Electronic Supplementary Information for Dalton Transactions

Structural and spectroscopic properties of a copper(I)–bis(N-heterocyclic)carbene complex

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Supplementary Information

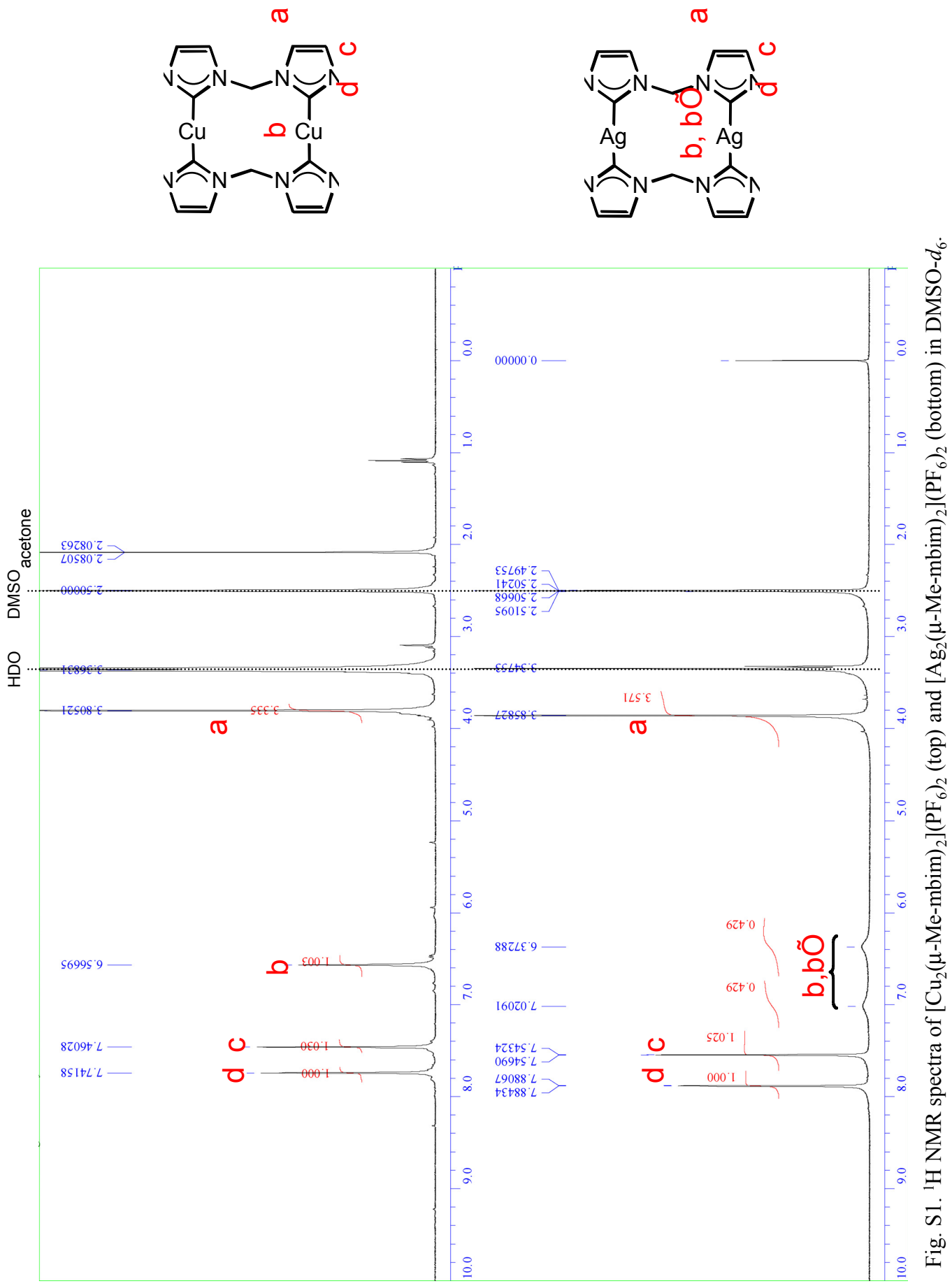

Fig. S1. ^{1}H NMR spectra of $[Cu_2(\mu\text{-Me-mbim})_2](PF_6)_2$ (top) and $[Ag_2(\mu\text{-Me-mbim})_2](PF_6)_2$ (bottom) in DMSO-d_6.

(i) Input file for the geometry optimization of $[Cu_2(\mu\text{-Me-mbim})_2](PF_6)_2$ in the singlet state.

```
%Nproc=4
%Mem=1024MB
%CHK=singlet_Cu2PF62Membim2_opt.chk
#P UB3LYP GEN OPT FREQ POP=FULL NOSYMM

geometry optimization of Cu2PF62Membim2 in the singlet state

0 1
H 0 0.41699 -0.90093 -4.92925
H 0 2.23039 -2.43031 -4.68403
H 0 0.52771 2.46543 -4.50527
C 0 0.88873 -1.06575 -4.14527
C 0 1.87491 -1.87799 -4.02461
H 0 1.58833 4.41223 -3.55938
C 0 0.63721 2.63999 -3.60075
H 0 -1.01564 0.61436 -3.37369
C 0 1.23925 3.69467 -3.08865
N 0 0.64252 -0.47720 -2.92891
H 0 3.50273 -3.35127 -2.62532
N 0 2.30303 -1.76615 -2.70458
C 0 -0.35836 0.60885 -2.66004
N 0 0.22208 1.85914 -2.57017
H 0 4.23071 -2.00638 -2.27829
F 0 -3.69072 1.09880 -2.30071
C 0 3.42399 -2.51267 -2.16312
C 0 1.54657 -0.87536 -2.00972
N 0 1.23409 3.53207 -1.77784
H 0 -0.82083 0.41358 -1.83093
H 0 2.64926 4.92523 -1.30628
F 0 -5.22959 2.27555 -1.12386
F 0 0.40206 -4.46692 -1.23500
C 0 0.58453 2.41923 -1.35565
H 0 3.27722 -2.67506 -1.22808
F 0 -5.06631 -0.02454 -0.97103
C 0 1.90731 4.51802 -0.85157
P 0 -4.11498 1.19694 -0.76531
H 0 1.27799 5.19523 -0.59539
F 0 -3.02448 2.31958 -0.58618
F 0 -2.98594 0.11334 -0.45345
H 0 2.22192 4.05934 -0.07072
Cu 0 1.83310 -0.36294 -0.18064
F 0 -0.59637 -2.96214 0.06627
F 0 -1.24818 -4.99698 0.28854
P 0 0.16647 -4.33694 0.33854
F 0 1.51213 -3.52226 0.42272
F 0 0.92147 -5.70153 0.65823
Cu 0 0.02198 1.83817 0.38115
H 0 4.39868 1.20562 0.78630
F 0 -4.39661 1.29030 0.80325
H 0 5.22420 -0.02444 1.29818
H 0 -2.03985 3.65907 1.36182
C 0 4.67163 0.71381 1.56265
C 0 2.28864 -0.13437 1.66619
F 0 -0.03851 -4.06442 1.89764
H 0 -0.01834 -1.08092 1.74023
H 0 5.16640 1.29008 2.15103
C 0 -0.77626 1.48795 2.09298
C 0 -1.97392 3.66582 2.31985
N 0 3.45030 0.19314 2.28415
H 0 -1.32464 4.31739 2.59239
H 0 -2.82890 3.88713 2.69816
C 0 0.16167 -0.76526 2.63878
N 0 -1.56560 2.35258 2.78428
N 0 1.50866 -0.48279 2.75724
N 0 -0.70764 0.42541 2.92187
H 0 -0.06912 -1.47700 3.25645
C 0 3.43637 0.02356 3.59401
C 0 2.21842 -0.36908 3.90940
C 0 -1.94003 1.82620 4.01757
H 0 4.14421 0.14650 4.17898
```

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C 0 -1.38364 0.67218 4.09178
H 0 -2.48409 2.22855 4.65661
H 0 1.90692 -0.52933 4.76842
H 0 -1.42939 0.09583 4.81982

Cu 0
6-311G
 P 1 1.5
 0.083141     1.000000000
 P 1 1.5
 0.018137     1.000000000
****
P 0
6-31+G*
****
F 0
6-31+G*
****
N 0
6-31G*
****
C 0
6-31G*
****
H 0
6-31G
****
```

(ii) Results for the geometry optimization of $[Cu_2(\mu\text{-Me-mbim})_2](PF_6)_2$ in the singlet state.

Item	Value	Threshold	Converged?
Maximum Force	0.000042	0.000450	YES
RMS Force	0.000006	0.000300	YES
Maximum Displacement	0.001390	0.001800	YES
RMS Displacement	0.000225	0.001200	YES

Predicted change in Energy=-3.494923D-08
Optimization completed.
-- Stationary point found.

Optimized Parameters (Angstroms and Degrees)

Name	Definition	Value	Derivative Info.
R1	R(1,4)	1.0793	-DE/DX = 0.0
R2	R(2,5)	1.0789	-DE/DX = 0.0
R3	R(3,7)	1.0786	-DE/DX = 0.0
R4	R(4,5)	1.3562	-DE/DX = 0.0
R5	R(4,10)	1.3884	-DE/DX = 0.0
R6	R(5,12)	1.3871	-DE/DX = 0.0
R7	R(6,9)	1.079	-DE/DX = 0.0
R8	R(7,9)	1.3561	-DE/DX = 0.0
R9	R(7,14)	1.3872	-DE/DX = 0.0
R10	R(8,13)	1.0916	-DE/DX = 0.0
R11	R(8,16)	2.6933	-DE/DX = 0.0
R12	R(9,19)	1.3877	-DE/DX = 0.0
R13	R(10,13)	1.4566	-DE/DX = 0.0
R14	R(10,18)	1.3691	-DE/DX = 0.0
R15	R(11,17)	1.0922	-DE/DX = 0.0
R16	R(12,17)	1.4645	-DE/DX = 0.0
R17	R(12,18)	1.3573	-DE/DX = 0.0
R18	R(13,14)	1.4539	-DE/DX = 0.0
R19	R(13,20)	1.0882	-DE/DX = 0.0
R20	R(14,24)	1.363	-DE/DX = 0.0
R21	R(15,17)	1.0944	-DE/DX = 0.0
R22	R(16,20)	3.3736	-DE/DX = 0.0
R23	R(16,28)	1.6495	-DE/DX = 0.0
R24	R(17,25)	1.0879	-DE/DX = 0.0
R25	R(18,33)	1.9214	-DE/DX = 0.0
R26	R(19,24)	1.3571	-DE/DX = 0.0
R27	R(19,27)	1.4593	-DE/DX = 0.0
R28	R(20,30)	4.137	-DE/DX = 0.0
R29	R(20,31)	2.5846	-DE/DX = 0.0
R30	R(21,27)	1.0926	-DE/DX = 0.0
R31	R(22,28)	1.623	-DE/DX = 0.0
R32	R(23,36)	1.6369	-DE/DX = 0.0
R33	R(24,39)	1.9222	-DE/DX = 0.0
R34	R(25,37)	2.2617	-DE/DX = 0.0
R35	R(26,28)	1.6249	-DE/DX = 0.0
R36	R(27,29)	1.0937	-DE/DX = 0.0
R37	R(27,32)	1.0916	-DE/DX = 0.0
R38	R(28,30)	1.6742	-DE/DX = 0.0
R39	R(28,31)	1.6766	-DE/DX = 0.0
R40	R(28,41)	1.6369	-DE/DX = 0.0
R41	R(30,39)	2.7683	-DE/DX = 0.0
R42	R(30,43)	2.2789	-DE/DX = 0.0
R43	R(33,37)	2.7754	-DE/DX = 0.0
R44	R(33,45)	1.9221	-DE/DX = 0.0
R45	R(34,36)	1.6772	-DE/DX = 0.0
R46	R(34,47)	2.5163	-DE/DX = 0.0
R47	R(35,36)	1.6252	-DE/DX = 0.0
R48	R(36,37)	1.6732	-DE/DX = 0.0
R49	R(36,38)	1.6226	-DE/DX = 0.0
R50	R(36,46)	1.6496	-DE/DX = 0.0
R51	R(37,47)	4.106	-DE/DX = 0.0
R52	R(39,49)	1.9213	-DE/DX = 0.0
R53	R(40,44)	1.0914	-DE/DX = 0.0
R54	R(42,44)	1.0938	-DE/DX = 0.0
R55	R(43,50)	1.088	-DE/DX = 0.0

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! R56   R(44,48)              1.0928         -DE/DX =    0.0                 !
! R57   R(44,51)              1.4591         -DE/DX =    0.0                 !
! R58   R(45,51)              1.3574         -DE/DX =    0.0                 !
! R59   R(45,56)              1.3632         -DE/DX =    0.0                 !
! R60   R(46,47)              3.3592         -DE/DX =    0.0                 !
! R61   R(46,58)              2.6596         -DE/DX =    0.0                 !
! R62   R(47,54)              1.0878         -DE/DX =    0.0                 !
! R63   R(49,55)              1.3573         -DE/DX =    0.0                 !
! R64   R(49,57)              1.3692         -DE/DX =    0.0                 !
! R65   R(50,52)              1.0943         -DE/DX =    0.0                 !
! R66   R(50,53)              1.0922         -DE/DX =    0.0                 !
! R67   R(50,55)              1.4646         -DE/DX =    0.0                 !
! R68   R(51,59)              1.3878         -DE/DX =    0.0                 !
! R69   R(54,56)              1.4546         -DE/DX =    0.0                 !
! R70   R(54,57)              1.4563         -DE/DX =    0.0                 !
! R71   R(54,58)              1.0915         -DE/DX =    0.0                 !
! R72   R(55,61)              1.3871         -DE/DX =    0.0                 !
! R73   R(56,60)              1.387          -DE/DX =    0.0                 !
! R74   R(57,63)              1.3884         -DE/DX =    0.0                 !
! R75   R(59,60)              1.356          -DE/DX =    0.0                 !
! R76   R(59,62)              1.079          -DE/DX =    0.0                 !
! R77   R(60,65)              1.0785         -DE/DX =    0.0                 !
! R78   R(61,63)              1.3562         -DE/DX =    0.0                 !
! R79   R(61,64)              1.079          -DE/DX =    0.0                 !
! R80   R(63,66)              1.0793         -DE/DX =    0.0                 !
! A1    A(1,4,5)            131.2937         -DE/DX =    0.0                 !
! A2    A(1,4,10)           122.4996         -DE/DX =    0.0                 !
! A3    A(5,4,10)           106.1879         -DE/DX =    0.0                 !
! A4    A(2,5,4)            130.9492         -DE/DX =    0.0                 !
! A5    A(2,5,12)           122.194          -DE/DX =    0.0                 !
! A6    A(4,5,12)           106.8508         -DE/DX =    0.0                 !
! A7    A(3,7,9)            131.0291         -DE/DX =    0.0                 !
! A8    A(3,7,14)           122.7639         -DE/DX =    0.0                 !
! A9    A(9,7,14)           106.2035         -DE/DX =    0.0                 !
! A10   A(13,8,16)          108.2478         -DE/DX =    0.0                 !
! A11   A(6,9,7)            130.8997         -DE/DX =    0.0                 !
! A12   A(6,9,19)           122.3865         -DE/DX =    0.0                 !
! A13   A(7,9,19)           106.7136         -DE/DX =    0.0                 !
! A14   A(4,10,13)          124.2226         -DE/DX =    0.0                 !
! A15   A(4,10,18)          111.5658         -DE/DX =    0.0                 !
! A16   A(13,10,18)         124.1998         -DE/DX =    0.0                 !
! A17   A(5,12,17)          123.0989         -DE/DX =    0.0                 !
! A18   A(5,12,18)          111.6048         -DE/DX =    0.0                 !
! A19   A(17,12,18)         125.2878         -DE/DX =    0.0                 !
! A20   A(8,13,10)          108.7683         -DE/DX =    0.0                 !
! A21   A(8,13,14)          109.605          -DE/DX =    0.0                 !
! A22   A(8,13,20)          108.2642         -DE/DX =    0.0                 !
! A23   A(10,13,14)         112.6789         -DE/DX =    0.0                 !
! A24   A(10,13,20)         110.2328         -DE/DX =    0.0                 !
! A25   A(14,13,20)         107.1964         -DE/DX =    0.0                 !
! A26   A(7,14,13)          124.9123         -DE/DX =    0.0                 !
! A27   A(7,14,24)          111.6577         -DE/DX =    0.0                 !
! A28   A(13,14,24)         123.0196         -DE/DX =    0.0                 !
! A29   A(8,16,20)           31.3757         -DE/DX =    0.0                 !
! A30   A(8,16,28)          119.9877         -DE/DX =    0.0                 !
! A31   A(20,16,28)          96.0203         -DE/DX =    0.0                 !
! A32   A(11,17,12)         109.6135         -DE/DX =    0.0                 !
! A33   A(11,17,15)         109.9556         -DE/DX =    0.0                 !
! A34   A(11,17,25)         108.0845         -DE/DX =    0.0                 !
! A35   A(12,17,15)         109.625          -DE/DX =    0.0                 !
! A36   A(12,17,25)         109.2661         -DE/DX =    0.0                 !
! A37   A(15,17,25)         110.2714         -DE/DX =    0.0                 !
! A38   A(10,18,12)         103.7898         -DE/DX =    0.0                 !
! A39   A(10,18,33)         126.1647         -DE/DX =    0.0                 !
! A40   A(12,18,33)         130.0014         -DE/DX =    0.0                 !
! A41   A(9,19,24)          111.5032         -DE/DX =    0.0                 !
! A42   A(9,19,27)          124.2219         -DE/DX =    0.0                 !
! A43   A(24,19,27)         123.856          -DE/DX =    0.0                 !
! A44   A(13,20,16)          71.9149         -DE/DX =    0.0                 !
! A45   A(13,20,30)          97.8511         -DE/DX =    0.0                 !
! A46   A(13,20,31)         115.2156         -DE/DX =    0.0                 !
! A47   A(16,20,30)          34.2891         -DE/DX =    0.0                 !
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! A48	A(16,20,31)	43.4457	-DE/DX = 0.0	!
! A49	A(30,20,31)	30.5473	-DE/DX = 0.0	!
! A50	A(14,24,19)	103.9137	-DE/DX = 0.0	!
! A51	A(14,24,39)	127.2817	-DE/DX = 0.0	!
! A52	A(19,24,39)	128.295	-DE/DX = 0.0	!
! A53	A(17,25,37)	164.3426	-DE/DX = 0.0	!
! A54	A(19,27,21)	109.3359	-DE/DX = 0.0	!
! A55	A(19,27,29)	110.033	-DE/DX = 0.0	!
! A56	A(19,27,32)	109.0372	-DE/DX = 0.0	!
! A57	A(21,27,29)	109.9108	-DE/DX = 0.0	!
! A58	A(21,27,32)	109.2052	-DE/DX = 0.0	!
! A59	A(29,27,32)	109.2988	-DE/DX = 0.0	!
! A60	A(16,28,22)	90.7507	-DE/DX = 0.0	!
! A61	A(16,28,26)	90.494	-DE/DX = 0.0	!
! A62	A(16,28,30)	89.0674	-DE/DX = 0.0	!
! A63	A(16,28,31)	88.6359	-DE/DX = 0.0	!
! A64	A(22,28,26)	92.2749	-DE/DX = 0.0	!
! A65	A(22,28,30)	90.1891	-DE/DX = 0.0	!
! A66	A(22,28,41)	91.3402	-DE/DX = 0.0	!
! A67	A(26,28,30)	177.5028	-DE/DX = 0.0	!
! A68	A(26,28,31)	89.941	-DE/DX = 0.0	!
! A69	A(26,28,41)	91.1418	-DE/DX = 0.0	!
! A70	A(30,28,31)	87.591	-DE/DX = 0.0	!
! A71	A(30,28,41)	89.2055	-DE/DX = 0.0	!
! A72	A(31,28,41)	89.2082	-DE/DX = 0.0	!
! A73	A(20,30,28)	70.3937	-DE/DX = 0.0	!
! A74	A(20,30,39)	39.8288	-DE/DX = 0.0	!
! A75	A(20,30,43)	100.7228	-DE/DX = 0.0	!
! A76	A(28,30,39)	104.3785	-DE/DX = 0.0	!
! A77	A(28,30,43)	112.7127	-DE/DX = 0.0	!
! A78	A(39,30,43)	68.7283	-DE/DX = 0.0	!
! A79	A(20,31,28)	131.8142	-DE/DX = 0.0	!
! A80	A(18,33,37)	106.929	-DE/DX = 0.0	!
! A81	A(18,33,45)	170.9599	-DE/DX = 0.0	!
! A82	A(37,33,45)	81.0152	-DE/DX = 0.0	!
! A83	A(36,34,47)	132.9761	-DE/DX = 0.0	!
! A84	A(23,36,34)	89.185	-DE/DX = 0.0	!
! A85	A(23,36,35)	91.1366	-DE/DX = 0.0	!
! A86	A(23,36,37)	89.228	-DE/DX = 0.0	!
! A87	A(23,36,38)	91.3304	-DE/DX = 0.0	!
! A88	A(34,36,35)	89.8515	-DE/DX = 0.0	!
! A89	A(34,36,37)	87.5752	-DE/DX = 0.0	!
! A90	A(34,36,46)	88.6225	-DE/DX = 0.0	!
! A91	A(35,36,37)	177.3957	-DE/DX = 0.0	!
! A92	A(35,36,38)	92.291	-DE/DX = 0.0	!
! A93	A(35,36,46)	90.4865	-DE/DX = 0.0	!
! A94	A(37,36,38)	90.2783	-DE/DX = 0.0	!
! A95	A(37,36,46)	89.052	-DE/DX = 0.0	!
! A96	A(38,36,46)	90.7995	-DE/DX = 0.0	!
! A97	A(25,37,33)	68.7628	-DE/DX = 0.0	!
! A98	A(25,37,36)	112.9755	-DE/DX = 0.0	!
! A99	A(25,37,47)	101.1648	-DE/DX = 0.0	!
! A100	A(33,37,36)	104.2703	-DE/DX = 0.0	!
! A101	A(33,37,47)	40.3538	-DE/DX = 0.0	!
! A102	A(36,37,47)	69.7288	-DE/DX = 0.0	!
! A103	A(24,39,30)	80.5001	-DE/DX = 0.0	!
! A104	A(24,39,49)	170.642	-DE/DX = 0.0	!
! A105	A(30,39,49)	107.5579	-DE/DX = 0.0	!
! A106	A(30,43,50)	162.2726	-DE/DX = 0.0	!
! A107	A(40,44,42)	109.2239	-DE/DX = 0.0	!
! A108	A(40,44,48)	109.2502	-DE/DX = 0.0	!
! A109	A(40,44,51)	108.9089	-DE/DX = 0.0	!
! A110	A(42,44,48)	109.8712	-DE/DX = 0.0	!
! A111	A(42,44,51)	110.1312	-DE/DX = 0.0	!
! A112	A(48,44,51)	109.4342	-DE/DX = 0.0	!
! A113	A(33,45,51)	128.4861	-DE/DX = 0.0	!
! A114	A(33,45,56)	127.1511	-DE/DX = 0.0	!
! A115	A(51,45,56)	103.897	-DE/DX = 0.0	!
! A116	A(36,46,47)	94.6235	-DE/DX = 0.0	!
! A117	A(36,46,58)	118.9441	-DE/DX = 0.0	!
! A118	A(47,46,58)	31.4769	-DE/DX = 0.0	!
! A119	A(34,47,37)	30.4364	-DE/DX = 0.0	!

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! A120  A(34,47,46)            43.7356          -DE/DX =    0.0                 !
! A121  A(34,47,54)           115.5743          -DE/DX =    0.0                 !
! A122  A(37,47,46)            34.573           -DE/DX =    0.0                 !
! A123  A(37,47,54)            98.0506          -DE/DX =    0.0                 !
! A124  A(46,47,54)            71.9484          -DE/DX =    0.0                 !
! A125  A(39,49,55)           130.0852          -DE/DX =    0.0                 !
! A126  A(39,49,57)           126.101           -DE/DX =    0.0                 !
! A127  A(55,49,57)           103.7738          -DE/DX =    0.0                 !
! A128  A(43,50,52)           110.211           -DE/DX =    0.0                 !
! A129  A(43,50,53)           108.0608          -DE/DX =    0.0                 !
! A130  A(43,50,55)           109.3062          -DE/DX =    0.0                 !
! A131  A(52,50,53)           109.9693          -DE/DX =    0.0                 !
! A132  A(52,50,55)           109.5334          -DE/DX =    0.0                 !
! A133  A(53,50,55)           109.7382          -DE/DX =    0.0                 !
! A134  A(44,51,45)           123.9811          -DE/DX =    0.0                 !
! A135  A(44,51,59)           124.1185          -DE/DX =    0.0                 !
! A136  A(45,51,59)           111.5098          -DE/DX =    0.0                 !
! A137  A(47,54,56)           107.2578          -DE/DX =    0.0                 !
! A138  A(47,54,57)           110.1646          -DE/DX =    0.0                 !
! A139  A(47,54,58)           108.2612          -DE/DX =    0.0                 !
! A140  A(56,54,57)           112.6821          -DE/DX =    0.0                 !
! A141  A(56,54,58)           109.5768          -DE/DX =    0.0                 !
! A142  A(57,54,58)           108.8023          -DE/DX =    0.0                 !
! A143  A(49,55,50)           125.317           -DE/DX =    0.0                 !
! A144  A(49,55,61)           111.614           -DE/DX =    0.0                 !
! A145  A(50,55,61)           123.0529          -DE/DX =    0.0                 !
! A146  A(45,56,54)           123.105           -DE/DX =    0.0                 !
! A147  A(45,56,60)           111.6607          -DE/DX =    0.0                 !
! A148  A(54,56,60)           124.8619          -DE/DX =    0.0                 !
! A149  A(49,57,54)           124.2087          -DE/DX =    0.0                 !
! A150  A(49,57,63)           111.5784          -DE/DX =    0.0                 !
! A151  A(54,57,63)           124.2007          -DE/DX =    0.0                 !
! A152  A(46,58,54)           109.5004          -DE/DX =    0.0                 !
! A153  A(51,59,60)           106.6981          -DE/DX =    0.0                 !
! A154  A(51,59,62)           122.3971          -DE/DX =    0.0                 !
! A155  A(60,59,62)           130.9047          -DE/DX =    0.0                 !
! A156  A(56,60,59)           106.2271          -DE/DX =    0.0                 !
! A157  A(56,60,65)           122.7458          -DE/DX =    0.0                 !
! A158  A(59,60,65)           131.0233          -DE/DX =    0.0                 !
! A159  A(55,61,63)           106.8486          -DE/DX =    0.0                 !
! A160  A(55,61,64)           122.1966          -DE/DX =    0.0                 !
! A161  A(63,61,64)           130.949           -DE/DX =    0.0                 !
! A162  A(57,63,61)           106.1841          -DE/DX =    0.0                 !
! A163  A(57,63,66)           122.4775          -DE/DX =    0.0                 !
! A164  A(61,63,66)           131.321           -DE/DX =    0.0                 !
! A165  L(16,28,41,22,-2)     181.7205          -DE/DX =    0.0                 !
! A166  L(22,28,31,16,-2)     177.7891          -DE/DX =    0.0                 !
! A167  L(23,36,46,34,-2)     181.629           -DE/DX =    0.0                 !
! A168  L(34,36,38,23,-2)     177.8462          -DE/DX =    0.0                 !
! D1    D(1,4,5,2)              0.7131          -DE/DX =    0.0                 !
! D2    D(1,4,5,12)          -178.3882          -DE/DX =    0.0                 !
! D3    D(10,4,5,2)           179.1262          -DE/DX =    0.0                 !
! D4    D(10,4,5,12)            0.0249          -DE/DX =    0.0                 !
! D5    D(1,4,10,13)           -0.4103          -DE/DX =    0.0                 !
! D6    D(1,4,10,18)          178.3834          -DE/DX =    0.0                 !
! D7    D(5,4,10,13)         -178.9967          -DE/DX =    0.0                 !
! D8    D(5,4,10,18)           -0.203           -DE/DX =    0.0                 !
! D9    D(2,5,12,17)           -0.0468          -DE/DX =    0.0                 !
! D10   D(2,5,12,18)         -179.0359          -DE/DX =    0.0                 !
! D11   D(4,5,12,17)          179.1511          -DE/DX =    0.0                 !
! D12   D(4,5,12,18)            0.162           -DE/DX =    0.0                 !
! D13   D(3,7,9,6)              0.7711          -DE/DX =    0.0                 !
! D14   D(3,7,9,19)          -179.3719          -DE/DX =    0.0                 !
! D15   D(14,7,9,6)          -179.9088          -DE/DX =    0.0                 !
! D16   D(14,7,9,19)           -0.0519          -DE/DX =    0.0                 !
! D17   D(3,7,14,13)           -7.1849          -DE/DX =    0.0                 !
! D18   D(3,7,14,24)         -179.9961          -DE/DX =    0.0                 !
! D19   D(9,7,14,13)          173.4251          -DE/DX =    0.0                 !
! D20   D(9,7,14,24)            0.6138          -DE/DX =    0.0                 !
! D21   D(16,8,13,10)        -165.6684          -DE/DX =    0.0                 !
! D22   D(16,8,13,14)         -42.0737          -DE/DX =    0.0                 !
! D23   D(16,8,13,20)          74.5443          -DE/DX =    0.0                 !
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! D24   D(13,8,16,20)          -34.5438         -DE/DX =    0.0                 !
! D25   D(13,8,16,28)          -79.0063         -DE/DX =    0.0                 !
! D26   D(6,9,19,24)           179.3452         -DE/DX =    0.0                 !
! D27   D(6,9,19,27)             6.5395         -DE/DX =    0.0                 !
! D28   D(7,9,19,24)            -0.5267         -DE/DX =    0.0                 !
! D29   D(7,9,19,27)          -173.3325         -DE/DX =    0.0                 !
! D30   D(4,10,13,8)            12.5093         -DE/DX =    0.0                 !
! D31   D(4,10,13,14)         -109.2312         -DE/DX =    0.0                 !
! D32   D(4,10,13,20)          131.0651         -DE/DX =    0.0                 !
! D33   D(18,10,13,8)         -166.1343         -DE/DX =    0.0                 !
! D34   D(18,10,13,14)          72.1252         -DE/DX =    0.0                 !
! D35   D(18,10,13,20)         -47.5785         -DE/DX =    0.0                 !
! D36   D(4,10,18,12)            0.292          -DE/DX =    0.0                 !
! D37   D(4,10,18,33)         -177.4833         -DE/DX =    0.0                 !
! D38   D(13,10,18,12)         179.086          -DE/DX =    0.0                 !
! D39   D(13,10,18,33)           1.3107         -DE/DX =    0.0                 !
! D40   D(5,12,17,11)          -55.7914         -DE/DX =    0.0                 !
! D41   D(5,12,17,15)           64.9874         -DE/DX =    0.0                 !
! D42   D(5,12,17,25)         -174.0626         -DE/DX =    0.0                 !
! D43   D(18,12,17,11)         123.0572         -DE/DX =    0.0                 !
! D44   D(18,12,17,15)        -116.1641         -DE/DX =    0.0                 !
! D45   D(18,12,17,25)           4.786          -DE/DX =    0.0                 !
! D46   D(5,12,18,10)           -0.2753         -DE/DX =    0.0                 !
! D47   D(5,12,18,33)          177.38           -DE/DX =    0.0                 !
! D48   D(17,12,18,10)        -179.2378         -DE/DX =    0.0                 !
! D49   D(17,12,18,33)          -1.5825         -DE/DX =    0.0                 !
! D50   D(8,13,14,7)           -59.4355         -DE/DX =    0.0                 !
! D51   D(8,13,14,24)          112.5914         -DE/DX =    0.0                 !
! D52   D(10,13,14,7)           61.8299         -DE/DX =    0.0                 !
! D53   D(10,13,14,24)        -126.1432         -DE/DX =    0.0                 !
! D54   D(20,13,14,7)         -176.725          -DE/DX =    0.0                 !
! D55   D(20,13,14,24)          -4.698          -DE/DX =    0.0                 !
! D56   D(8,13,20,16)          -50.2408         -DE/DX =    0.0                 !
! D57   D(8,13,20,30)          -72.9615         -DE/DX =    0.0                 !
! D58   D(8,13,20,31)          -46.5975         -DE/DX =    0.0                 !
! D59   D(10,13,20,16)        -169.1048         -DE/DX =    0.0                 !
! D60   D(10,13,20,30)         168.1745         -DE/DX =    0.0                 !
! D61   D(10,13,20,31)        -165.4615         -DE/DX =    0.0                 !
! D62   D(14,13,20,16)          67.9238         -DE/DX =    0.0                 !
! D63   D(14,13,20,30)          45.2031         -DE/DX =    0.0                 !
! D64   D(14,13,20,31)          71.567          -DE/DX =    0.0                 !
! D65   D(7,14,24,19)           -0.9059         -DE/DX =    0.0                 !
! D66   D(7,14,24,39)          171.3984         -DE/DX =    0.0                 !
! D67   D(13,14,24,19)        -173.8762         -DE/DX =    0.0                 !
! D68   D(13,14,24,39)          -1.5719         -DE/DX =    0.0                 !
! D69   D(8,16,20,13)           34.6303         -DE/DX =    0.0                 !
! D70   D(8,16,20,30)          171.852          -DE/DX =    0.0                 !
! D71   D(8,16,20,31)         -140.5742         -DE/DX =    0.0                 !
! D72   D(28,16,20,13)         177.0378         -DE/DX =    0.0                 !
! D73   D(28,16,20,30)         -45.7404         -DE/DX =    0.0                 !
! D74   D(28,16,20,31)           1.8334         -DE/DX =    0.0                 !
! D75   D(8,16,28,22)         -162.6424         -DE/DX =    0.0                 !
! D76   D(8,16,28,26)          -70.3608         -DE/DX =    0.0                 !
! D77   D(8,16,28,30)          107.1807         -DE/DX =    0.0                 !
! D78   D(8,16,28,31)           19.5685         -DE/DX =    0.0                 !
! D79   D(20,16,28,22)         175.845          -DE/DX =    0.0                 !
! D80   D(20,16,28,26)         -91.8734         -DE/DX =    0.0                 !
! D81   D(20,16,28,30)          85.6681         -DE/DX =    0.0                 !
! D82   D(20,16,28,31)          -1.9441         -DE/DX =    0.0                 !
! D83   D(11,17,25,37)         -47.7828         -DE/DX =    0.0                 !
! D84   D(12,17,25,37)          71.44           -DE/DX =    0.0                 !
! D85   D(15,17,25,37)        -168.0042         -DE/DX =    0.0                 !
! D86   D(10,18,33,37)         161.0761         -DE/DX =    0.0                 !
! D87   D(10,18,33,45)         -47.9826         -DE/DX =    0.0                 !
! D88   D(12,18,33,37)         -16.103          -DE/DX =    0.0                 !
! D89   D(12,18,33,45)         134.8383         -DE/DX =    0.0                 !
! D90   D(9,19,24,14)            0.8695         -DE/DX =    0.0                 !
! D91   D(9,19,24,39)         -171.3279         -DE/DX =    0.0                 !
! D92   D(27,19,24,14)         173.7064         -DE/DX =    0.0                 !
! D93   D(27,19,24,39)           1.509          -DE/DX =    0.0                 !
! D94   D(9,19,27,21)          -31.3496         -DE/DX =    0.0                 !
! D95   D(9,19,27,29)           89.4545         -DE/DX =    0.0                 !
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! D96   D(9,19,27,32)        -150.6813         -DE/DX =    0.0                 !
! D97   D(24,19,27,21)        156.7161         -DE/DX =    0.0                 !
! D98   D(24,19,27,29)        -82.4799         -DE/DX =    0.0                 !
! D99   D(24,19,27,32)         37.3843         -DE/DX =    0.0                 !
! D100  D(13,20,30,28)         88.8249         -DE/DX =    0.0                 !
! D101  D(13,20,30,39)       -124.1751         -DE/DX =    0.0                 !
! D102  D(13,20,30,43)       -160.7058         -DE/DX =    0.0                 !
! D103  D(16,20,30,28)         48.1536         -DE/DX =    0.0                 !
! D104  D(16,20,30,39)       -164.8464         -DE/DX =    0.0                 !
! D105  D(16,20,30,43)        158.6229         -DE/DX =    0.0                 !
! D106  D(31,20,30,28)        -38.9456         -DE/DX =    0.0                 !
! D107  D(31,20,30,39)        108.0544         -DE/DX =    0.0                 !
! D108  D(31,20,30,43)         71.5237         -DE/DX =    0.0                 !
! D109  D(13,20,31,28)         -7.4465         -DE/DX =    0.0                 !
! D110  D(16,20,31,28)         -2.4071         -DE/DX =    0.0                 !
! D111  D(30,20,31,28)         52.4977         -DE/DX =    0.0                 !
! D112  D(14,24,39,30)       -101.3346         -DE/DX =    0.0                 !
! D113  D(14,24,39,49)        108.7137         -DE/DX =    0.0                 !
! D114  D(19,24,39,30)         69.1322         -DE/DX =    0.0                 !
! D115  D(19,24,39,49)        -80.8195         -DE/DX =    0.0                 !
! D116  D(17,25,37,33)        -82.9743         -DE/DX =    0.0                 !
! D117  D(17,25,37,36)         14.0609         -DE/DX =    0.0                 !
! D118  D(17,25,37,47)        -58.4876         -DE/DX =    0.0                 !
! D119  D(16,28,30,20)        -59.1408         -DE/DX =    0.0                 !
! D120  D(16,28,30,39)        -80.2483         -DE/DX =    0.0                 !
! D121  D(16,28,30,43)       -152.8685         -DE/DX =    0.0                 !
! D122  D(22,28,30,20)       -149.8885         -DE/DX =    0.0                 !
! D123  D(22,28,30,39)       -170.996          -DE/DX =    0.0                 !
! D124  D(22,28,30,43)        116.3838         -DE/DX =    0.0                 !
! D125  D(26,28,30,20)         20.7594         -DE/DX =    0.0                 !
! D126  D(26,28,30,39)         -0.3481         -DE/DX =    0.0                 !
! D127  D(26,28,30,43)        -72.9683         -DE/DX =    0.0                 !
! D128  D(31,28,30,20)         29.533          -DE/DX =    0.0                 !
! D129  D(31,28,30,39)          8.4255         -DE/DX =    0.0                 !
! D130  D(31,28,30,43)        -64.1947         -DE/DX =    0.0                 !
! D131  D(41,28,30,20)        118.7738         -DE/DX =    0.0                 !
! D132  D(41,28,30,39)         97.6663         -DE/DX =    0.0                 !
! D133  D(41,28,30,43)         25.0461         -DE/DX =    0.0                 !
! D134  D(16,28,31,20)          3.3873         -DE/DX =    0.0                 !
! D135  D(26,28,31,20)         93.8829         -DE/DX =    0.0                 !
! D136  D(30,28,31,20)        -85.7364         -DE/DX =    0.0                 !
! D137  D(41,28,31,20)       -174.9744         -DE/DX =    0.0                 !
! D138  D(20,30,39,24)         61.5784         -DE/DX =    0.0                 !
! D139  D(20,30,39,49)       -123.3205         -DE/DX =    0.0                 !
! D140  D(28,30,39,24)         93.5603         -DE/DX =    0.0                 !
! D141  D(28,30,39,49)        -91.3386         -DE/DX =    0.0                 !
! D142  D(43,30,39,24)       -157.2963         -DE/DX =    0.0                 !
! D143  D(43,30,39,49)         17.8048         -DE/DX =    0.0                 !
! D144  D(20,30,43,50)        -59.5758         -DE/DX =    0.0                 !
! D145  D(28,30,43,50)         13.5083         -DE/DX =    0.0                 !
! D146  D(39,30,43,50)        -83.7261         -DE/DX =    0.0                 !
! D147  D(18,33,37,25)         18.7797         -DE/DX =    0.0                 !
! D148  D(18,33,37,36)        -90.6875         -DE/DX =    0.0                 !
! D149  D(18,33,37,47)       -122.3171         -DE/DX =    0.0                 !
! D150  D(45,33,37,25)       -156.7889         -DE/DX =    0.0                 !
! D151  D(45,33,37,36)         93.7439         -DE/DX =    0.0                 !
! D152  D(45,33,37,47)         62.1143         -DE/DX =    0.0                 !
! D153  D(18,33,45,51)        -80.7323         -DE/DX =    0.0                 !
! D154  D(18,33,45,56)        108.3853         -DE/DX =    0.0                 !
! D155  D(37,33,45,51)         71.2055         -DE/DX =    0.0                 !
! D156  D(37,33,45,56)        -99.677          -DE/DX =    0.0                 !
! D157  D(47,34,36,23)       -175.9256         -DE/DX =    0.0                 !
! D158  D(47,34,36,35)         92.9356         -DE/DX =    0.0                 !
! D159  D(47,34,36,37)        -86.6638         -DE/DX =    0.0                 !
! D160  D(47,34,36,46)          2.4454         -DE/DX =    0.0                 !
! D161  D(36,34,47,37)         53.3512         -DE/DX =    0.0                 !
! D162  D(36,34,47,46)         -1.7363         -DE/DX =    0.0                 !
! D163  D(36,34,47,54)         -6.1161         -DE/DX =    0.0                 !
! D164  D(23,36,37,25)         23.8406         -DE/DX =    0.0                 !
! D165  D(23,36,37,33)         96.4951         -DE/DX =    0.0                 !
! D166  D(23,36,37,47)        117.7175         -DE/DX =    0.0                 !
! D167  D(34,36,37,25)        -65.3763         -DE/DX =    0.0                 !
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! D168  D(34,36,37,33)          7.2782         -DE/DX =    0.0                 !
! D169  D(34,36,37,47)         28.5006         -DE/DX =    0.0                 !
! D170  D(35,36,37,25)        -74.2281         -DE/DX =    0.0                 !
! D171  D(35,36,37,33)         -1.5735         -DE/DX =    0.0                 !
! D172  D(35,36,37,47)         19.6488         -DE/DX =    0.0                 !
! D173  D(38,36,37,25)        115.1674         -DE/DX =    0.0                 !
! D174  D(38,36,37,33)       -172.1781         -DE/DX =    0.0                 !
! D175  D(38,36,37,47)       -150.9557         -DE/DX =    0.0                 !
! D176  D(46,36,37,25)       -154.0376         -DE/DX =    0.0                 !
! D177  D(46,36,37,33)        -81.3831         -DE/DX =    0.0                 !
! D178  D(46,36,37,47)        -60.1607         -DE/DX =    0.0                 !
! D179  D(34,36,46,47)         -1.3443         -DE/DX =    0.0                 !
! D180  D(34,36,46,58)         19.7418         -DE/DX =    0.0                 !
! D181  D(35,36,46,47)        -91.184          -DE/DX =    0.0                 !
! D182  D(35,36,46,58)        -70.0979         -DE/DX =    0.0                 !
! D183  D(37,36,46,47)         86.2527         -DE/DX =    0.0                 !
! D184  D(37,36,46,58)        107.3388         -DE/DX =    0.0                 !
! D185  D(38,36,46,47)        176.5178         -DE/DX =    0.0                 !
! D186  D(38,36,46,58)       -162.396          -DE/DX =    0.0                 !
! D187  D(25,37,47,34)         71.7159         -DE/DX =    0.0                 !
! D188  D(25,37,47,46)        159.2026         -DE/DX =    0.0                 !
! D189  D(25,37,47,54)       -159.9755         -DE/DX =    0.0                 !
! D190  D(33,37,47,34)        108.3463         -DE/DX =    0.0                 !
! D191  D(33,37,47,46)       -164.167          -DE/DX =    0.0                 !
! D192  D(33,37,47,54)       -123.3452         -DE/DX =    0.0                 !
! D193  D(36,37,47,34)        -38.8474         -DE/DX =    0.0                 !
! D194  D(36,37,47,46)         48.6393         -DE/DX =    0.0                 !
! D195  D(36,37,47,54)         89.4612         -DE/DX =    0.0                 !
! D196  D(24,39,49,55)        134.5578         -DE/DX =    0.0                 !
! D197  D(24,39,49,57)        -48.1246         -DE/DX =    0.0                 !
! D198  D(30,39,49,55)        -14.2443         -DE/DX =    0.0                 !
! D199  D(30,39,49,57)        163.0733         -DE/DX =    0.0                 !
! D200  D(30,43,50,52)       -164.3852         -DE/DX =    0.0                 !
! D201  D(30,43,50,53)        -44.1975         -DE/DX =    0.0                 !
! D202  D(30,43,50,55)         75.1843         -DE/DX =    0.0                 !
! D203  D(40,44,51,45)         33.6283         -DE/DX =    0.0                 !
! D204  D(40,44,51,59)       -154.1612         -DE/DX =    0.0                 !
! D205  D(42,44,51,45)        -86.1244         -DE/DX =    0.0                 !
! D206  D(42,44,51,59)         86.0862         -DE/DX =    0.0                 !
! D207  D(48,44,51,45)        152.9963         -DE/DX =    0.0                 !
! D208  D(48,44,51,59)        -34.7931         -DE/DX =    0.0                 !
! D209  D(33,45,51,44)          1.3599         -DE/DX =    0.0                 !
! D210  D(33,45,51,59)       -171.7131         -DE/DX =    0.0                 !
! D211  D(56,45,51,44)        173.884          -DE/DX =    0.0                 !
! D212  D(56,45,51,59)          0.811          -DE/DX =    0.0                 !
! D213  D(33,45,56,54)         -1.486          -DE/DX =    0.0                 !
! D214  D(33,45,56,60)        171.8117         -DE/DX =    0.0                 !
! D215  D(51,45,56,54)       -174.1449         -DE/DX =    0.0                 !
! D216  D(51,45,56,60)         -0.8472         -DE/DX =    0.0                 !
! D217  D(36,46,47,34)          1.2957         -DE/DX =    0.0                 !
! D218  D(36,46,47,37)        -45.7634         -DE/DX =    0.0                 !
! D219  D(36,46,47,54)        177.1408         -DE/DX =    0.0                 !
! D220  D(58,46,47,34)       -141.6229         -DE/DX =    0.0                 !
! D221  D(58,46,47,37)        171.318          -DE/DX =    0.0                 !
! D222  D(58,46,47,54)         34.2223         -DE/DX =    0.0                 !
! D223  D(36,46,58,54)        -77.8018         -DE/DX =    0.0                 !
! D224  D(47,46,58,54)        -34.4268         -DE/DX =    0.0                 !
! D225  D(34,47,54,56)         72.4501         -DE/DX =    0.0                 !
! D226  D(34,47,54,57)       -164.5768         -DE/DX =    0.0                 !
! D227  D(34,47,54,58)        -45.7128         -DE/DX =    0.0                 !
! D228  D(37,47,54,56)         46.3027         -DE/DX =    0.0                 !
! D229  D(37,47,54,57)        169.2759         -DE/DX =    0.0                 !
! D230  D(37,47,54,58)        -71.8602         -DE/DX =    0.0                 !
! D231  D(46,47,54,56)         69.2669         -DE/DX =    0.0                 !
! D232  D(46,47,54,57)       -167.76           -DE/DX =    0.0                 !
! D233  D(46,47,54,58)        -48.896          -DE/DX =    0.0                 !
! D234  D(39,49,55,50)         -1.1319         -DE/DX =    0.0                 !
! D235  D(39,49,55,61)        177.4415         -DE/DX =    0.0                 !
! D236  D(57,49,55,50)       -178.9006         -DE/DX =    0.0                 !
! D237  D(57,49,55,61)         -0.3273         -DE/DX =    0.0                 !
! D238  D(39,49,57,54)          1.2218         -DE/DX =    0.0                 !
! D239  D(39,49,57,63)       -177.5527         -DE/DX =    0.0                 !
```

```
 ! D240  D(55,49,57,54)        179.109          -DE/DX =    0.0                 !
 ! D241  D(55,49,57,63)          0.3345         -DE/DX =    0.0                 !
 ! D242  D(43,50,55,49)          0.9644         -DE/DX =    0.0                 !
 ! D243  D(43,50,55,61)       -177.4532         -DE/DX =    0.0                 !
 ! D244  D(52,50,55,49)       -119.8796         -DE/DX =    0.0                 !
 ! D245  D(52,50,55,61)         61.7029         -DE/DX =    0.0                 !
 ! D246  D(53,50,55,49)        119.3042         -DE/DX =    0.0                 !
 ! D247  D(53,50,55,61)        -59.1134         -DE/DX =    0.0                 !
 ! D248  D(44,51,59,60)       -173.551          -DE/DX =    0.0                 !
 ! D249  D(44,51,59,62)          6.3516         -DE/DX =    0.0                 !
 ! D250  D(45,51,59,60)         -0.4892         -DE/DX =    0.0                 !
 ! D251  D(45,51,59,62)        179.4133         -DE/DX =    0.0                 !
 ! D252  D(47,54,56,45)         -4.8323         -DE/DX =    0.0                 !
 ! D253  D(47,54,56,60)       -177.2359         -DE/DX =    0.0                 !
 ! D254  D(57,54,56,45)       -126.2359         -DE/DX =    0.0                 !
 ! D255  D(57,54,56,60)         61.3604         -DE/DX =    0.0                 !
 ! D256  D(58,54,56,45)        112.4731         -DE/DX =    0.0                 !
 ! D257  D(58,54,56,60)        -59.9306         -DE/DX =    0.0                 !
 ! D258  D(47,54,57,49)        -47.2296         -DE/DX =    0.0                 !
 ! D259  D(47,54,57,63)        131.3925         -DE/DX =    0.0                 !
 ! D260  D(56,54,57,49)         72.5071         -DE/DX =    0.0                 !
 ! D261  D(56,54,57,63)       -108.8708         -DE/DX =    0.0                 !
 ! D262  D(58,54,57,49)       -165.7622         -DE/DX =    0.0                 !
 ! D263  D(58,54,57,63)         12.8599         -DE/DX =    0.0                 !
 ! D264  D(47,54,58,46)         73.728          -DE/DX =    0.0                 !
 ! D265  D(56,54,58,46)        -42.9463         -DE/DX =    0.0                 !
 ! D266  D(57,54,58,46)       -166.549          -DE/DX =    0.0                 !
 ! D267  D(49,55,61,63)          0.2051         -DE/DX =    0.0                 !
 ! D268  D(49,55,61,64)       -179.006          -DE/DX =    0.0                 !
 ! D269  D(50,55,61,63)        178.8163         -DE/DX =    0.0                 !
 ! D270  D(50,55,61,64)         -0.3949         -DE/DX =    0.0                 !
 ! D271  D(45,56,60,59)          0.5763         -DE/DX =    0.0                 !
 ! D272  D(45,56,60,65)        179.9381         -DE/DX =    0.0                 !
 ! D273  D(54,56,60,59)        173.7334         -DE/DX =    0.0                 !
 ! D274  D(54,56,60,65)         -6.9049         -DE/DX =    0.0                 !
 ! D275  D(49,57,63,61)         -0.2209         -DE/DX =    0.0                 !
 ! D276  D(49,57,63,66)        178.4192         -DE/DX =    0.0                 !
 ! D277  D(54,57,63,61)       -178.9955         -DE/DX =    0.0                 !
 ! D278  D(54,57,63,66)         -0.3554         -DE/DX =    0.0                 !
 ! D279  D(51,59,60,56)         -0.0518         -DE/DX =    0.0                 !
 ! D280  D(51,59,60,65)       -179.3402         -DE/DX =    0.0                 !
 ! D281  D(62,59,60,56)       -179.9429         -DE/DX =    0.0                 !
 ! D282  D(62,59,60,65)          0.7687         -DE/DX =    0.0                 !
 ! D283  D(55,61,63,57)          0.0103         -DE/DX =    0.0                 !
 ! D284  D(55,61,63,66)       -178.4621         -DE/DX =    0.0                 !
 ! D285  D(64,61,63,57)        179.1265         -DE/DX =    0.0                 !
 ! D286  D(64,61,63,66)          0.6541         -DE/DX =    0.0                 !

--------------------------------------------------------------------------------
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Z-Matrix orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          1             0       -0.371412   -0.867572   -4.979902
    2          1             0        1.527993   -2.887600   -5.105490
    3          1             0        1.033652    1.949277   -4.316098
    4          6             0        0.338828   -1.222285   -4.248725
    5          6             0        1.264109   -2.212175   -4.306607
    6          1             0        1.900314    4.328728   -3.192239
    7          6             0        0.937785    2.334264   -3.313114
    8          1             0       -1.245257    0.542338   -3.177448
    9          6             0        1.366272    3.496310   -2.760917
   10          7             0        0.418455   -0.692422   -2.967853
   11          1             0        2.570647   -4.237130   -2.907438
   12          7             0        1.880230   -2.259774   -3.064793
   13          6             0       -0.424547    0.388173   -2.474444
   14          7             0        0.305945    1.632618   -2.296876
   15          1             0        3.816747   -3.028064   -3.345378
   16          9             0       -2.409466    2.903751   -2.609947
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17	6	0	2.932453	-3.221957	-2.730438
18	6	0	1.369971	-1.329978	-2.217757
19	7	0	0.982958	3.469724	-1.427488
20	1	0	-0.848608	0.123322	-1.507925
21	1	0	2.008149	5.179265	-0.790508
22	9	0	-4.046840	4.417204	-1.936429
23	9	0	1.940842	-5.020872	-0.228111
24	6	0	0.314190	2.328278	-1.124796
25	1	0	3.179970	-3.130874	-1.674968
26	9	0	-4.563065	2.145056	-2.169715
27	6	0	1.129475	4.594093	-0.508843
28	15	0	-3.466822	3.019799	-1.349183
29	1	0	0.236074	5.224061	-0.542244
30	9	0	-2.303220	3.859010	-0.486213
31	9	0	-2.812465	1.608936	-0.722755
32	1	0	1.263011	4.210870	0.504523
33	29	0	1.781076	-0.981477	-0.373494
34	9	0	0.824162	-3.125436	0.529947
35	9	0	0.715792	-5.109566	1.751265
36	15	0	1.935658	-4.196404	1.186028
37	9	0	3.140582	-3.203082	0.585227
38	9	0	3.055686	-5.189311	1.812626
39	29	0	-0.622607	1.890547	0.495623
40	1	0	4.417702	0.275145	0.087653
41	9	0	-4.460469	3.108285	-0.051398
42	1	0	5.102630	-0.971522	1.160226
43	1	0	-2.537319	3.620864	1.768107
44	6	0	4.642912	0.020366	1.124721
45	6	0	2.196656	-0.340960	1.390434
46	9	0	1.923718	-3.298850	2.570026
47	1	0	-0.237838	-1.013314	1.391897
48	1	0	5.330118	0.763266	1.537170
49	6	0	-1.275713	1.382781	2.229686
50	6	0	-2.854203	3.261329	2.744842
51	7	0	3.402673	0.026823	1.893238
52	1	0	-2.608444	3.997189	3.516541
53	1	0	-3.934088	3.101055	2.712668
54	6	0	-0.014103	-0.763696	2.426757
55	7	0	-2.175128	1.997494	3.039319
56	7	0	1.368939	-0.315455	2.473242
57	7	0	-0.947337	0.242862	2.913437
58	1	0	-0.126074	-1.667420	3.028458
59	6	0	3.334950	0.258605	3.259890
60	6	0	2.048219	0.041568	3.628589
61	6	0	-2.410232	1.263068	4.192356
62	1	0	4.196305	0.551547	3.839951
63	6	0	-1.635416	0.152612	4.115931
64	1	0	-3.108852	1.587247	4.948027
65	1	0	1.564630	0.118209	4.589593
66	1	0	-1.528113	-0.688807	4.783324

Rotational constants (GHZ): 0.1009773 0.0502822 0.0429480

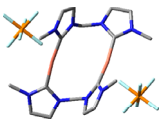

Fig. S2 Optimized structure of $[Cu_2(\mu\text{-Me-mbim})_2](PF_6)_2$ in the singlet state. Selected bond distances (Å) and angles (deg): Cu(33)–C(18), 1.921; Cu(33)–C(45), 1.922; Cu(39)–C(24), 1.922; Cu(39)–C(49), 1.921; Cu(33)···Cu(39), 3.844; Cu(33)···F(34), 2.516; Cu(39)···F(31), 2.522; Cu(33)···C(24), 3.697; Cu(39)···C(45), 3.705; C(18)–Cu(33)–C(45), 171.0; C(24)–Cu(39)–C(49), 170.6.

(iii) Input file for the singlet transition energy calculation of $[Cu_2(\mu\text{-Me-mbim})_2](PF_6)_2$.

```
%Nproc=4
%Mem=1024MB
%CHK=C:¥G03W¥data¥singlet_opt_Cu2PF62Membim2_pcm_TD_S.chk
#P B3LYP GEN TD=(ADD=10,SINGLETS,NSTATE=20) SCF=(TIGHT,VSHIFT=500,MAXCYC=256)
   SCRF=(PCM,SOLVENT=CH3OH) NOSYMM POP=FULL GUESS=CHECKPOINT

The calculation of the singlet transition energies of Cu2PF62Membim2

0 1
 H
 H                  1             B1
 H                  1             B2    2             A1
 C                  1             B3    2             A2    3             D1
 C                  4             B4    1             A3    2             D2
 H                  4             B5    1             A4    5             D3
 C                  4             B6    1             A5    5             D4
 H                  4             B7    1             A6    5             D5
 C                  7             B8    4             A7    1             D6
 N                  4             B9    1             A8    5             D7
 H                  5            B10    4             A9    1             D8
 N                  5            B11    4            A10    1             D9
 C                 10            B12    4            A11    1            D10
 N                  7            B13    4            A12    1            D11
 H                 12            B14    5            A13    4            D12
 F                 14            B15    7            A14    4            D13
 C                 12            B16    5            A15    4            D14
 C                 12            B17    5            A16    4            D15
 N                  9            B18    7            A17    4            D16
 H                 13            B19   10            A18    4            D17
 H                 19            B20    9            A19    7            D18
 F                 19            B21    9            A20    7            D19
 F                 17            B22   12            A21    5            D20
 C                 19            B23    9            A22    7            D21
 H                 17            B24   12            A23    5            D22
 F                 13            B25   10            A24    4            D23
 C                 19            B26    9            A25    7            D24
 P                 24            B27   19            A26    9            D25
 H                 27            B28   19            A27    9            D26
 F                 28            B29   24            A28   19            D27
 F                 28            B30   24            A29   19            D28
 H                 27            B31   19            A30    9            D29
 Cu                18            B32   12            A31    5            D30
 F                 33            B33   18            A32   12            D31
 F                 33            B34   18            A33   12            D32
 P                 33            B35   18            A34   12            D33
 F                 36            B36   33            A35   18            D34
 F                 36            B37   33            A36   18            D35
 Cu                24            B38   19            A37    9            D36
 H                 33            B39   18            A38   12            D37
 F                 28            B40   24            A39   19            D38
 H                 33            B41   18            A40   12            D39
 H                 39            B42   24            A41   19            D40
 C                 33            B43   18            A42   12            D41
 C                 33            B44   18            A43   12            D42
 F                 36            B45   33            A44   18            D43
 H                 45            B46   33            A45   18            D44
 H                 44            B47   33            A46   18            D45
 C                 39            B48   24            A47   19            D46
 C                 49            B49   39            A48   24            D47
 N                 45            B50   33            A49   18            D48
 H                 50            B51   49            A50   39            D49
 H                 50            B52   49            A51   39            D50
 C                 45            B53   33            A52   18            D51
 N                 49            B54   39            A53   24            D52
 N                 45            B55   33            A54   18            D53
 N                 49            B56   39            A55   24            D54
 H                 54            B57   45            A56   33            D55
 C                 51            B58   45            A57   33            D56
 C                 59            B59   51            A58   45            D57
 C                 55            B60   49            A59   39            D58
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H                59              B61   51              A60   45              D59
C                61              B62   55              A61   49              D60
H                61              B63   55              A62   49              D61
H                60              B64   59              A63   51              D62
H                63              B65   61              A64   55              D63

  B1            2.77561289
  B2            3.21706089
  B3            1.07929769
  B4            1.35623693
  B5            5.86243594
  B6            3.72601153
  B7            2.60208711
  B8            1.35605068
  B9            1.38842721
  B10           2.78660293
  B11           1.38707336
  B12           1.45663619
  B13           1.38717959
  B14           2.10216473
  B15           3.01450649
  B16           1.46450091
  B17           1.35733427
  B18           1.38768540
  B19           1.08817925
  B20           2.09267562
  B21           5.14350164
  B22           3.23744126
  B23           1.35711904
  B24           1.08792288
  B25           4.50630992
  B26           1.45930858
  B27           3.85027355
  B28           1.09368164
  B29           1.67420464
  B30           1.67664246
  B31           1.09160589
  B32           1.92139718
  B33           2.51564024
  B34           4.76345956
  B35           3.57655650
  B36           1.67316761
  B37           1.62263789
  B38           1.92222705
  B39           2.95695041
  B40           1.63689043
  B41           3.65856827
  B42           2.87738289
  B43           3.38207736
  B44           1.92208467
  B45           1.64960481
  B46           2.52563308
  B47           1.09282574
  B48           1.92128756
  B49           2.50718256
  B50           1.35740773
  B51           1.09426058
  B52           1.09218799
  B53           2.47792817
  B54           1.35732403
  B55           1.36317297
  B56           1.36921982
  B57           1.09146658
  B58           1.38782127
  B59           1.35599451
  B60           1.38713724
  B61           1.07898887
  B62           1.35620515
  B63           1.07898155
  B64           1.07854547
  B65           1.07931193
  A1          110.34650284
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A2	48.78742078
A3	131.29366153
A4	89.20755205
A5	87.83309399
A6	69.84391242
A7	166.16910521
A8	122.49961245
A9	145.97924813
A10	106.85083364
A11	124.22260790
A12	68.15691252
A13	107.59169625
A14	96.94544779
A15	123.09891293
A16	111.60481082
A17	106.71362465
A18	110.23280481
A19	98.13534098
A20	99.87565250
A21	108.75170745
A22	111.50318853
A23	109.26608002
A24	147.52512169
A25	124.22190475
A26	108.65454021
A27	110.03300194
A28	51.49907668
A29	56.20903298
A30	109.03719437
A31	130.00135775
A32	96.24292677
A33	102.89184940
A34	105.35170872
A35	48.76891941
A36	138.43928385
A37	128.29498536
A38	114.68044714
A39	124.02934571
A40	126.66459650
A41	124.06693591
A42	131.29838124
A43	170.95986859
A44	82.90191484
A45	72.74698022
A46	154.24569107
A47	170.64201580
A48	101.62154557
A49	128.48612328
A50	120.48860437
A51	120.43035683
A52	97.70406015
A53	130.08524602
A54	127.15111821
A55	126.10104119
A56	117.60276063
A57	111.50979399
A58	106.69813909
A59	111.61401737
A60	122.39711591
A61	106.84857851
A62	122.19658427
A63	131.02327063
A64	131.32103301
D1	-58.50247489
D2	-0.27829014
D3	132.54205683
D4	139.71979033
D5	-173.28271729
D6	-179.66654326
D7	-178.19299103
D8	-144.10896519
D9	-178.38821533

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   D11          112.08444677
   D12         -153.06240440
   D13         -107.46987608
   D14          179.15105263
   D15            0.16196620
   D16          -63.92017188
   D17          131.06508453
   D18          171.66147982
   D19          -75.21698701
   D20         -120.23582849
   D21           -0.52674495
   D22         -174.06255574
   D23           44.62794252
   D24         -173.33252324
   D25          -96.15859990
   D26           89.45450523
   D27          -52.63443191
   D28         -170.51995641
   D29         -150.68130756
   D30          177.37998922
   D31          -67.89125372
   D32          -59.88696632
   D33          -44.14518344
   D34           97.25542429
   D35          109.09312366
   D36         -171.32790588
   D37           71.99269972
   D38         -108.68110316
   D39           41.29453546
   D40           49.01887393
   D41           62.80905505
   D42          134.83834340
   D43         -167.75577117
   D44          105.03992880
   D45           94.51368023
   D46          -80.81945526
   D47          134.00705125
   D48          -80.73225299
   D49         -109.38993011
   D50          106.95304998
   D51          107.64796936
   D52          134.55784934
   D53          108.38526949
   D54          -48.12457987
   D55           99.55022926
   D56         -171.71311369
   D57           -0.48923967
   D58          177.44145899
   D59          179.41328355
   D60            0.20512091
   D61         -179.00602019
   D62         -179.34022457
   D63         -178.46210324

Cu 0
6-311G
 P 1 1.5
 0.083141     1.000000000
 P 1 1.5
 0.018137     1.000000000
****
P 0
6-31+G*
****
F 0
6-31+G*
****
N 0
6-31G*
****
C 0
```

```
6-31G*
****
H 0
6-31G
****
```

(iv) Results for the singlet transition energy calculation of $[Cu_2(\mu\text{-Me-mbim})_2](PF_6)_2$.

```
Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
Excited State   1:   Singlet-?Sym    3.8688 eV  320.47 nm  f=0.0214
    191 ->195        -0.14377
    192 ->193         0.67209
This state for optimization and/or second-order correction.
Total Energy, E(RPA) =  -6300.55602799
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited state symmetry could not be determined.
Excited State   2:   Singlet-?Sym    4.1148 eV  301.31 nm  f=0.0355
    191 ->193         0.58926
    192 ->195        -0.32216

Excited state symmetry could not be determined.
Excited State   3:   Singlet-?Sym    4.3043 eV  288.05 nm  f=0.0989
    188 ->193         0.12419
    191 ->196        -0.13670
    192 ->194         0.63934

Excited state symmetry could not be determined.
Excited State   4:   Singlet-?Sym    4.4333 eV  279.66 nm  f=0.0172
    187 ->193         0.12313
    189 ->195         0.17399
    190 ->193         0.62849

Excited state symmetry could not be determined.
Excited State   5:   Singlet-?Sym    4.4585 eV  278.08 nm  f=0.0778
    188 ->193        -0.13305
    189 ->193         0.62487
    190 ->195         0.14799

Excited state symmetry could not be determined.
Excited State   6:   Singlet-?Sym    4.4947 eV  275.85 nm  f=0.0068
    184 ->193        -0.29992
    188 ->195         0.10300
    191 ->193         0.16922
    191 ->194        -0.34854
    192 ->195         0.40747
    192 ->196         0.15827
    192 ->198         0.11034

Excited state symmetry could not be determined.
Excited State   7:   Singlet-?Sym    4.5565 eV  272.10 nm  f=0.0075
    183 ->193        -0.15597
    191 ->193         0.29672
    191 ->194         0.38659
    192 ->195         0.33351
    192 ->196        -0.27011

Excited state symmetry could not be determined.
Excited State   8:   Singlet-?Sym    4.6060 eV  269.18 nm  f=0.0231
    184 ->195        -0.23435
    186 ->193         0.57166
    188 ->193         0.24027

Excited state symmetry could not be determined.
Excited State   9:   Singlet-?Sym    4.6416 eV  267.12 nm  f=0.0169
    183 ->195        -0.23134
    185 ->193         0.58302
    187 ->195         0.11651
    188 ->193        -0.16833

Excited state symmetry could not be determined.
Excited State  10:   Singlet-?Sym    4.6552 eV  266.33 nm  f=0.0105
    183 ->193         0.40142
    184 ->193         0.30568
    185 ->195        -0.19962
    186 ->195        -0.15632
```

```
    187 ->193        -0.29384
    192 ->195         0.21225

Excited state symmetry could not be determined.
Excited State  11:   Singlet-?Sym    4.6947 eV  264.09 nm  f=0.0001
    183 ->193        -0.32808
    184 ->193         0.43527
    185 ->195         0.15110
    186 ->195        -0.18153
    188 ->195        -0.12446
    190 ->194        -0.11948
    191 ->194        -0.15786
    192 ->195         0.16942
    192 ->196         0.12035

Excited state symmetry could not be determined.
Excited State  12:   Singlet-?Sym    4.7617 eV  260.38 nm  f=0.0128
    187 ->195        -0.12061
    188 ->193         0.32980
    191 ->195        -0.53502
    191 ->196         0.10191
    192 ->193        -0.15139

Excited state symmetry could not be determined.
Excited State  13:   Singlet-?Sym    4.7837 eV  259.18 nm  f=0.0123
    181 ->193         0.17813
    182 ->195         0.12038
    183 ->193         0.27688
    187 ->193         0.48838
    188 ->195        -0.16142
    190 ->193        -0.12824
    192 ->195         0.11122
    192 ->196         0.16219

Excited state symmetry could not be determined.
Excited State  14:   Singlet-?Sym    4.8386 eV  256.24 nm  f=0.1034
    182 ->193         0.16225
    185 ->193        -0.18340
    186 ->193         0.24062
    187 ->195         0.10618
    188 ->193        -0.38462
    189 ->193        -0.12794
    191 ->195        -0.37196

Excited state symmetry could not be determined.
Excited State  15:   Singlet-?Sym    4.8762 eV  254.26 nm  f=0.0107
    189 ->196         0.11179
    190 ->194         0.50872
    191 ->194         0.12100
    192 ->196         0.37530

Excited state symmetry could not be determined.
Excited State  16:   Singlet-?Sym    4.9354 eV  251.21 nm  f=0.0086
    184 ->194         0.14201
    189 ->195         0.19946
    190 ->194         0.31624
    191 ->194        -0.31900
    192 ->196        -0.36008
    192 ->198        -0.15037

Excited state symmetry could not be determined.
Excited State  17:   Singlet-?Sym    4.9386 eV  251.05 nm  f=0.1546
    180 ->194         0.11870
    186 ->194        -0.17036
    189 ->194         0.56360
    190 ->195         0.16014
    191 ->196        -0.17448

Excited state symmetry could not be determined.
Excited State  18:   Singlet-?Sym    5.0140 eV  247.28 nm  f=0.0175
    184 ->196        -0.15818
    186 ->194         0.40909
```

```
    188 ->194         0.37223
    189 ->194         0.11510
    190 ->195         0.18116
    191 ->196         0.20590
    192 ->194         0.11295

Excited state symmetry could not be determined.
Excited State  19:   Singlet-?Sym    5.0528 eV  245.38 nm  f=0.0015
    183 ->196         0.14987
    185 ->194        -0.54680
    186 ->194        -0.11210
    187 ->196        -0.10015
    188 ->194         0.22376
    190 ->195        -0.17103

Excited state symmetry could not be determined.
Excited State  20:   Singlet-?Sym    5.0723 eV  244.43 nm  f=0.0033
    183 ->194         0.46508
    185 ->195        -0.11556
    185 ->196        -0.16616
    187 ->194        -0.39040
```

(v) Input file for the triplet excitation energy calculation based on the crystal structure of $[Cu_2(\mu\text{-Me-mbim})_2](PF_6)_2$.

```
%mem=1024MB
%chk=crystal_Cu2PF62Membim2_TD_T.chk
#P  B3LYP  GEN  TD=(TRIPLETS,NSTATE=10)  SCF=(TIGHT,VSHIFT=500,MAXCYC=256)  NOSYMM
POP=FULL

triplet excitation energy calculation using crystal structure of Cu2PF62Membim2

0 1
 H
 H                    1             B1
 H                    1             B2     2             A1
 C                    1             B3     2             A2     3             D1
 C                    4             B4     1             A3     2             D2
 H                    4             B5     1             A4     5             D3
 C                    4             B6     1             A5     5             D4
 H                    7             B7     4             A6     1             D5
 C                    7             B8     4             A7     1             D6
 N                    4             B9     1             A8     5             D7
 H                    5            B10     4             A9     1             D8
 N                    5            B11     4            A10     1             D9
 C                   10            B12     4            A11     1            D10
 N                    7            B13     4            A12     1            D11
 H                   12            B14     5            A13     4            D12
 F                   13            B15    10            A14     4            D13
 C                   12            B16     5            A15     4            D14
 C                   10            B17     4            A16     1            D15
 N                    9            B18     7            A17     4            D16
 H                   13            B19    10            A18     4            D17
 H                   19            B20     9            A19     7            D18
 F                   13            B21    10            A20     4            D19
 F                   12            B22     5            A21     4            D20
 C                   19            B23     9            A22     7            D21
 H                   17            B24    12            A23     5            D22
 F                   13            B25    10            A24     4            D23
 C                   19            B26     9            A25     7            D24
 P                   13            B27    10            A26     4            D25
 H                   27            B28    19            A27     9            D26
 F                   28            B29    13            A28    10            D27
 F                   28            B30    13            A29    10            D28
 H                   27            B31    19            A30     9            D29
 Cu                  18            B32    10            A31     4            D30
 F                   33            B33    18            A32    10            D31
 F                   18            B34    10            A33     4            D32
 P                   33            B35    18            A34    10            D33
 F                   36            B36    33            A35    18            D34
 F                   36            B37    33            A36    18            D35
 Cu                  24            B38    19            A37     9            D36
 H                   33            B39    18            A38    10            D37
 F                   28            B40    13            A39    10            D38
 H                   33            B41    18            A40    10            D39
 H                   39            B42    24            A41    19            D40
 C                   33            B43    18            A42    10            D41
 C                   33            B44    18            A43    10            D42
 F                   36            B45    33            A44    18            D43
 H                   45            B46    33            A45    18            D44
 H                   44            B47    33            A46    18            D45
 C                   39            B48    24            A47    19            D46
 C                   49            B49    39            A48    24            D47
 N                   45            B50    33            A49    18            D48
 H                   50            B51    49            A50    39            D49
 H                   50            B52    49            A51    39            D50
 C                   45            B53    33            A52    18            D51
 N                   49            B54    39            A53    24            D52
 N                   54            B55    45            A54    33            D53
 N                   49            B56    39            A55    24            D54
 H                   54            B57    45            A56    33            D55
 C                   51            B58    45            A57    33            D56
 C                   59            B59    51            A58    45            D57
```

C	55	B60	49	A59	39	D58
H	59	B61	51	A60	45	D59
C	61	B62	55	A61	49	D60
H	61	B63	55	A62	49	D61
H	60	B64	59	A63	51	D62
H	63	B65	61	A64	55	D63

B1	2.38485966
B2	3.39476032
B3	0.92969291
B4	1.28329406
B5	5.55346488
B6	3.75396767
B7	2.62424204
B8	1.31797135
B9	1.37351451
B10	2.60352922
B11	1.39221914
B12	1.50118502
B13	1.35799660
B14	1.98881467
B15	3.38729866
B16	1.45155860
B17	1.34935097
B18	1.32086647
B19	0.96924314
B20	2.04107074
B21	5.37276648
B22	3.61490123
B23	1.35594449
B24	0.96031857
B25	5.04169921
B26	1.51105880
B27	4.24829912
B28	0.95931498
B29	1.57530898
B30	1.59567445
B31	0.95869365
B32	1.92099124
B33	3.56638888
B34	5.48455814
B35	4.34049299
B36	1.57530651
B37	1.59195872
B38	1.91587251
B39	3.15872667
B40	1.59637465
B41	3.71497645
B42	2.92036529
B43	3.50081464
B44	1.91586586
B45	1.59595638
B46	2.49471352
B47	0.96076818
B48	1.92099013
B49	2.49579190
B50	1.35594665
B51	0.95936752
B52	0.96077436
B53	2.42238620
B54	1.35960964
B55	1.38137762
B56	1.34935488
B57	0.97023403
B58	1.32086511
B59	1.31796784
B60	1.39222051
B61	0.92646727
B62	1.28329230
B63	0.93073032
B64	0.92770021
B65	0.92968523

A1	126.74685177
A2	54.11033311
A3	125.55134028
A4	88.74006885
A5	85.02698416
A6	44.99046166
A7	144.65700205
A8	125.44067895
A9	152.76983192
A10	105.93916640
A11	126.02439210
A12	64.08399287
A13	119.44466294
A14	141.21999685
A15	123.35580527
A16	110.89937913
A17	106.57677361
A18	109.00086657
A19	98.19507109
A20	151.65753852
A21	99.42326528
A22	114.32384507
A23	109.39877777
A24	126.27800758
A25	121.75339923
A26	140.31722464
A27	109.39252673
A28	62.43455173
A29	50.76429180
A30	109.46968118
A31	132.05465294
A32	76.69734631
A33	99.54362982
A34	79.18684651
A35	37.33571479
A36	128.80841610
A37	132.20861578
A38	123.03017942
A39	127.03643246
A40	122.64844730
A41	108.82126950
A42	132.61939019
A43	170.10824927
A44	90.56314495
A45	76.31778252
A46	155.09266458
A47	170.10780159
A48	96.96821462
A49	132.20907788
A50	107.08008372
A51	131.59242815
A52	98.46389340
A53	125.33800264
A54	28.95323871
A55	132.05399583
A56	130.95896728
A57	114.32416853
A58	106.57678076
A59	111.47594336
A60	126.94469742
A61	105.93947659
A62	127.01240603
A63	125.68584618
A64	125.55193870
D1	-62.79366297
D2	0.94127067
D3	128.36198891
D4	139.05756221
D5	75.94155279
D6	-147.91666446
D7	179.93189600
D8	-161.87521868

```
   D9            177.66346787
   D10            -4.84135955
   D11           127.77550621
   D12          -147.53155273
   D13            75.57275760
   D14          -179.01664646
   D15          -176.71463125
   D16           -67.73915462
   D17           137.66293091
   D18           164.02696429
   D19            94.63487096
   D20            93.74887762
   D21            -3.05792585
   D22          -149.66472126
   D23            95.47746394
   D24           176.77884326
   D25           108.06874355
   D26            90.42386964
   D27           139.51707605
   D28            26.84896462
   D29          -149.46241289
   D30           175.83603213
   D31            86.82153317
   D32           -95.06142388
   D33           107.56092201
   D34           106.28810402
   D35           101.36825974
   D36          -168.49407043
   D37          -112.78328093
   D38            75.49963401
   D39          -142.27459930
   D40            65.95176058
   D41          -128.23312671
   D42           161.38804710
   D43          -167.36229532
   D44           -97.62107674
   D45           131.60195730
   D46            73.70858353
   D47           -19.38259363
   D48            73.70574161
   D49           -78.60106125
   D50           143.67947366
   D51          -102.52645333
   D52           -20.49365108
   D53           167.62825842
   D54           161.38598719
   D55           119.96829838
   D56          -168.49347858
   D57            -3.05833087
   D58          -177.37333584
   D59           176.33992479
   D60             0.68305127
   D61          -179.20379612
   D62          -177.20438445
   D63           177.66317869

Cu 0
6-311G
 P 1 1.5
 0.083141     1.000000000
 P 1 1.5
 0.018137     1.000000000
****
P 0
6-31+G*
****
F 0
6-31+G*
****
N 0
6-31G*
****
```

```
C 0
6-31G*
****
H 0
6-31G
****
```

(iv) Results for the triplet excitation energy calculation based on the crystal structure of $[Cu_2(\mu\text{-Me-mbim})_2](PF_6)_2$.

```
 Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:   Triplet-?Sym    3.2174 eV  385.36 nm  f=0.0000
     192 ->193         0.70949
 This state for optimization and/or second-order correction.
 Total Energy, E(RPA) =  -6300.00532595
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited state symmetry could not be determined.
 Excited State   2:   Triplet-?Sym    3.7663 eV  329.19 nm  f=0.0000
     192 ->194         0.69406

 Excited state symmetry could not be determined.
 Excited State   3:   Triplet-?Sym    3.9627 eV  312.88 nm  f=0.0000
     189 ->193         0.46776
     191 ->193        -0.41084
     192 ->195        -0.15841
     192 ->196         0.27326

 Excited state symmetry could not be determined.
 Excited State   4:   Triplet-?Sym    3.9796 eV  311.55 nm  f=0.0000
     187 ->193        -0.19624
     188 ->195        -0.15341
     189 ->193         0.26225
     190 ->196         0.13046
     191 ->193         0.40708
     192 ->195        -0.37971

 Excited state symmetry could not be determined.
 Excited State   5:   Triplet-?Sym    4.0113 eV  309.09 nm  f=0.0000
     174 ->195        -0.10143
     186 ->193        -0.10034
     187 ->195        -0.10778
     188 ->193        -0.32305
     188 ->194         0.11100
     190 ->193         0.55505
     191 ->196         0.13199

 Excited state symmetry could not be determined.
 Excited State   6:   Triplet-?Sym    4.0829 eV  303.67 nm  f=0.0000
     189 ->193         0.35509
     189 ->194        -0.14471
     190 ->196         0.10201
     191 ->193         0.19740
     191 ->194         0.10183
     192 ->195         0.51917

 Excited state symmetry could not be determined.
 Excited State   7:   Triplet-?Sym    4.2235 eV  293.55 nm  f=0.0000
     187 ->196         0.12130
     188 ->193         0.50848
     189 ->195        -0.10127
     190 ->193         0.32745
     190 ->194         0.18402
     191 ->195        -0.19897
     191 ->196         0.11331

 Excited state symmetry could not be determined.
 Excited State   8:   Triplet-?Sym    4.2826 eV  289.51 nm  f=0.0000
     187 ->193         0.50816
     188 ->196         0.16284
     189 ->194         0.15687
     190 ->195        -0.22085
     190 ->196         0.10622
     191 ->193         0.20958
     191 ->194         0.17028
     192 ->196         0.12399
```

```
Excited state symmetry could not be determined.
Excited State   9:   Triplet-?Sym    4.3047 eV  288.02 nm  f=0.0000
    186 ->193         0.65573
    188 ->193        -0.10494

Excited state symmetry could not be determined.
Excited State  10:   Triplet-?Sym    4.3492 eV  285.07 nm  f=0.0000
    184 ->196         0.12229
    185 ->193         0.66644
```

(vii) Input file for the triplet excitation energy calculation based on the singlet optimized geometry of $[Cu_2(\mu\text{-Me-mbim})_2](PF_6)_2$.

```
%nproc=4
%mem=1024MB
%chk=singlet_opt_Cu2PF62Membim2_TD_T.chk
#P B3LYP GEN TD=(TRIPLETS,NSTATE=10) SCF=(TIGHT,VSHIFT=500,MAXCYC=256)
   NOSYMM POP=FULL

triplet excitation energy calculation using Cu2PF62Membim2 singlet optimized
structure

0 1
 H
 H                  1             B1
 H                  1             B2     2             A1
 C                  1             B3     2             A2     3             D1
 C                  4             B4     1             A3     2             D2
 H                  4             B5     1             A4     5             D3
 C                  4             B6     1             A5     5             D4
 H                  4             B7     1             A6     5             D5
 C                  7             B8     4             A7     1             D6
 N                  4             B9     1             A8     5             D7
 H                  5            B10     4             A9     1             D8
 N                  5            B11     4            A10     1             D9
 C                 10            B12     4            A11     1            D10
 N                  7            B13     4            A12     1            D11
 H                 12            B14     5            A13     4            D12
 F                 14            B15     7            A14     4            D13
 C                 12            B16     5            A15     4            D14
 C                 12            B17     5            A16     4            D15
 N                  9            B18     7            A17     4            D16
 H                 13            B19    10            A18     4            D17
 H                 19            B20     9            A19     7            D18
 F                 19            B21     9            A20     7            D19
 F                 17            B22    12            A21     5            D20
 C                 19            B23     9            A22     7            D21
 H                 17            B24    12            A23     5            D22
 F                 13            B25    10            A24     4            D23
 C                 19            B26     9            A25     7            D24
 P                 24            B27    19            A26     9            D25
 H                 27            B28    19            A27     9            D26
 F                 28            B29    24            A28    19            D27
 F                 28            B30    24            A29    19            D28
 H                 27            B31    19            A30     9            D29
 Cu                18            B32    12            A31     5            D30
 F                 33            B33    18            A32    12            D31
 F                 33            B34    18            A33    12            D32
 P                 33            B35    18            A34    12            D33
 F                 36            B36    33            A35    18            D34
 F                 36            B37    33            A36    18            D35
 Cu                24            B38    19            A37     9            D36
 H                 33            B39    18            A38    12            D37
 F                 28            B40    24            A39    19            D38
 H                 33            B41    18            A40    12            D39
 H                 39            B42    24            A41    19            D40
 C                 33            B43    18            A42    12            D41
 C                 33            B44    18            A43    12            D42
 F                 36            B45    33            A44    18            D43
 H                 45            B46    33            A45    18            D44
 H                 44            B47    33            A46    18            D45
 C                 39            B48    24            A47    19            D46
 C                 49            B49    39            A48    24            D47
 N                 45            B50    33            A49    18            D48
 H                 50            B51    49            A50    39            D49
 H                 50            B52    49            A51    39            D50
 C                 45            B53    33            A52    18            D51
 N                 49            B54    39            A53    24            D52
 N                 45            B55    33            A54    18            D53
 N                 49            B56    39            A55    24            D54
 H                 54            B57    45            A56    33            D55
```

C	51	B58	45	A57	33	D56
C	59	B59	51	A58	45	D57
C	55	B60	49	A59	39	D58
H	59	B61	51	A60	45	D59
C	61	B62	55	A61	49	D60
H	61	B63	55	A62	49	D61
H	60	B64	59	A63	51	D62
H	63	B65	61	A64	55	D63

B1	2.77561289
B2	3.21706089
B3	1.07929769
B4	1.35623693
B5	5.86243594
B6	3.72601153
B7	2.60208711
B8	1.35605068
B9	1.38842721
B10	2.78660293
B11	1.38707336
B12	1.45663619
B13	1.38717959
B14	2.10216473
B15	3.01450649
B16	1.46450091
B17	1.35733427
B18	1.38768540
B19	1.08817925
B20	2.09267562
B21	5.14350164
B22	3.23744126
B23	1.35711904
B24	1.08792288
B25	4.50630992
B26	1.45930858
B27	3.85027355
B28	1.09368164
B29	1.67420464
B30	1.67664246
B31	1.09160589
B32	1.92139718
B33	2.51564024
B34	4.76345956
B35	3.57655650
B36	1.67316761
B37	1.62263789
B38	1.92222705
B39	2.95695041
B40	1.63689043
B41	3.65856827
B42	2.87738289
B43	3.38207736
B44	1.92208467
B45	1.64960481
B46	2.52563308
B47	1.09282574
B48	1.92128756
B49	2.50718256
B50	1.35740773
B51	1.09426058
B52	1.09218799
B53	2.47792817
B54	1.35732403
B55	1.36317297
B56	1.36921982
B57	1.09146658
B58	1.38782127
B59	1.35599451
B60	1.38713724
B61	1.07898887
B62	1.35620515
B63	1.07898155

B64	1.07854547
B65	1.07931193
A1	110.34650284
A2	48.78742078
A3	131.29366153
A4	89.20755205
A5	87.83309399
A6	69.84391242
A7	166.16910521
A8	122.49961245
A9	145.97924813
A10	106.85083364
A11	124.22260790
A12	68.15691252
A13	107.59169625
A14	96.94544779
A15	123.09891293
A16	111.60481082
A17	106.71362465
A18	110.23280481
A19	98.13534098
A20	99.87565250
A21	108.75170745
A22	111.50318853
A23	109.26608002
A24	147.52512169
A25	124.22190475
A26	108.65454021
A27	110.03300194
A28	51.49907668
A29	56.20903298
A30	109.03719437
A31	130.00135775
A32	96.24292677
A33	102.89184940
A34	105.35170872
A35	48.76891941
A36	138.43928385
A37	128.29498536
A38	114.68044714
A39	124.02934571
A40	126.66459650
A41	124.06693591
A42	131.29838124
A43	170.95986859
A44	82.90191484
A45	72.74698022
A46	154.24569107
A47	170.64201580
A48	101.62154557
A49	128.48612328
A50	120.48860437
A51	120.43035683
A52	97.70406015
A53	130.08524602
A54	127.15111821
A55	126.10104119
A56	117.60276063
A57	111.50979399
A58	106.69813909
A59	111.61401737
A60	122.39711591
A61	106.84857851
A62	122.19658427
A63	131.02327063
A64	131.32103301
D1	-58.50247489
D2	-0.27829014
D3	132.54205683
D4	139.71979033
D5	-173.28271729
D6	-179.66654326

```
   D7          -178.19299103
   D8          -144.10896519
   D9          -178.38821533
   D10           -0.41034128
   D11          112.08444677
   D12         -153.06240440
   D13         -107.46987608
   D14          179.15105263
   D15            0.16196620
   D16          -63.92017188
   D17          131.06508453
   D18          171.66147982
   D19          -75.21698701
   D20         -120.23582849
   D21           -0.52674495
   D22         -174.06255574
   D23           44.62794252
   D24         -173.33252324
   D25          -96.15859990
   D26           89.45450523
   D27          -52.63443191
   D28         -170.51995641
   D29         -150.68130756
   D30          177.37998922
   D31          -67.89125372
   D32          -59.88696632
   D33          -44.14518344
   D34           97.25542429
   D35          109.09312366
   D36         -171.32790588
   D37           71.99269972
   D38         -108.68110316
   D39           41.29453546
   D40           49.01887393
   D41           62.80905505
   D42          134.83834340
   D43         -167.75577117
   D44          105.03992880
   D45           94.51368023
   D46          -80.81945526
   D47          134.00705125
   D48          -80.73225299
   D49         -109.38993011
   D50          106.95304998
   D51          107.64796936
   D52          134.55784934
   D53          108.38526949
   D54          -48.12457987
   D55           99.55022926
   D56         -171.71311369
   D57           -0.48923967
   D58          177.44145899
   D59          179.41328355
   D60            0.20512091
   D61         -179.00602019
   D62         -179.34022457
   D63         -178.46210324

Cu 0
6-311G
 P 1 1.5
 0.083141     1.000000000
 P 1 1.5
 0.018137     1.000000000
****
P 0
6-31+G*
****
F 0
6-31+G*
****
N 0
```

```
6-31G*
****
C 0
6-31G*
****
H 0
6-31G
****
```

(viii) Results for the triplet excitation energy calculation based on the singlet optimized geometry of $[Cu_2(\mu\text{-Me-mbim})_2](PF_6)_2$.

```
 Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:   Triplet-?Sym    3.5505 eV  349.20 nm  f=0.0000
     191 ->194         0.25221
     192 ->193         0.66465
 This state for optimization and/or second-order correction.
 Total Energy, E(RPA) =  -6300.50331002
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited state symmetry could not be determined.
 Excited State   2:   Triplet-?Sym    3.7130 eV  333.92 nm  f=0.0000
     191 ->193         0.56708
     192 ->194         0.42365

 Excited state symmetry could not be determined.
 Excited State   3:   Triplet-?Sym    3.9541 eV  313.56 nm  f=0.0000
     191 ->196        -0.17846
     192 ->195         0.67541

 Excited state symmetry could not be determined.
 Excited State   4:   Triplet-?Sym    4.1197 eV  300.95 nm  f=0.0000
     183 ->193        -0.12931
     184 ->194        -0.15145
     189 ->193        -0.19581
     189 ->194         0.27038
     190 ->193         0.49062
     191 ->195         0.25925
     192 ->196        -0.11857

 Excited state symmetry could not be determined.
 Excited State   5:   Triplet-?Sym    4.1500 eV  298.76 nm  f=0.0000
     184 ->193        -0.18497
     189 ->193         0.37451
     190 ->193         0.28646
     190 ->194         0.30485
     191 ->195        -0.25302
     192 ->196         0.15139

 Excited state symmetry could not be determined.
 Excited State   6:   Triplet-?Sym    4.1604 eV  298.01 nm  f=0.0000
     184 ->193        -0.11325
     189 ->193         0.30515
     189 ->194        -0.11700
     190 ->194         0.16012
     191 ->195         0.46702
     192 ->196        -0.26699

 Excited state symmetry could not be determined.
 Excited State   7:   Triplet-?Sym    4.3676 eV  283.87 nm  f=0.0000
     181 ->196        -0.11329
     184 ->193        -0.15151
     185 ->194        -0.15007
     188 ->193         0.35932
     189 ->193        -0.12131
     189 ->195         0.25082
     190 ->195         0.14994
     190 ->196        -0.22305
     191 ->194         0.17762
     191 ->196         0.11072
     192 ->194        -0.11740

 Excited state symmetry could not be determined.
 Excited State   8:   Triplet-?Sym    4.3767 eV  283.28 nm  f=0.0000
     182 ->196        -0.10101
     183 ->193         0.12017
     185 ->193         0.22889
     188 ->193         0.16916
```

```
    188 ->194        -0.14110
    189 ->195         0.11511
    189 ->196         0.21339
    190 ->195        -0.18417
    191 ->193        -0.25393
    192 ->194         0.34768

Excited state symmetry could not be determined.
Excited State   9:   Triplet-?Sym    4.4086 eV  281.23 nm  f=0.0000
    184 ->193         0.15170
    185 ->193        -0.10920
    185 ->194        -0.12743
    186 ->193        -0.19202
    186 ->194        -0.19143
    187 ->193         0.35224
    187 ->194         0.12605
    188 ->193         0.30721
    189 ->195        -0.13138
    190 ->196         0.12943
    191 ->194         0.10564
    192 ->194        -0.10467

Excited state symmetry could not be determined.
Excited State  10:   Triplet-?Sym    4.4218 eV  280.39 nm  f=0.0000
    183 ->193        -0.12501
    185 ->193         0.18105
    186 ->193         0.35792
    187 ->194        -0.17529
    188 ->193         0.18028
    188 ->194        -0.10700
    189 ->195        -0.12310
    189 ->196        -0.18636
    190 ->195         0.13207
    192 ->194         0.14679
    192 ->196        -0.12442
```