	100.38	100.15	-0.62
OP(1 & 2)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002
OP(1 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.004
OP(1 & 4)	0.000	0.000	0.000	0.000	0.000	0.002	0.000	-0.006	-0.002	-0.016
OP(2 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(3 & 4)	0.000	0.000	0.000	0.000	0.000	0.007	-0.009	-0.003	-0.002	-0.003
Alpha MO:	41	42	43	44	45	46	47	48	49	50
Energy(eV):	-30.19	-30.01	-29.98	-29.48	-29.32	-27.99	-26.20	-25.73	-25.54	-25.50
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	3.32	37.06	43.51	0.05	0.02	56.71	98.28	0.30	0.17	0.11
FRAG# 2:	0.35	7.54	9.30	0.00	0.00	42.17	0.10	0.00	0.00	0.00
FRAG# 3:	97.28	55.42	48.25	99.14	99.10	0.18	0.47	98.58	98.84	99.67
FRAG# 4:	-0.95	-0.02	-1.06	0.80	0.88	0.95	1.16	1.12	0.98	0.22
OP(1 & 2)	0.003	0.055	0.068	0.000	0.000	0.207	0.001	0.000	0.000	0.000
OP(1 & 3)	0.004	0.004	0.001	0.001	0.000	0.002	0.001	0.000	0.000	0.000
OP(1 & 4)	-0.003	0.001	-0.015	0.000	0.000	0.015	0.015	0.000	-0.001	0.000
OP(2 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)	0.000	0.000	-0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(3 & 4)	-0.024	-0.010	-0.014	0.011	0.013	0.000	0.000	0.012	0.012	0.001
Alpha MO:	51	52	53	54	55	56	57	58	59	60
HOMO-76	HOMO-75	HOMO-74	HOMO-73	HOMO-72	HOMO-71	HOMO-70	HOMO-69	HOMO-68	HOMO-67	
Energy(eV):	-25.48	-25.33	-25.31	-25.07	-24.01	-23.84	-23.62	-21.67	-21.51	-21.38
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	0.02	0.01	0.04	98.07	0.18	0.01	96.74	0.01	0.22	1.67
FRAG# 2:	0.00	0.00	0.00	1.16	0.00	0.00	2.71	0.00	0.03	0.14
FRAG# 3:	99.54	100.01	99.45	0.33	99.97	100.13	0.20	98.90	98.48	97.36
FRAG# 4:	0.44	-0.03	0.51	0.45	-0.16	-0.15	0.35	1.09	1.26	0.83
OP(1 & 2)	0.000	0.000	0.000	0.011	0.000	0.000	0.023	0.000	0.000	0.000
OP(1 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(1 & 4)	0.000	0.000	0.000	0.005	0.000	0.000	0.002	-0.002	-0.002	0.000
OP(2 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(3 & 4)	0.006	-0.002	0.007	0.000	-0.004	-0.003	-0.001	0.014	0.015	0.009
Alpha MO:	61	62	63	64	65	66	67	68	69	70
HOMO-66	HOMO-65	HOMO-64	HOMO-63	HOMO-62	HOMO-61	HOMO-60	HOMO-59	HOMO-58	HOMO-57	
Energy(eV):	-21.25	-21.21	-21.06	-20.51	-20.36	-20.18	-20.01	-18.75	-18.54	-18.41
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	80.97	8.47	90.32	0.10	0.15	0.04	-0.01	91.36	7.14	83.36
FRAG# 2:	7.09	0.76	8.68	0.00	0.00	0.01	0.00	3.01	0.30	2.91
FRAG# 3:	11.40	90.05	0.25	99.76	99.59	98.34	98.26	3.99	90.30	11.67
FRAG# 4:	0.54	0.72	0.76	0.14	0.25	1.61	1.75	1.64	2.26	2.06
OP(1 & 2)	-0.010	-0.001	0.048	0.000	0.000	0.000	0.000	0.011	-0.001	-0.008
OP(1 & 3)	0.000	-0.003	-0.001	0.000	0.000	0.000	0.000	0.001	-0.001	-0.002
OP(1 & 4)	0.002	-0.002	0.010	0.000	0.000	-0.001	-0.001	0.020	0.000	0.015
OP(2 & 3)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(3 & 4)	-0.003	0.007	-0.002	0.001	0.003	0.018	0.019	-0.001	0.025	0.004
Alpha MO:	71	72	73	74	75	76	77	78	79	80
HOMO-56	HOMO-55	HOMO-54	HOMO-53	HOMO-52	HOMO-51	HOMO-50	HOMO-49	HOMO-48	HOMO-47	
Energy(eV):	-18.30	-17.38	-17.35	-17.23	-17.21	-17.05	-17.02	-16.75	-16.59	-16.41
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	9.38	0.44	0.26	3.34	0.56	87.71	85.86	0.43	0.53	0.22
FRAG# 2:	0.34	0.04	0.01	0.12	0.02	3.85	11.35	0.02	0.02	0.01

OP(3 & 4)		-0.021	-0.059	0.008	-0.001	0.005	0.007	-0.001	-0.001	-0.034	-0.029
Alpha MO:		121	122	123	124	125	126	127	128	129	130
Energy (eV):		HOMO-6	HOMO-5	HOMO-4	HOMO-3	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2
Symmetry:		na	na	na	na	na	na	na	na	na	na
=====											
FRAG#	1:	16.66	36.56	98.52	74.84	14.79	6.59	33.06	1.09	1.01	63.60
FRAG#	2:	0.11	59.87	0.02	0.55	1.51	0.53	0.03	0.21	0.18	20.74
FRAG#	3:	81.71	1.46	0.61	4.36	14.20	17.37	7.55	94.39	93.80	11.85
FRAG#	4:	1.52	2.11	0.86	20.25	69.50	75.51	59.36	4.31	5.01	3.81
OP(1 & 2)		0.000	-0.036	-0.002	-0.001	-0.003	-0.001	0.000	-0.002	-0.002	-0.266
OP(1 & 3)		-0.006	0.001	-0.006	0.001	0.005	0.001	0.005	-0.004	-0.005	-0.007
OP(1 & 4)		0.009	0.003	0.009	0.009	-0.042	-0.034	-0.085	-0.002	-0.005	-0.027
OP(2 & 3)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)		0.000	-0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.001
OP(3 & 4)		-0.006	-0.014	-0.007	-0.026	-0.071	-0.083	-0.048	-0.037	-0.045	-0.005
=====											
Alpha MO:		131	132	133	134	135	136	137	138	139	140
Energy (eV):		LUMO+3	LUMO+4	LUMO+5	LUMO+6	LUMO+7	LUMO+8	LUMO+9	LUMO+10	LUMO+11	LUMO+12
Symmetry:		na	na	na	na	na	na	na	na	na	na
=====											
FRAG#	1:	9.05	0.21	1.84	4.53	88.85	0.22	0.34	9.05	13.57	0.20
FRAG#	2:	1.75	0.01	0.00	0.09	1.69	0.03	0.01	0.02	0.02	0.40
FRAG#	3:	86.44	97.90	95.39	93.16	8.90	99.13	99.27	24.24	19.76	-8.06
FRAG#	4:	2.76	1.88	2.77	2.22	0.56	0.62	0.39	66.69	66.66	107.46
OP(1 & 2)		-0.025	0.000	0.000	-0.001	-0.027	-0.001	0.000	-0.013	-0.001	-0.013
OP(1 & 3)		0.006	0.000	0.001	0.001	-0.010	0.002	-0.002	-0.215	-0.245	0.144
OP(1 & 4)		-0.009	-0.002	-0.002	-0.002	0.002	-0.002	0.000	-0.570	-0.530	-0.578
OP(2 & 3)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)		0.000	0.000	0.000	0.000	-0.001	0.000	0.000	0.002	-0.004	0.007
OP(3 & 4)		-0.019	-0.019	-0.026	-0.023	-0.006	-0.015	-0.010	-1.296	-1.386	-2.845
=====											
Alpha MO:		141	142	143	144	145	146	147	148	149	150
Energy (eV):		LUMO+13	LUMO+14	LUMO+15	LUMO+16	LUMO+17	LUMO+18	LUMO+19	LUMO+20	LUMO+21	LUMO+22
Symmetry:		na	na	na	na	na	na	na	na	na	na
=====											
FRAG#	1:	-2.23	-2.37	87.85	91.07	1.24	-9.67	0.42	1.18	2.10	7.93
FRAG#	2:	0.01	0.14	4.54	7.10	0.02	-0.33	0.00	-0.01	0.01	0.12
FRAG#	3:	-7.98	-5.27	1.18	1.76	97.58	-0.86	98.59	95.35	94.78	90.30
FRAG#	4:	110.20	107.50	6.44	0.06	1.16	110.87	1.00	3.49	3.11	1.65
OP(1 & 2)		0.002	-0.003	-0.151	-0.336	-0.005	-0.064	-0.001	-0.003	-0.010	-0.011
OP(1 & 3)		0.067	0.327	-0.005	0.008	0.011	1.241	0.003	0.142	0.182	0.039
OP(1 & 4)		-0.771	-1.866	-0.035	-0.006	-0.059	-4.294	-0.011	-0.362	-0.413	-0.178
OP(2 & 3)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP(2 & 4)		-0.017	-0.027	-0.008	-0.003	-0.002	-0.044	0.000	0.000	0.002	0.001
OP(3 & 4)		-2.754	-2.905	-0.137	-0.008	-0.083	-10.7	-0.102	-0.997	-1.592	-0.534
=====											
Alpha MO:		151	152	153	154	155	156	157	158	159	160
Energy (eV):		LUMO+23	LUMO+24	LUMO+25	LUMO+26	LUMO+27	LUMO+28	LUMO+29	LUMO+30	LUMO+31	LUMO+32
Symmetry:		na	na	na	na	na	na	na	na	na	na
=====											
FRAG#	1:	17.59	7.77	7.10	22.57	5.79	66.84	28.12	13.63	13.72	1.01
FRAG#	2:	-0.36	-0.07	0.35	0.21	0.02	4.01	-0.75	0.35	-0.07	-0.04
FRAG#	3:	80.83	91.12	93.48	75.08	93.59	28.59	73.53	84.80	85.10	99.98
FRAG#	4:	1.95	1.17	-0.93	2.14	0.61	0.56	-0.90	1.22	1.25	-0.94
OP(1 & 2)		-0.230	-0.108	-0.062	-0.243	-0.048	-0.340	-0.501	-0.147	-0.490	-0.023
OP(1 & 3)		0.016	0.087	-0.035	-0.006	0.002	0.030	-0.070	0.049	-0.051	-0.003
OP(1 & 4)		-0.084	-0.180	-0.010	-0.660	-0.128	-0.056	-0.287	-0.092	-0.136	-0.002
OP(2 & 3)		-0.001	-0.001	0.000	-0.001	0.000	0.001	-0.001	-0.002	-0.003	0.000
OP(2 & 4)		0.008	0.010	0.005	0.029	-0.004	0.005	-0.001	0.018	0.056	-0.002
OP(3 & 4)		-0.252	-0.988	-0.836	-0.207	-0.075	-0.134	-0.346	-0.323	-0.324	-0.586
=====											
Alpha MO:		161	162	163	164	165	166	167	168	169	170
Energy (eV):		LUMO+33	LUMO+34	LUMO+35	LUMO+36	LUMO+37	LUMO+38	LUMO+39	LUMO+40	LUMO+41	LUMO+42
Symmetry:		na	na	na	na	na	na	na	na	na	na

FRAG#	1:	2.66	1.85	11.26	40.44	75.81	51.07	7.16	31.05	46.33	40.46
FRAG#	2:	0.07	0.01	0.10	-0.08	-1.11	0.11	-0.45	0.53	0.40	-0.83
FRAG#	3:	94.91	97.63	88.89	58.42	23.57	47.71	89.27	54.66	42.37	58.20
FRAG#	4:	2.35	0.51	-0.25	1.23	1.73	1.12	4.03	13.76	10.89	2.17
OP (1 & 2)		-0.006	-0.002	-0.039	-1.568	-0.389	-0.326	-0.279	-0.016	-0.109	-0.142
OP (1 & 3)		-0.078	0.007	-0.009	0.083	0.061	-0.011	0.010	0.089	0.019	0.047
OP (1 & 4)		-0.132	-0.027	-0.234	-0.076	-0.731	-0.447	-0.033	-0.800	-0.266	-0.112
OP (2 & 3)		0.000	0.000	0.000	0.006	-0.002	0.001	0.000	0.000	0.000	0.000
OP (2 & 4)		0.001	0.000	0.002	-0.019	0.010	-0.010	-0.018	-0.009	-0.014	0.016
OP (3 & 4)		-0.020	-0.082	-1.387	-0.295	-0.239	-0.465	-0.347	-0.479	-0.324	-0.416

Alpha MO:	171	172	173	174	175	176	177	178	179	180
	LUMO+43	LUMO+44	LUMO+45	LUMO+46	LUMO+47	LUMO+48	LUMO+49	LUMO+50	LUMO+51	LUMO+52
Energy (eV) :	2.68	2.83	2.93	3.00	3.10	3.15	3.26	3.33	3.42	3.45
Symmetry:	na	na	na	na	na	na	na	na	na	na

FRAG#	1:	14.35	67.14	74.86	16.72	27.65	3.59	15.89	56.25	12.86	37.53
FRAG#	2:	-1.46	-1.11	-1.78	-0.27	-0.77	0.02	-0.82	-1.15	-0.43	-1.40
FRAG#	3:	81.64	29.22	17.25	82.28	78.22	95.92	82.57	41.26	89.65	64.97
FRAG#	4:	5.47	4.75	9.66	1.27	-5.09	0.47	2.36	3.64	-2.08	-1.10
OP (1 & 2)		-0.676	-0.325	-0.988	-0.090	-0.349	-0.032	-0.322	-0.942	-0.238	-0.616
OP (1 & 3)		0.227	0.023	0.068	0.484	0.602	0.035	0.042	0.115	0.083	0.056
OP (1 & 4)		-0.919	-0.290	-0.486	-1.739	-1.184	-0.115	-0.041	-0.323	-0.303	-0.121
OP (2 & 3)		0.002	0.000	-0.001	0.001	0.002	0.000	-0.001	-0.001	0.000	0.000
OP (2 & 4)		-0.035	0.042	0.017	-0.016	-0.024	0.003	-0.025	0.031	0.003	-0.063
OP (3 & 4)		-1.137	-0.207	-0.286	-2.163	-3.414	-0.359	-0.258	-1.034	-0.874	-0.233

Alpha MO:	181	182	183	184	185	186	187	188	189	190
	LUMO+53	LUMO+54	LUMO+55	LUMO+56	LUMO+57	LUMO+58	LUMO+59	LUMO+60	LUMO+61	LUMO+62
Energy (eV) :	3.74	3.76	3.84	3.93	4.07	4.10	4.19	4.41	4.48	4.66
Symmetry:	na	na	na	na	na	na	na	na	na	na

FRAG#	1:	10.59	9.29	15.73	24.94	23.66	9.20	9.20	26.07	13.34	44.04
FRAG#	2:	-0.23	0.03	0.19	-0.22	-1.08	-0.17	-0.13	0.21	-0.21	-4.67
FRAG#	3:	84.04	80.29	83.60	69.67	74.00	87.05	89.05	68.98	61.66	42.78
FRAG#	4:	5.60	10.38	0.48	5.61	3.42	3.92	1.88	4.73	25.22	17.84
OP (1 & 2)		-0.180	-0.179	-0.161	-0.731	-0.206	-0.088	-0.072	-0.189	-0.117	-0.675
OP (1 & 3)		-0.003	0.079	-0.062	-0.014	-0.021	-0.024	0.048	-0.012	-0.604	0.073
OP (1 & 4)		-0.113	-0.342	-0.099	-0.103	-0.139	-0.364	-0.402	-0.570	-1.234	-0.451
OP (2 & 3)		0.001	0.000	0.000	-0.001	0.000	0.000	0.000	-0.001	-0.001	0.000
OP (2 & 4)		-0.014	0.000	-0.002	-0.012	-0.015	-0.002	0.003	0.004	0.028	-0.030
OP (3 & 4)		-0.196	-0.746	-0.021	-0.666	-0.251	-0.294	-0.080	-0.269	-2.279	-2.190

Alpha MO:	191	192	193	194	195	196	197	198	199	200
	LUMO+63	LUMO+64	LUMO+65	LUMO+66	LUMO+67	LUMO+68	LUMO+69	LUMO+70	LUMO+71	LUMO+72
Energy (eV) :	4.76	4.85	4.98	5.14	5.21	5.39	5.53	5.54	5.59	5.70
Symmetry:	na	na	na	na	na	na	na	na	na	na

FRAG#	1:	31.48	36.02	29.91	58.88	9.95	15.86	6.87	17.51	16.50	19.37
FRAG#	2:	-0.69	0.31	-1.65	-2.94	-0.35	-0.14	0.05	-1.28	-0.80	-1.30
FRAG#	3:	59.86	60.68	71.61	27.54	83.95	80.07	93.41	84.52	76.37	71.84
FRAG#	4:	9.35	3.00	0.13	16.52	6.45	4.21	-0.33	-0.74	7.93	10.09
OP (1 & 2)		-0.099	-0.127	-0.498	-0.632	-0.131	-0.062	-0.053	-0.182	-0.395	-0.109
OP (1 & 3)		0.015	-0.057	0.059	0.331	-0.052	0.073	0.034	0.082	0.088	-0.013
OP (1 & 4)		-0.695	-0.128	-0.506	-1.312	-0.441	-0.411	-0.122	-0.474	-0.843	-0.240
OP (2 & 3)		-0.001	-0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OP (2 & 4)		0.004	0.002	0.022	0.026	-0.007	-0.005	-0.001	0.007	0.006	0.008
OP (3 & 4)		-0.964	-0.870	-0.139	-1.956	-0.751	-0.418	-0.514	-0.160	-0.837	-1.944

Alpha MO:	201	202	203	204	205	206	207	208	209	210
	LUMO+73	LUMO+74	LUMO+75	LUMO+76	LUMO+77	LUMO+78	LUMO+79	LUMO+80	LUMO+81	LUMO+82
Energy (eV) :	5.78	5.86	5.96	6.20	6.23	6.39	6.39	6.48	6.65	6.77
Symmetry:	na	na	na	na	na	na	na	na	na	na

FRAG#	1:	17.78	54.48	41.33	21.75	52.17	21.31	18.90	29.57	28.94	16.48
FRAG#	2:	-0.47	-3.69	-5.25	-0.89	-6.78	-1.88	-3.44	-5.24	-0.52	-2.09
FRAG#	3:	78.14	44.18	62.49	75.20	48.86	74.81	67.45	72.65	64.23	71.44
FRAG#	4:	4.55	5.03	1.44	3.94	5.75	5.76	17.09	3.02	7.35	14.17
OP (1 & 2)		-0.056	-0.430	-0.622	-0.044	-1.164	-0.154	-0.558	-0.547	-0.097	-0.294
OP (1 & 3)		-0.028	0.123	0.050	-0.029	-0.161	-0.025	0.124	-0.013	0.024	0.079
OP (1 & 4)		-0.093	-0.443	-0.158	-0.112	-0.771	-0.495	-0.200	-0.091	-0.200	-0.733

OP(2 & 3)	0.000	0.000	0.001	0.001	0.000	0.001	0.000	-0.003	0.000	-0.001
OP(2 & 4)	0.002	-0.022	-0.009	-0.002	0.000	0.005	0.000	-0.003	0.002	0.004
OP(3 & 4)	-0.770	-1.187	-0.547	-0.518	-1.206	-0.887	-2.934	-0.202	-1.053	-1.727
Alpha MO:	211	212	213	214	215	216	217	218	219	220
Energy(eV):	6.85	6.93	7.17	7.19	7.36	7.39	7.49	7.56	7.59	7.65
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	17.42	35.40	31.49	51.24	23.28	41.15	18.84	21.43	17.69	20.46
FRAG# 2:	-0.21	0.17	0.17	0.04	-0.32	-1.64	-0.10	-0.04	-0.17	-0.22
FRAG# 3:	79.99	59.67	66.03	42.88	76.20	58.42	78.58	72.44	81.17	75.50
FRAG# 4:	2.80	4.77	2.31	5.84	0.84	2.08	2.68	6.17	1.30	4.27
OP(1 & 2)	-0.130	-0.106	-0.049	-0.209	-0.198	-0.233	-0.062	-0.194	-0.027	-0.072
OP(1 & 3)	-0.029	0.001	0.176	0.247	-0.081	-0.034	0.042	-0.425	0.036	0.051
OP(1 & 4)	-0.143	-0.205	-0.444	-1.248	-0.207	-0.062	-0.096	-1.340	-0.061	-0.739
OP(2 & 3)	0.000	-0.001	0.000	0.000	0.002	0.001	0.000	0.001	-0.001	-0.001
OP(2 & 4)	0.003	0.008	0.002	0.005	-0.011	-0.006	0.005	-0.004	0.002	0.008
OP(3 & 4)	-0.716	-0.413	-1.036	-1.257	-0.867	-0.119	-0.264	-0.989	-0.415	-1.392
Alpha MO:	221	222	223	224	225	226	227	228	229	230
Energy(eV):	7.70	7.80	7.82	7.87	7.97	8.00	8.09	8.21	8.31	8.32
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	15.33	24.60	22.15	12.35	19.74	14.62	39.10	11.79	9.46	36.73
FRAG# 2:	-0.01	-0.84	-0.06	-0.51	-1.13	0.17	0.50	-0.01	0.13	-1.15
FRAG# 3:	82.41	71.65	77.59	81.57	77.74	81.52	58.35	84.24	87.89	63.79
FRAG# 4:	2.28	4.59	0.32	6.59	3.65	3.69	2.06	3.98	2.52	0.63
OP(1 & 2)	-0.005	-0.197	-0.062	-0.248	-0.205	-0.063	-0.032	-0.296	-0.072	-0.522
OP(1 & 3)	-0.073	-0.055	-0.033	-0.021	0.008	-0.054	0.064	0.035	0.012	0.070
OP(1 & 4)	-0.177	-0.662	-0.055	-0.348	-0.462	-0.139	-0.171	-0.279	-0.054	-0.288
OP(2 & 3)	0.000	0.000	0.000	0.000	0.003	0.000	0.002	-0.002	0.000	0.000
OP(2 & 4)	0.000	0.032	0.007	0.020	0.006	0.010	-0.012	0.022	0.007	-0.033
OP(3 & 4)	-0.332	-0.140	-0.341	-0.756	-0.282	-0.782	-1.358	-1.225	-0.098	-0.381
Alpha MO:	231	232	233	234	235	236	237	238	239	240
Energy(eV):	8.39	8.58	8.70	8.80	8.97	9.03	9.19	9.27	9.37	9.47
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	19.04	28.95	16.93	36.93	42.92	30.47	11.96	32.02	19.88	25.63
FRAG# 2:	-0.20	1.27	0.20	3.01	1.17	1.46	0.32	-0.81	-0.72	-1.84
FRAG# 3:	78.70	60.44	80.95	59.12	56.56	66.67	86.35	66.12	78.56	73.99
FRAG# 4:	2.45	9.34	1.92	0.94	-0.65	1.40	1.37	2.67	2.28	2.22
OP(1 & 2)	-0.122	-0.224	-0.016	-0.954	-0.115	-0.422	-0.163	-0.178	-0.539	-0.498
OP(1 & 3)	0.053	0.002	0.022	0.045	-0.126	-0.072	0.130	-0.070	0.039	-0.013
OP(1 & 4)	-0.127	-0.160	-0.115	-0.179	-0.169	-0.193	-0.521	-0.144	-0.216	-0.157
OP(2 & 3)	0.001	-0.003	0.000	-0.001	0.000	0.000	-0.001	0.000	0.000	-0.002
OP(2 & 4)	-0.011	0.037	-0.002	0.008	0.000	0.007	0.014	-0.003	-0.002	0.041
OP(3 & 4)	-0.214	-1.488	-0.422	-1.202	-0.920	-0.504	-0.648	-0.523	-0.289	-0.913
Alpha MO:	241	242	243	244	245	246	247	248	249	250
Energy(eV):	9.64	9.74	9.86	9.92	10.00	10.11	10.32	10.37	10.49	10.52
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	20.46	9.01	30.60	35.12	29.99	41.04	33.82	33.91	39.15	13.33
FRAG# 2:	-0.34	-0.49	-0.32	0.04	1.71	0.43	-0.16	2.70	-0.60	0.35
FRAG# 3:	78.04	92.73	70.39	61.33	59.97	57.39	53.12	61.26	53.09	75.04
FRAG# 4:	1.84	-1.24	-0.67	3.52	8.33	1.13	13.22	2.12	8.35	11.28
OP(1 & 2)	-0.310	-0.185	-0.299	-0.260	-1.030	-0.057	-0.429	-0.089	-1.515	-0.103
OP(1 & 3)	0.020	0.008	-0.019	-0.009	-0.158	0.044	-0.037	0.118	-0.180	0.080
OP(1 & 4)	-0.347	-0.072	-0.380	-0.420	-0.712	-0.207	-0.617	-1.043	-2.044	-0.884
OP(2 & 3)	0.000	0.000	0.000	-0.001	0.000	0.002	-0.001	0.001	0.002	0.000
OP(2 & 4)	0.008	0.011	0.035	-0.018	-0.026	-0.014	0.016	-0.020	0.054	0.006
OP(3 & 4)	-0.605	-0.509	-1.418	-1.495	-1.584	-1.183	-1.826	-0.600	-2.427	-0.885
Alpha MO:	251	252	253	254	255	256	257	258	259	260
Energy(eV):	10.68	10.88	10.97	11.32	11.45	11.49	11.68	11.92	12.07	12.09
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	37.96	50.00	23.97	40.56	23.79	23.77	42.02	45.90	9.40	39.62
FRAG# 2:	1.87	0.70	0.15	2.16	0.73	4.05	1.69	1.83	0.68	3.30
FRAG# 3:	52.05	42.84	69.98	53.20	69.83	53.36	50.19	43.82	87.41	47.17

FRAG#	1:	52.50	15.13	18.57	33.23	39.96	39.97	36.08	17.98	35.81	46.01
FRAG#	2:	5.26	0.47	2.37	1.26	9.82	0.56	13.67	59.06	19.62	1.71
FRAG#	3:	39.56	83.21	64.83	58.43	44.98	45.12	31.87	14.32	33.07	58.78
FRAG#	4:	2.68	1.19	14.24	7.08	5.23	14.34	18.37	8.64	11.50	-6.49
OP (1 & 2)		-0.581	-0.035	-0.206	-0.146	-1.624	-0.375	-4.473	-16.4	-5.828	-0.425
OP (1 & 3)		-0.087	-0.237	1.036	0.886	1.205	0.253	0.217	-0.166	-1.192	1.835
OP (1 & 4)		-2.607	0.053	-2.096	-2.689	-8.098	-2.912	-1.642	-0.504	-1.035	-8.772
OP (2 & 3)		-0.001	0.002	-0.013	-0.003	-0.011	-0.002	0.004	0.002	-0.012	-0.002
OP (2 & 4)		0.030	-0.015	0.021	0.025	0.112	0.009	0.005	0.001	0.046	0.023
OP (3 & 4)		-2.482	-2.091	-9.118	-8.114	-7.965	-4.219	-1.636	-0.761	-6.655	-11.6
Alpha MO:		311	312	313	314	315	316	317	318	319	320
Energy(eV):		23.03	23.67	24.16	24.47	24.62	24.68	25.28	25.52	25.63	25.89
Symmetry:		na	na	na	na	na	na	na	na	na	na
FRAG#	1:	44.07	32.35	12.12	47.26	29.06	13.16	10.02	9.19	15.71	20.60
FRAG#	2:	2.94	58.10	-0.16	5.34	0.10	4.06	0.28	0.03	0.52	0.42
FRAG#	3:	62.52	8.99	45.83	47.93	39.39	52.85	91.22	100.39	84.17	76.30
FRAG#	4:	-9.53	0.56	42.21	-0.54	31.45	29.93	-1.52	-9.63	-0.40	2.67
OP (1 & 2)		-1.370	-25.6	-0.324	-1.865	-0.006	-0.943	-0.052	0.011	-0.098	-0.087
OP (1 & 3)		0.710	-2.510	-0.130	-8.383	0.194	0.890	0.660	1.827	-1.374	0.039
OP (1 & 4)		-6.339	-6.971	-5.441	-18.0	-3.686	-6.909	-1.448	-5.954	-2.004	-1.755
OP (2 & 3)		0.001	0.005	-0.003	-0.004	0.000	0.004	0.002	0.002	0.001	0.000
OP (2 & 4)		0.037	-0.054	0.013	0.084	-0.001	-0.059	-0.007	-0.019	-0.017	-0.003
OP (3 & 4)		-21.7	-3.419	-23.3	-32.0	-18.5	-13.7	-18.5	-11.3	-8.030	-1.963
Alpha MO:		321	322	323	324	325	326	327	328	329	330
Energy(eV):		26.09	26.19	26.35	26.71	26.96	27.22	27.60	27.83	27.89	28.18
Symmetry:		na	na	na	na	na	na	na	na	na	na
FRAG#	1:	6.34	25.44	15.64	24.05	9.55	16.64	44.73	29.47	20.65	8.54
FRAG#	2:	0.02	0.53	1.32	0.50	0.27	0.95	0.79	-0.07	-0.29	-0.21
FRAG#	3:	95.41	47.53	83.39	80.44	85.64	72.69	52.35	72.90	83.46	92.57
FRAG#	4:	-1.77	26.50	-0.35	-4.98	4.53	9.72	2.12	-2.30	-3.82	-0.91
OP (1 & 2)		-0.026	-0.176	-0.179	-0.281	-0.077	-0.238	-0.231	-0.073	-0.293	-0.269
OP (1 & 3)		-0.926	-3.253	-0.896	-3.556	0.875	1.445	2.734	0.155	0.128	1.469
OP (1 & 4)		-2.097	-10.5	-1.256	-6.563	-3.262	-4.823	-9.343	-0.823	-2.219	-6.149
OP (2 & 3)		-0.001	0.000	0.000	0.001	0.001	0.006	-0.005	0.000	-0.001	-0.005
OP (2 & 4)		0.011	-0.003	-0.006	-0.003	-0.010	-0.048	0.036	-0.012	-0.014	0.070
OP (3 & 4)		-9.013	-11.8	-19.3	-6.866	-12.5	-17.0	-12.8	-1.748	-3.384	-5.628
Alpha MO:		331	332	333	334	335	336	337	338	339	340
Energy(eV):		28.28	28.36	28.67	28.80	28.87	28.89	29.22	29.44	29.58	30.02
Symmetry:		na	na	na	na	na	na	na	na	na	na
FRAG#	1:	8.95	17.61	23.76	6.11	12.19	25.12	19.50	42.90	42.48	29.90
FRAG#	2:	1.16	1.11	0.43	0.15	0.58	2.56	1.38	0.15	2.72	0.69
FRAG#	3:	83.24	83.06	80.65	93.49	86.48	71.31	76.59	63.94	61.07	75.96
FRAG#	4:	6.65	-1.79	-4.83	0.26	0.75	1.02	2.52	-6.99	-6.27	-6.55
OP (1 & 2)		-0.447	-0.272	-0.642	-0.063	-0.150	-0.375	-0.407	-0.856	-0.576	-0.078
OP (1 & 3)		1.332	-0.262	-1.092	0.125	-0.004	-0.388	-0.347	-1.518	-0.075	-1.426
OP (1 & 4)		-7.871	-0.678	-0.167	-1.354	-0.310	-0.125	-2.919	-13.7	-3.457	-7.126
OP (2 & 3)		0.001	0.001	0.007	-0.002	0.002	-0.005	0.001	-0.002	-0.001	0.000
OP (2 & 4)		0.007	-0.020	-0.015	0.001	-0.017	-0.003	0.020	0.133	0.016	-0.005
OP (3 & 4)		-2.925	-1.653	-8.578	-9.213	-1.831	-1.460	-0.500	-7.194	-10.3	-6.915
Alpha MO:		341	342	343	344	345	346	347	348	349	350
Energy(eV):		30.42	30.49	30.56	30.71	31.56	31.61	31.72	32.11	32.20	32.99
Symmetry:		na	na	na	na	na	na	na	na	na	na
FRAG#	1:	10.02	19.66	8.63	3.89	49.40	44.02	46.18	12.99	21.11	56.26
FRAG#	2:	1.01	-0.07	0.14	0.00	0.37	0.72	0.32	0.08	0.04	2.88
FRAG#	3:	88.87	65.03	70.74	92.28	45.48	56.17	53.22	85.74	78.61	40.02
FRAG#	4:	0.11	15.38	20.49	3.84	4.76	-0.91	0.28	1.19	0.24	0.83
OP (1 & 2)		-0.264	-0.083	-0.076	-0.021	-0.570	-0.014	-0.047	-0.208	-0.177	-0.823
OP (1 & 3)		0.262	1.407	-2.531	-1.360	-2.511	-1.666	1.595	0.968	2.025	-1.083
OP (1 & 4)		-1.218	-4.246	-5.562	-0.894	-30.1	-1.917	-4.072	-2.869	-6.407	-18.5
OP (2 & 3)		-0.001	0.002	0.004	0.000	-0.004	0.000	-0.001	-0.011	0.003	0.001
OP (2 & 4)		-0.006	0.016	-0.006	0.003	0.091	-0.002	0.015	0.038	-0.018	0.209
OP (3 & 4)		-4.587	-19.3	-26.3	-10.1	-18.5	-5.235	-19.6	-27.9	-27.6	-9.999

Alpha MO:	351	352	353	354	355	356	357	358	359	360	
Energy(eV):	34.27	34.53	34.67	35.19	35.76	36.17	36.23	36.53	37.10	37.26	
Symmetry:	na	na	na	na	na	na	na	na	na	na	
=====											
FRAG#	1:	34.36	11.11	36.48	12.46	12.49	9.65	8.39	12.61	18.40	68.96
FRAG#	2:	8.95	0.09	3.42	0.22	1.96	-0.20	2.93	-0.22	0.42	-2.72
FRAG#	3:	57.00	86.32	61.50	89.29	78.56	90.32	83.57	87.26	79.01	33.27
FRAG#	4:	-0.31	2.47	-1.39	-1.98	6.99	0.24	5.12	0.36	2.17	0.48
OP(1 & 2)		-0.308	-0.360	-0.776	-0.076	-0.149	-0.121	-0.512	-1.084	-0.296	-2.981
OP(1 & 3)		0.156	-1.996	0.398	-0.267	4.398	-0.126	-0.889	0.305	0.748	0.183
OP(1 & 4)		-1.316	-6.508	-1.497	-2.005	-9.030	-0.719	-7.176	-1.940	-3.889	-1.144
OP(2 & 3)		0.000	0.012	0.003	0.002	0.000	-0.002	-0.001	0.002	0.003	-0.005
OP(2 & 4)		0.024	0.045	0.016	0.013	-0.008	0.008	0.089	0.005	0.025	0.021
OP(3 & 4)		-7.642	-10.3	-5.126	-7.911	-90.5	-2.162	-13.3	-19.8	-17.5	-3.199
=====											
Alpha MO:	361	362	363	364	365	366	367	368	369	370	
Energy(eV):	39.15	39.96	40.11	40.19	40.65	41.62	42.87	43.31	43.56	44.16	
Symmetry:	na	na	na	na	na	na	na	na	na	na	
=====											
FRAG#	1:	57.98	4.66	10.79	7.39	17.65	64.63	17.11	5.85	57.88	86.14
FRAG#	2:	-1.54	-0.20	0.04	0.21	0.78	31.14	4.15	1.98	19.24	4.54
FRAG#	3:	42.99	96.84	88.46	92.56	83.56	12.31	80.95	97.13	34.14	9.79
FRAG#	4:	0.55	-1.31	0.71	-0.15	-2.01	-8.09	-2.20	-4.98	-11.26	-0.47
OP(1 & 2)		-3.685	-0.315	-0.605	-0.622	-1.133	-11.9	-2.122	-0.883	-9.312	-2.989
OP(1 & 3)		-0.271	-0.075	-0.243	-0.024	0.635	-1.551	-0.628	0.228	1.225	-0.432
OP(1 & 4)		-1.679	-0.723	-0.243	-0.335	-3.906	-20.4	-0.604	-1.799	-9.289	-2.287
OP(2 & 3)		0.001	-0.001	-0.001	0.001	0.004	0.042	-0.021	0.015	0.011	-0.001
OP(2 & 4)		0.037	-0.001	-0.005	0.013	-0.070	-0.676	0.128	-0.056	0.175	-0.077
OP(3 & 4)		-2.144	-0.767	-0.996	-0.192	-10.9	-16.6	-6.229	-11.1	-12.6	-4.227
=====											
Alpha MO:	371	372	373	374	375	376	377				
Energy(eV):	46.85	47.35	48.29	49.76	50.49	51.20	334.85				
Symmetry:	na	na	na	na	na	na	na				
=====											
FRAG#	1:	21.35	6.49	39.04	30.47	76.25	7.96	13.04			
FRAG#	2:	33.40	0.66	15.56	1.48	0.03	0.26	0.00			
FRAG#	3:	57.82	114.42	48.14	68.74	36.26	109.99	19.37			
FRAG#	4:	-12.56	-21.57	-2.74	-0.69	-12.54	-18.19	67.59			
OP(1 & 2)		-19.4	-0.381	-8.682	-1.524	-1.165	-0.080	-0.958			
OP(1 & 3)		1.179	1.030	0.019	-0.831	0.004	-7.086	3.515			
OP(1 & 4)		-8.220	-2.124	-1.264	-3.382	-2.772	-24.8	-12.1			
OP(2 & 3)		-0.014	0.004	-0.007	0.001	0.000	0.002	-0.009			
OP(2 & 4)		0.532	-0.026	-0.022	0.155	0.032	-0.061	0.180			
OP(3 & 4)		-5.160	-23.7	-5.806	-7.697	-26.7	-24.0	-13.7			
=====											
Alpha-spin HOMO-LUMO gap: 2.855 eV (23027.3 cm-1)											
The sum of energies of the occupied orbitals:											
alpha-spin MOs: -12620.530 eV											
--- COMPOSITIONS OF ALPHA-SPIN MOLECULAR ORBITALS ---											
Orbital	E(eV)	Fragments									
		1	2	3	4						
377	334.85	13.0	0.0	19.4	67.6						
376	51.20	8.0	0.3	110.0	-18.2						
375	50.49	76.3	0.0	36.3	-12.5						
374	49.76	30.5	1.5	68.7	-0.7						
373	48.29	39.0	15.6	48.1	-2.7						
372	47.35	6.5	0.7	114.4	-21.6						
371	46.85	21.4	33.4	57.8	-12.6						
370	44.16	86.1	4.5	9.8	-0.5						
369	43.56	57.9	19.2	34.1	-11.3						
368	43.31	5.8	2.0	97.1	-5.0						
367	42.87	17.1	4.1	80.9	-2.2						
366	41.62	64.6	31.1	12.3	-8.1						
365	40.65	17.7	0.8	83.6	-2.0						
364	40.19	7.4	0.2	92.6	-0.2						
363	40.11	10.8	0.0	88.5	0.7						
362	39.96	4.7	-0.2	96.8	-1.3						
361	39.15	58.0	-1.5	43.0	0.6						

360	37.26	69.0	-2.7	33.3	0.5
359	37.10	18.4	0.4	79.0	2.2
358	36.53	12.6	-0.2	87.3	0.4
357	36.23	8.4	2.9	83.6	5.1
356	36.17	9.6	-0.2	90.3	0.2
355	35.76	12.5	2.0	78.6	7.0
354	35.19	12.5	0.2	89.3	-2.0
353	34.67	36.5	3.4	61.5	-1.4
352	34.53	11.1	0.1	86.3	2.5
351	34.27	34.4	8.9	57.0	-0.3
350	32.99	56.3	2.9	40.0	0.8
349	32.20	21.1	0.0	78.6	0.2
348	32.11	13.0	0.1	85.7	1.2
347	31.72	46.2	0.3	53.2	0.3
346	31.61	44.0	0.7	56.2	-0.9
345	31.56	49.4	0.4	45.5	4.8
344	30.71	3.9	0.0	92.3	3.8
343	30.56	8.6	0.1	70.7	20.5
342	30.49	19.7	-0.1	65.0	15.4
341	30.42	10.0	1.0	88.9	0.1
340	30.02	29.9	0.7	76.0	-6.5
339	29.58	42.5	2.7	61.1	-6.3
338	29.44	42.9	0.1	63.9	-7.0
337	29.22	19.5	1.4	76.6	2.5
336	28.89	25.1	2.6	71.3	1.0
335	28.87	12.2	0.6	86.5	0.7
334	28.80	6.1	0.1	93.5	0.3
333	28.67	23.8	0.4	80.7	-4.8
332	28.36	17.6	1.1	83.1	-1.8
331	28.28	9.0	1.2	83.2	6.7
330	28.18	8.5	-0.2	92.6	-0.9
329	27.89	20.7	-0.3	83.5	-3.8
328	27.83	29.5	-0.1	72.9	-2.3
327	27.60	44.7	0.8	52.4	2.1
326	27.22	16.6	0.9	72.7	9.7
325	26.96	9.6	0.3	85.6	4.5
324	26.71	24.0	0.5	80.4	-5.0
323	26.35	15.6	1.3	83.4	-0.3
322	26.19	25.4	0.5	47.5	26.5
321	26.09	6.3	0.0	95.4	-1.8
320	25.89	20.6	0.4	76.3	2.7
319	25.63	15.7	0.5	84.2	-0.4
318	25.52	9.2	0.0	100.4	-9.6
317	25.28	10.0	0.3	91.2	-1.5
316	24.68	13.2	4.1	52.9	29.9
315	24.62	29.1	0.1	39.4	31.4
314	24.47	47.3	5.3	47.9	-0.5
313	24.16	12.1	-0.2	45.8	42.2
312	23.67	32.3	58.1	9.0	0.6
311	23.03	44.1	2.9	62.5	-9.5
310	22.50	46.0	1.7	58.8	-6.5
309	22.13	35.8	19.6	33.1	11.5
308	21.79	18.0	59.1	14.3	8.6
307	21.42	36.1	13.7	31.9	18.4
306	20.85	40.0	0.6	45.1	14.3
305	20.41	40.0	9.8	45.0	5.2
304	20.20	33.2	1.3	58.4	7.1
303	19.99	18.6	2.4	64.8	14.2
302	19.57	15.1	0.5	83.2	1.2
301	19.25	52.5	5.3	39.6	2.7
300	18.92	16.5	1.0	56.8	25.6
299	18.71	14.2	0.3	65.6	19.9
298	18.59	29.7	7.8	62.0	0.5
297	18.30	24.0	0.3	70.5	5.3
296	17.87	17.9	0.7	75.5	5.9
295	17.77	12.9	0.0	87.0	0.1
294	17.64	26.2	0.4	69.7	3.7
293	17.38	45.4	26.8	30.1	-2.3
292	17.11	32.5	3.5	62.1	1.9
291	17.02	47.8	6.3	45.1	0.7
290	16.67	49.1	5.2	42.4	3.4

289	16.35	24.0	1.9	74.1	0.0
288	16.18	12.4	8.8	77.5	1.4
287	15.88	8.1	9.3	83.7	-1.1
286	15.76	59.7	4.4	39.5	-3.6
285	15.67	39.8	6.5	53.9	-0.2
284	15.56	22.2	15.2	61.2	1.4
283	15.36	49.3	20.2	30.5	0.0
282	15.30	8.2	42.5	49.4	-0.2
281	15.16	29.1	0.8	66.6	3.5
280	14.90	10.8	0.9	87.0	1.3
279	14.85	31.1	7.8	59.1	2.1
278	14.72	11.3	2.0	87.4	-0.7
277	14.53	11.6	1.8	86.5	0.2
276	14.47	38.9	1.7	58.1	1.3
275	14.11	13.8	8.1	77.9	0.1
274	14.05	30.6	3.5	64.6	1.3
273	13.96	21.2	2.4	68.4	7.9
272	13.85	23.8	1.3	68.5	6.4
271	13.72	30.7	6.5	61.0	1.9
270	13.58	17.3	0.8	79.5	2.3
269	13.46	13.6	5.3	76.8	4.2
268	13.39	21.9	0.6	68.0	9.5
267	13.18	12.5	-0.1	84.1	3.4
266	12.93	51.1	1.8	39.9	7.2
265	12.81	25.0	2.7	68.1	4.2
264	12.73	22.6	2.3	73.1	2.0
263	12.57	34.7	1.0	56.8	7.5
262	12.48	44.9	2.5	44.4	8.2
261	12.35	23.0	1.1	60.8	15.1
260	12.09	39.6	3.3	47.2	9.9
259	12.07	9.4	0.7	87.4	2.5
258	11.92	45.9	1.8	43.8	8.4
257	11.68	42.0	1.7	50.2	6.1
256	11.49	23.8	4.0	53.4	18.8
255	11.45	23.8	0.7	69.8	5.6
254	11.32	40.6	2.2	53.2	4.1
253	10.97	24.0	0.2	70.0	5.9
252	10.88	50.0	0.7	42.8	6.4
251	10.68	38.0	1.9	52.0	8.1
250	10.52	13.3	0.4	75.0	11.3
249	10.49	39.2	-0.6	53.1	8.4
248	10.37	33.9	2.7	61.3	2.1
247	10.32	33.8	-0.2	53.1	13.2
246	10.11	41.0	0.4	57.4	1.1
245	10.00	30.0	1.7	60.0	8.3
244	9.92	35.1	0.0	61.3	3.5
243	9.86	30.6	-0.3	70.4	-0.7
242	9.74	9.0	-0.5	92.7	-1.2
241	9.64	20.5	-0.3	78.0	1.8
240	9.47	25.6	-1.8	74.0	2.2
239	9.37	19.9	-0.7	78.6	2.3
238	9.27	32.0	-0.8	66.1	2.7
237	9.19	12.0	0.3	86.4	1.4
236	9.03	30.5	1.5	66.7	1.4
235	8.97	42.9	1.2	56.6	-0.7
234	8.80	36.9	3.0	59.1	0.9
233	8.70	16.9	0.2	80.9	1.9
232	8.58	28.9	1.3	60.4	9.3
231	8.39	19.0	-0.2	78.7	2.4
230	8.32	36.7	-1.1	63.8	0.6
229	8.31	9.5	0.1	87.9	2.5
228	8.21	11.8	0.0	84.2	4.0
227	8.09	39.1	0.5	58.3	2.1
226	8.00	14.6	0.2	81.5	3.7
225	7.97	19.7	-1.1	77.7	3.7
224	7.87	12.3	-0.5	81.6	6.6
223	7.82	22.1	-0.1	77.6	0.3
222	7.80	24.6	-0.8	71.6	4.6
221	7.70	15.3	0.0	82.4	2.3
220	7.65	20.5	-0.2	75.5	4.3
219	7.59	17.7	-0.2	81.2	1.3

218	7.56	21.4	0.0	72.4	6.2
217	7.49	18.8	-0.1	78.6	2.7
216	7.39	41.1	-1.6	58.4	2.1
215	7.36	23.3	-0.3	76.2	0.8
214	7.19	51.2	0.0	42.9	5.8
213	7.17	31.5	0.2	66.0	2.3
212	6.93	35.4	0.2	59.7	4.8
211	6.85	17.4	-0.2	80.0	2.8
210	6.77	16.5	-2.1	71.4	14.2
209	6.65	28.9	-0.5	64.2	7.4
208	6.48	29.6	-5.2	72.7	3.0
207	6.39	18.9	-3.4	67.5	17.1
206	6.39	21.3	-1.9	74.8	5.8
205	6.23	52.2	-6.8	48.9	5.8
204	6.20	21.8	-0.9	75.2	3.9
203	5.96	41.3	-5.3	62.5	1.4
202	5.86	54.5	-3.7	44.2	5.0
201	5.78	17.8	-0.5	78.1	4.5
200	5.70	19.4	-1.3	71.8	10.1
199	5.59	16.5	-0.8	76.4	7.9
198	5.54	17.5	-1.3	84.5	-0.7
197	5.53	6.9	0.0	93.4	-0.3
196	5.39	15.9	-0.1	80.1	4.2
195	5.21	10.0	-0.4	83.9	6.5
194	5.14	58.9	-2.9	27.5	16.5
193	4.98	29.9	-1.6	71.6	0.1
192	4.85	36.0	0.3	60.7	3.0
191	4.76	31.5	-0.7	59.9	9.4
190	4.66	44.0	-4.7	42.8	17.8
189	4.48	13.3	-0.2	61.7	25.2
188	4.41	26.1	0.2	69.0	4.7
187	4.19	9.2	-0.1	89.0	1.9
186	4.10	9.2	-0.2	87.1	3.9
185	4.07	23.7	-1.1	74.0	3.4
184	3.93	24.9	-0.2	69.7	5.6
183	3.84	15.7	0.2	83.6	0.5
182	3.76	9.3	0.0	80.3	10.4
181	3.74	10.6	-0.2	84.0	5.6
180	3.45	37.5	-1.4	65.0	-1.1
179	3.42	12.9	-0.4	89.6	-2.1
178	3.33	56.3	-1.2	41.3	3.6
177	3.26	15.9	-0.8	82.6	2.4
176	3.15	3.6	0.0	95.9	0.5
175	3.10	27.6	-0.8	78.2	-5.1
174	3.00	16.7	-0.3	82.3	1.3
173	2.93	74.9	-1.8	17.3	9.7
172	2.83	67.1	-1.1	29.2	4.8
171	2.68	14.3	-1.5	81.6	5.5
170	2.62	40.5	-0.8	58.2	2.2
169	2.43	46.3	0.4	42.4	10.9
168	2.30	31.0	0.5	54.7	13.8
167	2.28	7.2	-0.5	89.3	4.0
166	2.11	51.1	0.1	47.7	1.1
165	1.95	75.8	-1.1	23.6	1.7
164	1.72	40.4	-0.1	58.4	1.2
163	1.56	11.3	0.1	88.9	-0.2
162	1.45	1.9	0.0	97.6	0.5
161	1.39	2.7	0.1	94.9	2.4
160	1.29	1.0	0.0	100.0	-0.9
159	1.24	13.7	-0.1	85.1	1.3
158	1.11	13.6	0.4	84.8	1.2
157	1.02	28.1	-0.8	73.5	-0.9
156	0.98	66.8	4.0	28.6	0.6
155	0.92	5.8	0.0	93.6	0.6
154	0.81	22.6	0.2	75.1	2.1
153	0.78	7.1	0.4	93.5	-0.9
152	0.70	7.8	-0.1	91.1	1.2
151	0.62	17.6	-0.4	80.8	1.9
150	0.55	7.9	0.1	90.3	1.6
149	0.30	2.1	0.0	94.8	3.1
148	0.09	1.2	0.0	95.3	3.5

147	-0.36	0.4	0.0	98.6	1.0
146	-0.49	-9.7	-0.3	-0.9	110.9
145	-0.58	1.2	0.0	97.6	1.2
144	-0.91	91.1	7.1	1.8	0.1
143	-1.46	87.8	4.5	1.2	6.4
142	-1.63	-2.4	0.1	-5.3	107.5
141	-1.67	-2.2	0.0	-8.0	110.2
140	-1.85	0.2	0.4	-8.1	107.5
139	-2.24	13.6	0.0	19.8	66.7
138	-2.46	9.0	0.0	24.2	66.7
137	-2.76	0.3	0.0	99.3	0.4
136	-3.01	0.2	0.0	99.1	0.6
135	-3.89	88.8	1.7	8.9	0.6
134	-4.07	4.5	0.1	93.2	2.2
133	-4.23	1.8	0.0	95.4	2.8
132	-4.29	0.2	0.0	97.9	1.9
131	-4.54	9.0	1.7	86.4	2.8
130	-4.71	63.6	20.7	11.8	3.8
129	-5.12	1.0	0.2	93.8	5.0
128	-5.35	1.1	0.2	94.4	4.3
----- E(gap) = 2.855 eV					
127	-8.21	33.1	0.0	7.6	59.4
126	-8.53	6.6	0.5	17.4	75.5
125	-8.65	14.8	1.5	14.2	69.5
124	-9.01	74.8	0.5	4.4	20.2
123	-9.24	98.5	0.0	0.6	0.9
122	-9.62	36.6	59.9	1.5	2.1
121	-9.98	16.7	0.1	81.7	1.5
120	-10.11	63.2	1.5	26.0	9.3
119	-10.20	79.7	5.7	9.5	5.2
118	-10.23	4.6	0.1	94.1	1.1
117	-11.00	97.9	0.0	1.9	0.1
116	-11.31	2.4	0.0	96.5	1.1
115	-11.47	1.5	0.1	96.9	1.5
114	-11.53	10.3	5.0	83.5	1.2
113	-11.60	5.8	0.1	91.0	3.1
112	-11.72	3.7	0.2	96.9	-0.8
111	-11.74	2.6	0.3	94.4	2.7
110	-11.88	3.3	0.8	91.3	4.6
109	-12.03	22.3	3.0	75.8	-1.1
108	-12.11	34.7	0.9	66.0	-1.6
107	-12.18	48.1	30.8	16.8	4.3
106	-12.89	2.8	1.5	86.7	9.0
105	-13.17	47.1	0.9	38.9	13.0
104	-13.23	55.3	5.3	32.7	6.7
103	-13.47	0.6	0.1	98.9	0.4
102	-13.55	78.2	6.6	13.8	1.4
101	-13.60	8.2	0.5	90.4	0.9
100	-13.75	3.7	0.4	94.1	1.8
99	-13.89	23.8	1.0	73.3	1.8
98	-13.97	47.8	2.9	49.3	0.1
97	-14.15	15.0	2.0	82.3	0.7
96	-14.21	89.6	4.1	5.9	0.4
95	-14.40	9.9	0.1	88.4	1.6
94	-14.59	13.6	1.8	84.0	0.6
93	-14.82	4.2	0.5	89.1	6.2
92	-14.92	24.1	1.5	72.4	2.0
91	-15.02	26.3	1.4	68.1	4.2
90	-15.18	14.1	0.4	82.1	3.4
89	-15.25	13.0	0.5	84.8	1.6
88	-15.31	7.4	0.1	90.9	1.6
87	-15.48	33.7	0.6	64.5	1.3
86	-15.59	7.2	0.1	91.8	1.0
85	-15.64	52.4	0.7	45.4	1.5
84	-15.78	4.2	0.1	94.6	1.1
83	-15.90	3.7	0.1	95.3	1.0
82	-16.25	1.2	0.0	98.2	0.5
81	-16.27	91.5	1.7	5.6	1.2
80	-16.41	0.2	0.0	99.2	0.6
79	-16.59	0.5	0.0	99.3	0.2
78	-16.75	0.4	0.0	99.4	0.1

77	-17.02	85.9	11.3	1.8	0.9
76	-17.05	87.7	3.8	6.5	2.0
75	-17.21	0.6	0.0	97.7	1.7
74	-17.23	3.3	0.1	95.8	0.8
73	-17.35	0.3	0.0	98.6	1.2
72	-17.38	0.4	0.0	98.4	1.1
71	-18.30	9.4	0.3	89.9	0.4
70	-18.41	83.4	2.9	11.7	2.1
69	-18.54	7.1	0.3	90.3	2.3
68	-18.75	91.4	3.0	4.0	1.6
67	-20.01	0.0	0.0	98.3	1.8
66	-20.18	0.0	0.0	98.3	1.6
65	-20.36	0.2	0.0	99.6	0.3
64	-20.51	0.1	0.0	99.8	0.1
63	-21.06	90.3	8.7	0.2	0.8
62	-21.21	8.5	0.8	90.1	0.7
61	-21.25	81.0	7.1	11.4	0.5
60	-21.38	1.7	0.1	97.4	0.8
59	-21.51	0.2	0.0	98.5	1.3
58	-21.67	0.0	0.0	98.9	1.1
57	-23.62	96.7	2.7	0.2	0.4
56	-23.84	0.0	0.0	100.1	-0.1
55	-24.01	0.2	0.0	100.0	-0.2
54	-25.07	98.1	1.2	0.3	0.4
53	-25.31	0.0	0.0	99.5	0.5
52	-25.33	0.0	0.0	100.0	0.0
51	-25.48	0.0	0.0	99.5	0.4
50	-25.50	0.1	0.0	99.7	0.2
49	-25.54	0.2	0.0	98.8	1.0
48	-25.73	0.3	0.0	98.6	1.1
47	-26.20	98.3	0.1	0.5	1.2
46	-27.99	56.7	42.2	0.2	0.9
45	-29.32	0.0	0.0	99.1	0.9
44	-29.48	0.1	0.0	99.1	0.8
43	-29.98	43.5	9.3	48.2	-1.1
42	-30.01	37.1	7.5	55.4	0.0
41	-30.19	3.3	0.4	97.3	-0.9
40	-31.03	99.9	0.2	0.5	-0.6
39	-50.61	-0.1	0.0	-0.1	100.2
38	-50.88	-0.3	0.0	-0.1	100.4
37	-50.93	0.0	0.0	-0.4	100.4
36	-81.34	0.1	0.0	0.4	99.5
35	-280.49	100.0	0.0	0.0	0.0
34	-281.03	0.0	0.0	100.0	0.0
33	-281.10	0.0	0.0	100.0	0.0
32	-281.10	100.0	0.0	0.0	0.0
31	-281.14	0.0	0.0	100.0	0.0
30	-281.15	0.0	0.0	100.0	0.0
29	-281.18	0.0	0.0	100.0	0.0
28	-281.20	0.0	0.0	100.0	0.0
27	-281.25	0.0	0.0	100.0	0.0
26	-281.31	0.0	0.0	100.0	0.0
25	-281.35	0.0	0.0	100.0	0.0
24	-281.36	0.0	0.0	100.0	0.0
23	-281.38	100.0	0.0	0.0	0.0
22	-281.41	100.0	0.0	0.0	0.0
21	-281.43	0.0	0.0	100.0	0.0
20	-281.46	0.0	0.0	100.0	0.0
19	-281.80	100.0	0.0	0.0	0.0
18	-281.83	0.0	0.0	100.0	0.0
17	-281.88	0.0	0.0	100.0	0.0
16	-281.90	0.0	0.0	100.0	0.0
15	-282.03	100.0	0.0	0.0	0.0
14	-282.09	0.0	0.0	100.0	0.0
13	-282.27	0.0	0.0	100.0	0.0
12	-282.33	0.0	0.0	100.0	0.0
11	-282.47	0.0	0.0	100.0	0.0
10	-282.53	0.0	0.0	100.0	0.0
9	-392.01	100.0	0.0	0.0	0.0
8	-392.75	100.0	0.0	0.0	0.0
7	-393.28	0.1	99.9	0.0	0.0

6	-393.41	100.0	0.0	0.0	0.0
5	-394.41	100.0	0.0	0.0	0.0
4	-394.43	0.0	0.0	100.0	0.0
3	-394.48	0.0	0.0	100.0	0.0
2	-394.56	0.0	0.0	100.0	0.0
1	-394.64	0.0	0.0	100.0	0.0

----- Density-of-States Calculations -----
Using Gaussian functions with the half-widths 0.50 eV
The data window: from -18.0 to 4.6 eV

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Using Gaussian functions with the half-widths 0.50 eV
The data window: from -18.0 to 4.6 eV