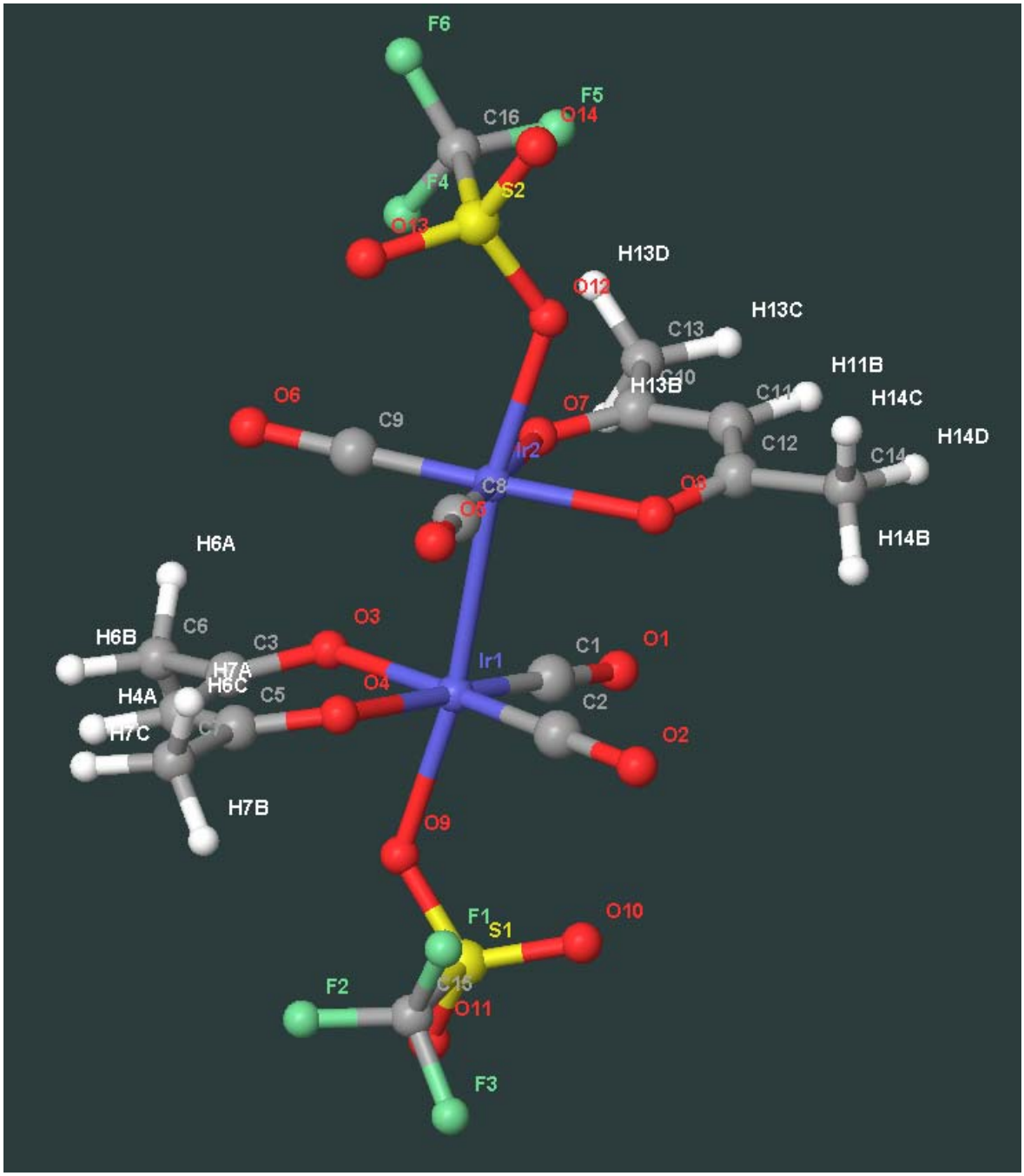



```
+-------------------------------------------------------------------+
|  Jaguar version 7.0, release 207                                  |
|                                                                   |
|  Copyright (c) 2007 Schrodinger,  LLC.                            |
|  All Rights Reserved.                                             |
|                                                                   |
|  Use of this program should be acknowledged in publications as:   |
|  Jaguar, version 7.0, Schrodinger, LLC, New York, NY, 2007.       |
+-------------------------------------------------------------------+

basis set:             lacv3p**++
net molecular charge:    0
multiplicity:            1
```

```
 This run will use ECP on           2  atoms
 number of basis functions....        1022

Final geometry:
                                angstroms
 atom              x                 y                 z
 Ir1          5.7007545686      4.9151182841      3.5012469294
 Ir2          3.8764658271      2.9141712731      3.1142218584
 S1           8.2942491126      7.0203142198      3.3489137737
 S2           1.1556530745      0.9791368316      2.9036292124
 F1           7.0094575113      7.4149492330      1.0573814563
 F2           6.9468800475      9.1164870600      2.4086419421
 F3           8.7689806751      8.6699985107      1.3062766774
 F4           1.4941447128      1.2490584874      5.5247398421
 F5           1.7893570611     -0.7793450359      4.7985486627
 F6          -0.2224037397      0.0284277102      4.9808193654
 O1           7.5715377912      3.0541547476      4.9823091718
 O2           6.8543420950      4.2156358862      0.7824440435
 O3           4.8864691795      5.4818566262      5.3181846888
 O4           4.4542343340      6.2860134406      2.5785416496
 O5           2.8561098997      4.2372022921      0.5869978065
 O6           1.9359706520      4.4316544045      4.8839485925
 O7           4.5487788774      1.8867493933      4.7786886605
 O8           5.1980794179      1.8121385651      1.9639880796
 O9           6.9328448366      6.6697517410      3.9712027863
 O10          8.9073606120      5.8609501327      2.6991633214
 O11          9.0793890798      7.8630507412      4.2313657946
 O12          2.6823045520      1.1046636467      2.7759452266
 O13          0.5067260992      2.2907714533      2.9377826800
 O14          0.6334175755     -0.0714207709      2.0499625183
 C1           6.8600622669      3.7231149052      4.4049944612
 C2           6.4481223581      4.4613692362      1.8103924950
 C3           4.2861333237      6.5971144006      5.5299176391
 C4           3.8095491351      7.4735166852      4.5485798093
 H4A          3.3076073654      8.3664073542      4.8910953341
 C5           3.8752636797      7.2727065028      3.1685080000
 C6           4.0950420264      6.9195306493      6.9838788209
 H6A          3.6567448061      6.0611913923      7.4975875094
 H6B          3.4691758292      7.7982054018      7.1313739479
 H6C          5.0783731945      7.1004679442      7.4287514559
 C7           3.2263475659      8.2473785321      2.2271715468
 H7A          2.5343910401      7.7167017430      1.5683153728
 H7B          3.9982059990      8.6940004361      1.5943033881
 H7C          2.6934965775      9.0353690788      2.7569367441
 C8           3.2369685194      3.7774266952      1.5507167893
 C9           2.6550109711      3.8736750659      4.2094827024
 C10          5.1823042217      0.7690281459      4.7503366861
 C11          5.7169291222      0.1593080578      3.6118483475
 H11B         6.2070000733     -0.7932649132      3.7498188023
 C12          5.7144125363      0.6891685091      2.3181480333
 C13          5.3411799939      0.1272547069      6.0992239403
 H13B         5.8321676575      0.8278703195      6.7793930715
 H13C         5.9165978392     -0.7956930135      6.0492225259
 H13D         4.3499585649     -0.0835804688      6.5095686180
 C14          6.3551453415     -0.0681240007      1.1907814133
 H14B         6.9667543981      0.6059747542      0.5880575636
 H14C         5.5594007714     -0.4530437908      0.5447352659
 H14D         6.9575715138     -0.9030842455      1.5452976752
 C15          7.7277252601      8.1341248997      1.9404544224
 C16          1.0377928145      0.3206352204      4.6630799297

 Stoichiometry: Ir2C16H14S2O14F6
 Molecular Point Group: C1
```

Point Group used: C1 (symmetry turned off)

bond lengths (angstroms):

Ir1	-Ir2	:	2.735253	Ir1	-O3	:	2.070149
Ir1	-O4	:	2.069916	Ir1	-O9	:	2.194913
Ir1	-C1	:	1.892518	Ir1	-C2	:	1.903532
Ir2	-O7	:	2.068345	Ir2	-O8	:	2.069825
Ir2	-O12	:	2.194258	Ir2	-C8	:	1.897028
Ir2	-C9	:	1.900578	S1	-O9	:	1.537387
S1	-O10	:	1.463628	S1	-O11	:	1.450990
S1	-C15	:	1.882892	S2	-O12	:	1.537116
S2	-O13	:	1.463782	S2	-O14	:	1.450913
S2	-C16	:	1.882334	F1	-C15	:	1.346455
F2	-C15	:	1.339386	F3	-C15	:	1.331749
F4	-C16	:	1.346360	F5	-C16	:	1.339088
F6	-C16	:	1.332081	O1	-C1	:	1.134459
O2	-C2	:	1.132289	O3	-C3	:	1.284147
O4	-C5	:	1.287179	O5	-C8	:	1.133667
O6	-C9	:	1.132812	O7	-C10	:	1.285091
O8	-C12	:	1.285726	C3	-C4	:	1.399370
C3	-C6	:	1.501490	C4	-H4A	:	1.080054
C4	-C5	:	1.396152	C5	-C7	:	1.502395
C6	-H6A	:	1.092130	C6	-H6B	:	1.088822
C6	-H6C	:	1.094345	C7	-H7A	:	1.092938
C7	-H7B	:	1.093508	C7	-H7C	:	1.088811
C10	-C11	:	1.397762	C10	-C13	:	1.502202
C11	-H11B	:	1.080093	C11	-C12	:	1.398005
C12	-C14	:	1.501661	C13	-H13B	:	1.092960
C13	-H13C	:	1.088778	C13	-H13D	:	1.093323
C14	-H14B	:	1.091673	C14	-H14C	:	1.094874
C14	-H14D	:	1.088925				

bond angles:

O3	-Ir1	-Ir2	:	93.561255	O4	-Ir1	-Ir2	:	91.133145
O4	-Ir1	-O3	:	88.455928	O9	-Ir1	-Ir2	:	171.683049
O9	-Ir1	-O3	:	79.282109	O9	-Ir1	-O4	:	84.493567
C1	-Ir1	-Ir2	:	90.880519	C1	-Ir1	-O3	:	89.671069
C1	-Ir1	-O4	:	177.331171	C1	-Ir1	-O9	:	93.290603
C2	-Ir1	-Ir2	:	87.810521	C2	-Ir1	-O3	:	177.882716
C2	-Ir1	-O4	:	89.905351	C2	-Ir1	-O9	:	99.227340
C2	-Ir1	-C1	:	91.921727	O7	-Ir2	-Ir1	:	91.875272
O8	-Ir2	-Ir1	:	92.422231	O8	-Ir2	-O7	:	88.577673
O12	-Ir2	-Ir1	:	171.134460	O12	-Ir2	-O7	:	83.760962
O12	-Ir2	-O8	:	79.790480	C8	-Ir2	-Ir1	:	90.490441
C8	-Ir2	-O7	:	177.275365	C8	-Ir2	-O8	:	89.972388
C8	-Ir2	-O12	:	93.712233	C9	-Ir2	-Ir1	:	88.726658
C9	-Ir2	-O7	:	89.766649	C9	-Ir2	-O8	:	178.014495
C9	-Ir2	-O12	:	98.940590	C9	-Ir2	-C8	:	91.637549
O10	-S1	-O9	:	111.716589	O11	-S1	-O9	:	111.434262
O11	-S1	-O10	:	120.223906	C15	-S1	-O9	:	99.859257
C15	-S1	-O10	:	105.220522	C15	-S1	-O11	:	105.912589
O13	-S2	-O12	:	111.658065	O14	-S2	-O12	:	111.576407
O14	-S2	-O13	:	120.196465	C16	-S2	-O12	:	99.694846
C16	-S2	-O13	:	105.301787	C16	-S2	-O14	:	105.909358
C3	-O3	-Ir1	:	124.497100	C5	-O4	-Ir1	:	125.046647
C10	-O7	-Ir2	:	125.066735	C12	-O8	-Ir2	:	124.637002
S1	-O9	-Ir1	:	126.349009	S2	-O12	-Ir2	:	126.516519
O1	-C1	-Ir1	:	176.962618	O2	-C2	-Ir1	:	177.446635
C4	-C3	-O3	:	125.980096	C6	-C3	-O3	:	113.931874
C6	-C3	-C4	:	120.082519	H4A	-C4	-C3	:	116.977300
C5	-C4	-C3	:	125.950409	C5	-C4	-H4A	:	117.017113

```
 C4      -C5      -O4      : 125.766761  C7      -C5      -O4      : 113.853496
 C7      -C5      -C4      : 120.377894  H6A     -C6      -C3      : 109.742637
 H6B     -C6      -C3      : 112.186150  H6B     -C6      -H6A     : 109.867158
 H6C     -C6      -C3      : 108.348590  H6C     -C6      -H6A     : 107.418011
 H6C     -C6      -H6B     : 109.147684  H7A     -C7      -C5      : 109.643396
 H7B     -C7      -C5      : 108.827128  H7B     -C7      -H7A     : 107.236338
 H7C     -C7      -C5      : 112.088034  H7C     -C7      -H7A     : 109.564697
 H7C     -C7      -H7B     : 109.356352  O5      -C8      -Ir2     : 176.798317
 O6      -C9      -Ir2     : 178.620976  C11     -C10     -O7      : 125.868578
 C13     -C10     -O7      : 113.822751  C13     -C10     -C11     : 120.302659
 H11B    -C11     -C10     : 117.014231  C12     -C11     -C10     : 125.995369
 C12     -C11     -H11B    : 116.954947  C11     -C12     -O8      : 125.920376
 C14     -C12     -O8      : 113.892324  C14     -C12     -C11     : 120.187299
 H13B    -C13     -C10     : 109.417885  H13C    -C13     -C10     : 112.136214
 H13C    -C13     -H13B    : 109.545505  H13D    -C13     -C10     : 108.875548
 H13D    -C13     -H13B    : 107.296874  H13D    -C13     -H13C    : 109.445654
 H14B    -C14     -C12     : 110.007333  H14C    -C14     -C12     : 108.069789
 H14C    -C14     -H14B    : 107.367062  H14D    -C14     -C12     : 112.229889
 H14D    -C14     -H14B    : 110.076708  H14D    -C14     -H14C    : 108.942304
 F1      -C15     -S1      : 109.581201  F2      -C15     -S1      : 110.352488
 F2      -C15     -F1      : 108.059829  F3      -C15     -S1      : 111.038132
 F3      -C15     -F1      : 108.644634  F3      -C15     -F2      : 109.096077
 F4      -C16     -S2      : 109.618230  F5      -C16     -S2      : 110.290785
 F5      -C16     -F4      : 108.147641  F6      -C16     -S2      : 111.034607
 F6      -C16     -F4      : 108.618921  F6      -C16     -F5      : 109.064986

SCF type: DFT=Becke_3_Parameter/HF+Slater+Becke88+VWN+LYP (B3LYP)

SCFE: SCF energy: DFT(b3lyp)     -3276.96677944305 hartrees   iterations:  13

  Thermodynamic properties calculated assuming an ideal gas

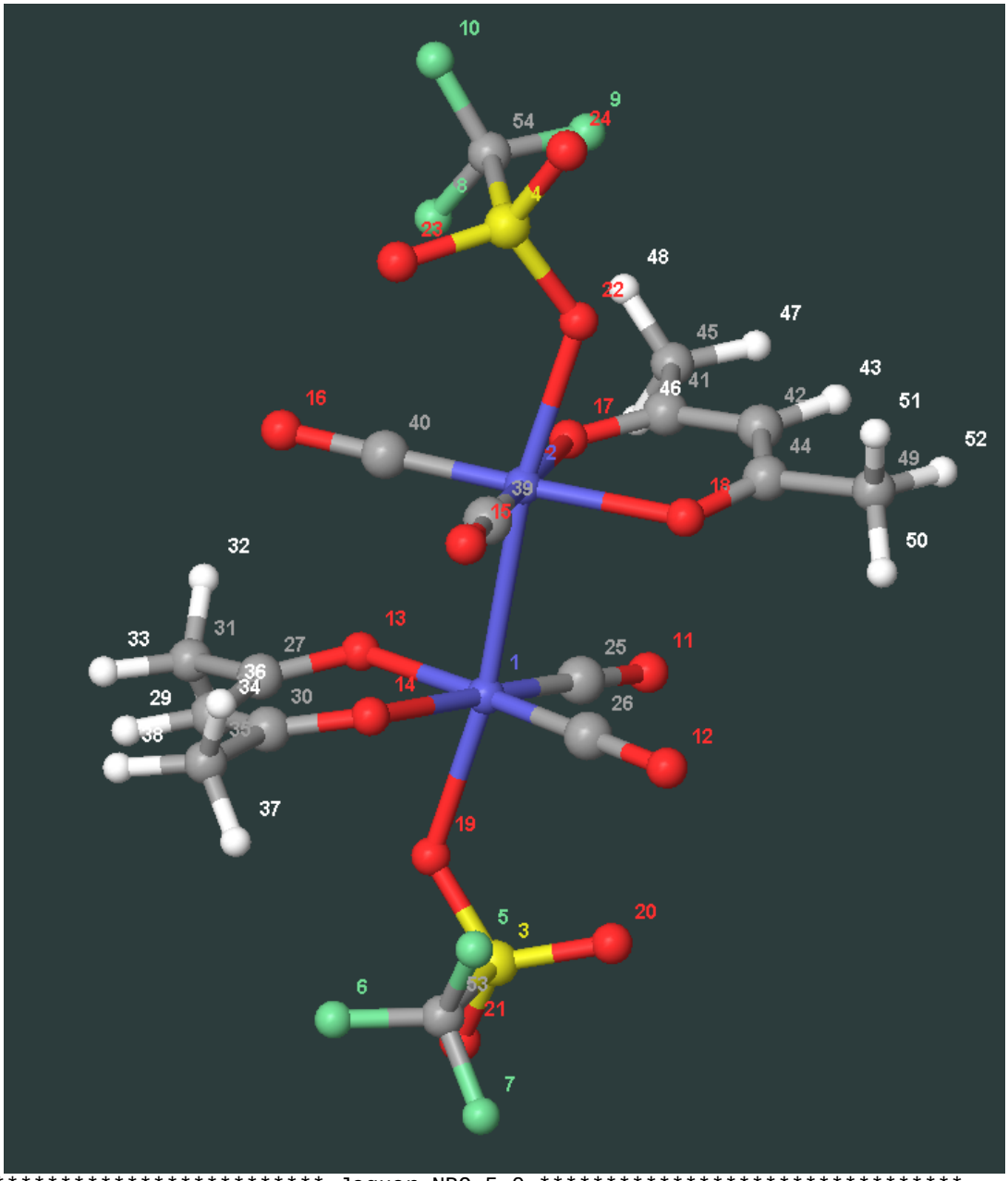
  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):    199.830 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G
         ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     46.563      1.481    -12.402
    rot.      0.889      2.981     38.168      0.889    -10.491
    vib.     26.637    150.195    190.220     26.637    -30.077
   elec.      0.000      0.000      0.000      0.000      0.000
   total     28.414    156.157    274.951     29.007    -52.970

  Total internal energy, Utot (SCFE + ZPE + U):   -3276.603050 hartrees
              Total enthalpy, Htot (Utot + pV):   -3276.602106 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):   -3276.732743 hartrees
```



********** Jaguar NBO 5.0 **********

N A T U R A L A T O M I C O R B I T A L A N D
N A T U R A L B O N D O R B I T A L A N A L Y S I S

****

Cite this program as:

NBO 5.0. E. D. Glendening, J. K. Badenhoop, A. E. Reed,
J. E. Carpenter, J. A. Bohmann, C. M. Morales, and F. Weinhold
(Theoretical Chemistry Institute, University of Wisconsin,
Madison, WI, 2001); http://www.chem.wisc.edu/~nbo5

Job title: Ir2_ACAC_2_CO_4_OTf_2_rph448_01: Input generated by Jaguar v7.0

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population			
		Core	Valence	Rydberg	Total
Ir 1	**0.61698**	**67.97766**	**8.34686**	**0.05850**	**76.38302**
Ir 2	**0.61681**	**67.97778**	**8.34697**	**0.05845**	**76.38319**
S 3	2.21798	9.99887	3.55790	0.22525	13.78202
S 4	2.21809	9.99887	3.55784	0.22520	13.78191
F 5	-0.34768	1.99991	7.34006	0.00771	9.34768
F 6	-0.33626	1.99991	7.33036	0.00600	9.33626
F 7	-0.32473	1.99991	7.31889	0.00593	9.32473
F 8	-0.34761	1.99991	7.34003	0.00766	9.34761
F 9	-0.33583	1.99991	7.32992	0.00599	9.33583
F 10	-0.32534	1.99991	7.31951	0.00592	9.32534
O 11	**-0.38786**	**1.99973**	**6.36547**	**0.02266**	**8.38786**
O 12	**-0.37773**	**1.99973**	**6.35348**	**0.02452**	**8.37773**
O 13	-0.66241	1.99973	6.63782	0.02486	8.66241
O 14	-0.67775	1.99973	6.65056	0.02747	8.67775
O 15	**-0.37913**	**1.99973**	**6.35659**	**0.02281**	**8.37913**
O 16	**-0.38498**	**1.99973**	**6.36088**	**0.02437**	**8.38498**
O 17	-0.66585	1.99973	6.63994	0.02618	8.66585
O 18	-0.67230	1.99973	6.64598	0.02659	8.67230
O 19	-0.96979	1.99983	6.94527	0.02469	8.96979
O 20	-0.92528	1.99981	6.91221	0.01326	8.92528
O 21	-0.87617	1.99980	6.86384	0.01253	8.87617
O 22	-0.97004	1.99983	6.94555	0.02466	8.97004
O 23	-0.92593	1.99981	6.91286	0.01326	8.92593
O 24	-0.87611	1.99980	6.86380	0.01251	8.87611
C 25	**0.64524**	**1.99958**	**3.29452**	**0.06066**	**5.35476**
C 26	**0.63456**	**1.99957**	**3.30455**	**0.06132**	**5.36544**
C 27	0.53538	1.99925	3.43323	0.03214	5.46462
C 28	-0.45723	1.99899	4.44441	0.01382	6.45723
H 29	0.22689	0.00000	0.77199	0.00112	0.77311
C 30	0.52695	1.99924	3.44238	0.03142	5.47305
C 31	-0.63856	1.99937	4.62774	0.01145	6.63856
H 32	0.23572	0.00000	0.76318	0.00110	0.76428
H 33	0.21718	0.00000	0.78207	0.00074	0.78282
H 34	0.24354	0.00000	0.75542	0.00105	0.75646
C 35	-0.63800	1.99938	4.62711	0.01151	6.63800
H 36	0.23504	0.00000	0.76385	0.00110	0.76496
H 37	0.24290	0.00000	0.75586	0.00124	0.75710
H 38	0.21781	0.00000	0.78147	0.00072	0.78219
C 39	**0.63943**	**1.99958**	**3.30064**	**0.06035**	**5.36057**
C 40	**0.64099**	**1.99957**	**3.29774**	**0.06170**	**5.35901**
C 41	0.52854	1.99925	3.44006	0.03215	5.47146
C 42	-0.45870	1.99899	4.44588	0.01382	6.45870
H 43	0.22682	0.00000	0.77206	0.00113	0.77318
C 44	0.53278	1.99925	3.43680	0.03117	5.46722
C 45	-0.63829	1.99937	4.62732	0.01160	6.63829
H 46	0.23592	0.00000	0.76297	0.00112	0.76408
H 47	0.21717	0.00000	0.78209	0.00074	0.78283
H 48	0.24212	0.00000	0.75664	0.00124	0.75788
C 49	-0.63899	1.99937	4.62827	0.01134	6.63899
H 50	0.23509	0.00000	0.76381	0.00111	0.76491
H 51	0.24532	0.00000	0.75369	0.00100	0.75468
H 52	0.21783	0.00000	0.78144	0.00073	0.78217
C 53	0.82267	1.99983	3.09891	0.07858	5.17733
C 54	0.82281	1.99983	3.09871	0.07865	5.17719
* Total *	0.00000	227.93979	232.53740	1.52281	462.00000

```
                                Natural Population
 ------------------------------------------------------------
   Effective Core           120.00000
   Core                     107.93979 ( 99.9442% of 108)
   Valence                  232.53740 ( 99.3750% of 234)
   Natural Minimal Basis    460.47719 ( 99.6704% of 462)
   Natural Rydberg Basis      1.52281 (  0.3296% of 462)
 ------------------------------------------------------------

NATURAL BOND ORBITAL ANALYSIS:

                     Occupancies       Lewis Structure    Low   High
           Occ.    -------------------  ----------------   occ   occ
 Cycle   Thresh.    Lewis    Non-Lewis     CR  BD  3C  LP    (L)   (NL)   Dev
=================================================================================
  1(1)    1.90   447.61938  14.38062      54  79   0  38     31     43    0.68
  2(2)    1.90   447.78461  14.21539      54  78   0  39     32     41    0.94
  3(3)    1.90   448.01598  13.98402      54  79   0  38     32     41    0.68
  4(4)    1.90   448.18377  13.81623      54  78   0  39     33     39    0.94
  5(5)    1.90   448.41059  13.58941      54  79   0  38     33     39    0.38
  6(6)    1.90   448.41059  13.58941      54  79   0  38     33     39    0.38
  7(1)    1.80   451.41214  10.58786      54  69   0  48     15     33    0.50
  8(2)    1.80   451.87462  10.12538      54  67   0  50     16     33    0.38
  9(3)    1.80   451.87462  10.12538      54  67   0  50     16     33    0.38
 10(1)    1.70   452.44586   9.55414      54  63   0  54      6     31    0.38
 11(2)    1.70   452.44586   9.55414      54  63   0  54      6     31    0.38
 12(1)    1.60   452.82707   9.17293      54  59   0  58      0     29    0.38
 13(2)    1.60   452.84108   9.15892      54  59   0  58      0     29    0.37
 14(3)    1.60   452.84013   9.15987      54  59   0  58      0     29    0.37
 15(4)    1.60   452.84108   9.15892      54  59   0  58      0     29    0.37
 16(1)    1.50   450.47145  11.52855      54  54   0  63      0     29    1.21
 17(2)    1.50   450.47145  11.52855      54  54   0  63      0     29    1.21
 18(1)    1.60   452.84108   9.15892      54  59   0  58      0     29    0.37
---------------------------------------------------------------------------------

 Strongly delocalized structure accepted

          4 low occupancy (<1.9990e) core orbitals found on Ir 1
          4 low occupancy (<1.9990e) core orbitals found on Ir 2
          1 low occupancy (<1.9990e) core orbital  found on  C28
          1 low occupancy (<1.9990e) core orbital  found on  C42

 ------------------------------------------------------------
   Effective Core          120.00000
   Core                    107.93928 ( 99.944% of 108)
   Valence Lewis           224.90180 ( 96.112% of 234)
  ==================       ============================
   Total Lewis             452.84108 ( 98.018% of 462)
  ------------------------------------------------------
   Valence non-Lewis         7.93580 (  1.718% of 462)
   Rydberg non-Lewis         1.22312 (  0.265% of 462)
  ==================       ============================
   Total non-Lewis           9.15892 (  1.982% of 462)
 ------------------------------------------------------------


     (Occupancy)   Bond orbital/ Coefficients/ Hybrids
 ---------------------------------------------------------------------------------
   1. (1.83044) BD ( 1)Ir  1-Ir  2
              ( 50.00%)   0.7071*Ir  1 s( 27.78%)p 0.03(  0.73%)d 2.57( 71.49%)
                                       0.0008  0.5268 -0.0142  0.0091 -0.0008
                                       0.0013 -0.0004  0.0011 -0.0598  0.0021
```

```
                                     0.0080  0.0007 -0.0598 -0.0027  0.0023
                                     0.0001 -0.0098  0.0000 -0.0003  0.7130
                                     0.0423 -0.0106 -0.0026  0.1618  0.0091
                                    -0.0021 -0.0003  0.1563  0.0142 -0.0048
                                    -0.0006 -0.1426 -0.0035  0.0066  0.0013
                                    -0.3642 -0.0247  0.0061  0.0016
              ( 50.00%)   0.7071*Ir  2 s( 27.77%)p 0.03(  0.74%)d 2.57( 71.49%)
                                     0.0008  0.5267 -0.0138  0.0092 -0.0009
                                     0.0013 -0.0004 -0.0011  0.0609 -0.0019
                                    -0.0079 -0.0007  0.0593  0.0020 -0.0019
                                    -0.0003  0.0100  0.0012 -0.0005  0.7224
                                     0.0412 -0.0107 -0.0029  0.1095  0.0087
                                    -0.0008  0.0004  0.1491  0.0122 -0.0008
                                    -0.0001 -0.1495 -0.0040  0.0066  0.0013
                                    -0.3654 -0.0267  0.0075  0.0013
 2. (1.95572) BD ( 1)Ir  1- C 25
              ( 32.74%)   0.5722*Ir  1 s( 35.57%)p 0.00(  0.08%)d 1.81( 64.34%)
                                    -0.0006  0.5964  0.0016 -0.0003  0.0011
                                     0.0019  0.0000 -0.0002 -0.0026 -0.0033
                                     0.0159  0.0005 -0.0162  0.0018 -0.0133
                                     0.0002  0.0079 -0.0025  0.0077 -0.5255
                                    -0.0095 -0.0078 -0.0032  0.3891  0.0159
                                     0.0066  0.0009 -0.4304 -0.0113 -0.0083
                                    -0.0003 -0.0060 -0.0068  0.0024  0.0005
                                    -0.1719 -0.0191  0.0040  0.0002
              ( 67.26%)   0.8201* C 25 s( 61.54%)p 0.62( 38.43%)d 0.00(  0.03%)
                                     0.0002  0.7835 -0.0388  0.0035 -0.0008
                                     0.0000 -0.3811 -0.0276  0.0110  0.0004
                                     0.3741  0.0286 -0.0096 -0.0013 -0.3109
                                    -0.0225  0.0091  0.0002 -0.0123  0.0071
                                    -0.0083 -0.0015 -0.0027
 3. (1.95423) BD ( 1)Ir  1- C 26
              ( 32.48%)   0.5699*Ir  1 s( 36.02%)p 0.00(  0.08%)d 1.77( 63.90%)
                                    -0.0004  0.6001  0.0017  0.0004  0.0022
                                     0.0018 -0.0001 -0.0002 -0.0064 -0.0039
                                     0.0106  0.0005 -0.0081 -0.0002 -0.0072
                                     0.0003 -0.0148  0.0037 -0.0180 -0.1107
                                     0.0079 -0.0008 -0.0020 -0.5054 -0.0166
                                    -0.0082 -0.0009  0.2997  0.0245 -0.0004
                                     0.0008  0.1022 -0.0032  0.0008  0.0004
                                     0.5194  0.0106  0.0116  0.0024
              ( 67.52%)   0.8217* C 26 s( 61.68%)p 0.62( 38.29%)d 0.00(  0.03%)
                                     0.0002  0.7844 -0.0380 -0.0036 -0.0006
                                     0.0000 -0.2265 -0.0179  0.0071  0.0006
                                     0.1424  0.0111 -0.0028 -0.0008  0.5559
                                     0.0395 -0.0165 -0.0011 -0.0048 -0.0093
                                     0.0073  0.0012  0.0110
 4. (1.95489) BD ( 1)Ir  2- C 39
              ( 32.63%)   0.5712*Ir  2 s( 35.56%)p 0.00(  0.09%)d 1.81( 64.36%)
                                    -0.0006  0.5963  0.0020 -0.0002  0.0014
                                     0.0018  0.0000  0.0002  0.0070  0.0019
                                    -0.0106 -0.0005  0.0122 -0.0009  0.0107
                                     0.0001 -0.0127  0.0046 -0.0156 -0.1987
                                     0.0035 -0.0031 -0.0026  0.3961  0.0174
                                     0.0031  0.0021 -0.5433 -0.0232 -0.0062
                                    -0.0008 -0.0461 -0.0075  0.0012  0.0001
                                     0.3857  0.0030  0.0113  0.0011
              ( 67.37%)   0.8208* C 39 s( 61.60%)p 0.62( 38.37%)d 0.00(  0.03%)
                                     0.0002  0.7839 -0.0388 -0.0034 -0.0009
                                     0.0001  0.2061  0.0154 -0.0073 -0.0007
                                    -0.2638 -0.0204  0.0067  0.0011  0.5189
                                     0.0368 -0.0158 -0.0001 -0.0060  0.0068
                                    -0.0119 -0.0015  0.0075
```

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 5. (1.95461) BD ( 1)Ir  2- C 40
            ( 32.56%)   0.5706*Ir  2 s( 36.05%)p 0.00(  0.08%)d 1.77( 63.87%)
                                     -0.0005  0.6004  0.0012  0.0004  0.0018
                                      0.0018 -0.0001  0.0002  0.0029  0.0053
                                     -0.0146 -0.0006  0.0129 -0.0008  0.0125
                                      0.0000  0.0111 -0.0011  0.0106 -0.4389
                                     -0.0055 -0.0055 -0.0031 -0.5010 -0.0161
                                     -0.0116 -0.0004  0.4150  0.0217  0.0029
                                      0.0018  0.1422 -0.0043  0.0042 -0.0002
                                     -0.0369 -0.0158  0.0040  0.0008
            ( 67.44%)   0.8212* C 40 s( 61.62%)p 0.62( 38.35%)d 0.00(  0.03%)
                                      0.0002  0.7840 -0.0382  0.0039 -0.0007
                                      0.0000  0.3899  0.0290 -0.0107 -0.0010
                                     -0.3077 -0.0231  0.0070  0.0009 -0.3667
                                     -0.0269  0.0102  0.0009 -0.0108 -0.0100
                                      0.0081  0.0007  0.0001
20. (1.99833) BD ( 1) O 11- C 25
            ( 73.65%)   0.8582* O 11 s(  0.12%)p99.99( 99.67%)d 1.77(  0.21%)
                                      0.0000 -0.0343  0.0013 -0.0004  0.0002
                                      0.0000 -0.1571  0.0011  0.0002  0.0003
                                      0.4996 -0.0025 -0.0034 -0.0004  0.8499
                                     -0.0050 -0.0030 -0.0005 -0.0180 -0.0214
                                      0.0115 -0.0087 -0.0331
            ( 26.35%)   0.5133* C 25 s(  0.15%)p99.99( 99.31%)d 3.68(  0.54%)
                                      0.0000 -0.0382 -0.0038 -0.0001  0.0007
                                      0.0000 -0.2048  0.0035 -0.0028 -0.0016
                                      0.5441 -0.0044  0.0047  0.0013  0.8092
                                     -0.0086  0.0115  0.0012  0.0333  0.0311
                                     -0.0162  0.0149  0.0536
21. (1.99677) BD ( 2) O 11- C 25
            ( 72.90%)   0.8538* O 11 s( 11.40%)p 7.75( 88.36%)d 0.02(  0.24%)
                                      0.0000  0.3372 -0.0179  0.0013 -0.0003
                                     -0.0003  0.4301 -0.0002 -0.0083  0.0000
                                      0.7579 -0.0061 -0.0016 -0.0004 -0.3523
                                      0.0040 -0.0021  0.0004 -0.0167  0.0054
                                     -0.0320 -0.0321  0.0040
            ( 27.10%)   0.5206* C 25 s(  9.17%)p 9.85( 90.38%)d 0.05(  0.45%)
                                      0.0000  0.2942  0.0719 -0.0027  0.0034
                                     -0.0001  0.8941 -0.0360  0.0060  0.0022
                                      0.3185  0.0198  0.0052 -0.0019  0.0263
                                     -0.0198 -0.0032  0.0011 -0.0115  0.0245
                                      0.0215  0.0562 -0.0124
22. (1.99548) BD ( 3) O 11- C 25
            ( 69.58%)   0.8341* O 11 s( 34.80%)p 1.87( 64.90%)d 0.01(  0.30%)
                                      0.0000 -0.5893  0.0262 -0.0024  0.0007
                                      0.0006  0.7798 -0.0076  0.0032 -0.0009
                                     -0.0967  0.0060 -0.0084  0.0002  0.1771
                                     -0.0048  0.0052 -0.0003  0.0343 -0.0324
                                      0.0155 -0.0205  0.0115
            ( 30.42%)   0.5516* C 25 s( 30.01%)p 2.33( 69.80%)d 0.01(  0.19%)
                                      0.0001 -0.5357 -0.1145  0.0043 -0.0028
                                      0.0001 -0.0391  0.0405  0.0110 -0.0020
                                      0.6734 -0.0401 -0.0023  0.0012 -0.4882
                                      0.0365  0.0031 -0.0019  0.0115 -0.0054
                                      0.0289  0.0298 -0.0075
23. (1.99700) BD ( 1) O 12- C 26
            ( 72.48%)   0.8513* O 12 s( 11.86%)p 7.41( 87.89%)d 0.02(  0.25%)
                                      0.0000  0.3439 -0.0186  0.0011 -0.0004
                                     -0.0003  0.6254 -0.0029 -0.0051 -0.0003
                                      0.4419 -0.0044 -0.0026  0.0000  0.5408
                                     -0.0068  0.0040 -0.0004 -0.0029  0.0116
                                      0.0271 -0.0145  0.0371
            ( 27.52%)   0.5246* C 26 s(  9.92%)p 9.04( 89.66%)d 0.04(  0.42%)
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                                     0.0000  0.3063  0.0733  0.0031  0.0020
                                     0.0001  0.8930 -0.0272  0.0097  0.0026
                                     0.2787  0.0037  0.0030 -0.0020 -0.1385
                                     0.0366  0.0051 -0.0018 -0.0051 -0.0527
                                    -0.0244  0.0250 -0.0142
 24. (1.99752) BD ( 2) O 12- C 26
             ( 73.04%)   0.8546* O 12 s(  2.35%)p41.51( 97.43%)d 0.09(  0.22%)
                                     0.0000  0.1530 -0.0079  0.0008  0.0000
                                    -0.0001 -0.4858  0.0031 -0.0002  0.0006
                                     0.8317 -0.0058 -0.0040 -0.0003 -0.2157
                                     0.0000  0.0029  0.0000 -0.0194 -0.0192
                                     0.0344  0.0005 -0.0169
             ( 26.96%)   0.5192* C 26 s(  1.71%)p57.18( 97.79%)d 0.29(  0.50%)
                                     0.0000  0.1272  0.0304  0.0017  0.0014
                                     0.0000 -0.3636 -0.0009 -0.0083 -0.0025
                                     0.7574 -0.0074  0.0100  0.0004 -0.5209
                                     0.0224 -0.0028 -0.0012  0.0266  0.0160
                                    -0.0449  0.0029  0.0452
 25. (1.99545) BD ( 3) O 12- C 26
             ( 70.10%)   0.8373* O 12 s( 32.96%)p 2.03( 66.74%)d 0.01(  0.30%)
                                     0.0000  0.5734 -0.0276  0.0021 -0.0005
                                    -0.0006 -0.5566  0.0052 -0.0001  0.0005
                                    -0.2964  0.0008  0.0053  0.0000  0.5192
                                    -0.0083  0.0075 -0.0007 -0.0029 -0.0411
                                    -0.0019  0.0136  0.0333
             ( 29.90%)   0.5468* C 26 s( 27.55%)p 2.62( 72.23%)d 0.01(  0.22%)
                                    -0.0001  0.5135  0.1089  0.0039  0.0036
                                    -0.0002 -0.1048 -0.0200 -0.0065  0.0014
                                    -0.5678  0.0186 -0.0033 -0.0003 -0.6201
                                     0.0595  0.0067 -0.0035 -0.0088  0.0107
                                     0.0370 -0.0138  0.0203
 28. (1.99759) BD ( 1) O 15- C 39
             ( 72.95%)   0.8541* O 15 s(  7.58%)p12.17( 92.19%)d 0.03(  0.23%)
                                     0.0000  0.2749 -0.0139  0.0008 -0.0003
                                    -0.0003 -0.7458  0.0029 -0.0060  0.0003
                                    -0.4127  0.0038 -0.0006  0.0002  0.4420
                                    -0.0054 -0.0025 -0.0004  0.0055 -0.0184
                                    -0.0289 -0.0197  0.0269
             ( 27.05%)   0.5201* C 39 s(  6.25%)p14.91( 93.27%)d 0.08(  0.48%)
                                     0.0000  0.2432  0.0582  0.0018  0.0023
                                     0.0001 -0.9478  0.0209 -0.0105 -0.0022
                                    -0.1654 -0.0095 -0.0033  0.0010 -0.0739
                                     0.0278  0.0044 -0.0013 -0.0206  0.0543
                                     0.0189  0.0290 -0.0141
 29. (1.99760) BD ( 2) O 15- C 39
             ( 73.16%)   0.8553* O 15 s(  4.41%)p21.62( 95.37%)d 0.05(  0.22%)
                                     0.0000 -0.2097  0.0108 -0.0007  0.0001
                                     0.0002 -0.3744  0.0025  0.0002  0.0006
                                     0.8522 -0.0050  0.0019 -0.0005  0.2951
                                     0.0009  0.0044  0.0002  0.0216 -0.0130
                                     0.0314  0.0102  0.0223
             ( 26.84%)   0.5181* C 39 s(  3.32%)p28.94( 96.17%)d 0.15(  0.50%)
                                     0.0000 -0.1771 -0.0430 -0.0014 -0.0024
                                     0.0001 -0.2178 -0.0073 -0.0058 -0.0012
                                     0.6619  0.0025  0.0094  0.0009  0.6894
                                    -0.0269  0.0038  0.0016 -0.0261  0.0020
                                    -0.0290 -0.0151 -0.0572
 30. (1.99571) BD ( 3) O 15- C 39
             ( 69.60%)   0.8343* O 15 s( 34.44%)p 1.89( 65.26%)d 0.01(  0.30%)
                                     0.0000  0.5862 -0.0276  0.0025 -0.0004
                                    -0.0006  0.4993 -0.0049  0.0000 -0.0005
                                     0.1508  0.0028  0.0060  0.0001  0.6167
                                    -0.0099 -0.0058 -0.0007 -0.0110  0.0371
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                                    -0.0153  0.0099  0.0346
              ( 30.40%)   0.5514* C 39 s( 29.70%)p 2.36( 70.11%)d 0.01(  0.20%)
                                    -0.0001  0.5328  0.1143  0.0036  0.0034
                                    -0.0002  0.0640  0.0212  0.0058 -0.0010
                                     0.6764 -0.0303  0.0016  0.0008 -0.4844
                                     0.0576  0.0081 -0.0023 -0.0072 -0.0098
                                    -0.0372 -0.0199  0.0051
 31. (1.99723) BD ( 1) O 16- C 40
              ( 73.12%)   0.8551* O 16 s(  7.65%)p12.04( 92.12%)d 0.03(  0.23%)
                                     0.0000 -0.2761  0.0160 -0.0008  0.0002
                                     0.0003  0.3022 -0.0008 -0.0074  0.0000
                                     0.9092 -0.0081 -0.0049 -0.0003  0.0546
                                    -0.0017  0.0028 -0.0001  0.0247 -0.0016
                                    -0.0299  0.0281  0.0044
              ( 26.88%)   0.5185* C 40 s(  6.16%)p15.16( 93.37%)d 0.08(  0.47%)
                                     0.0000 -0.2403 -0.0618  0.0038 -0.0021
                                     0.0000  0.6818 -0.0316  0.0049  0.0014
                                     0.6131  0.0096  0.0062 -0.0023 -0.3019
                                     0.0246 -0.0016 -0.0016 -0.0115  0.0333
                                     0.0245 -0.0527 -0.0096
 32. (1.99725) BD ( 2) O 16- C 40
              ( 72.79%)   0.8531* O 16 s(  6.41%)p14.57( 93.36%)d 0.04(  0.23%)
                                     0.0000 -0.2528  0.0133 -0.0009  0.0005
                                     0.0003  0.2596 -0.0012 -0.0042 -0.0001
                                    -0.2178  0.0009  0.0032  0.0002  0.9048
                                    -0.0075  0.0004 -0.0005 -0.0082  0.0245
                                    -0.0176  0.0020 -0.0362
              ( 27.21%)   0.5217* C 40 s(  5.38%)p17.49( 94.15%)d 0.09(  0.47%)
                                     0.0000 -0.2265 -0.0502  0.0020 -0.0014
                                     0.0000  0.6091 -0.0272  0.0043  0.0033
                                    -0.4889  0.0185 -0.0045 -0.0029  0.5746
                                     0.0046  0.0114 -0.0003  0.0373 -0.0087
                                     0.0082 -0.0080  0.0554
 33. (1.99521) BD ( 3) O 16- C 40
              ( 70.09%)   0.8372* O 16 s( 32.95%)p 2.03( 66.75%)d 0.01(  0.30%)
                                     0.0000  0.5734 -0.0260  0.0021 -0.0008
                                    -0.0006  0.8070 -0.0072  0.0037 -0.0010
                                    -0.0876  0.0038 -0.0075  0.0001 -0.0916
                                     0.0038 -0.0070  0.0003 -0.0294 -0.0353
                                     0.0126  0.0240 -0.0115
              ( 29.91%)   0.5469* C 40 s( 27.70%)p 2.60( 72.08%)d 0.01(  0.22%)
                                    -0.0001  0.5149  0.1089 -0.0042  0.0031
                                    -0.0001  0.0062  0.0365  0.0114 -0.0019
                                     0.5316 -0.0321 -0.0027  0.0010  0.6587
                                    -0.0423 -0.0018  0.0028 -0.0065 -0.0085
                                     0.0309 -0.0253  0.0214

114. (1.86212) LP ( 1)Ir  1           s(  0.04%)p 0.40(  0.01%)d99.99( 99.95%)
                                     0.0000  0.0190  0.0002  0.0006 -0.0001
                                     0.0000  0.0001 -0.0004  0.0062 -0.0025
                                    -0.0017 -0.0006  0.0048 -0.0034 -0.0002
                                     0.0001  0.0073 -0.0003 -0.0031  0.1925
                                    -0.0022 -0.0021  0.0008 -0.6431  0.0175
                                    -0.0018 -0.0018 -0.7058  0.0123 -0.0016
                                    -0.0009  0.0700  0.0006  0.0001 -0.0002
                                    -0.2129  0.0002 -0.0018  0.0000
115. (1.84666) LP ( 2)Ir  1           s(  0.03%)p 1.60(  0.05%)d99.99( 99.93%)
                                    -0.0007  0.0166  0.0024 -0.0016 -0.0004
                                     0.0004  0.0001 -0.0016  0.0092 -0.0031
                                     0.0014 -0.0014  0.0184 -0.0033 -0.0010
                                    -0.0004 -0.0003 -0.0012  0.0012  0.1440
                                     0.0057 -0.0017  0.0000  0.1666 -0.0022
                                     0.0012 -0.0001 -0.0119 -0.0039  0.0010
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                                    -0.0001  0.9747 -0.0195  0.0011  0.0016
                                    -0.0111  0.0019  0.0000 -0.0006
 116. (1.79189) LP ( 3)Ir  1         s(  0.04%)p 0.44(  0.02%)d99.99( 99.95%)
                                     0.0015  0.0156 -0.0104  0.0040  0.0002
                                     0.0004  0.0001 -0.0010  0.0098 -0.0023
                                    -0.0002  0.0008 -0.0068  0.0032  0.0000
                                     0.0005 -0.0019  0.0001 -0.0011 -0.3753
                                    -0.0050  0.0028  0.0012 -0.3524 -0.0005
                                     0.0012  0.0006  0.4480 -0.0019 -0.0023
                                    -0.0003  0.1126 -0.0082 -0.0001 -0.0003
                                    -0.7217  0.0070 -0.0007  0.0010
 117. (1.86046) LP ( 1)Ir  2         s(  0.01%)p 1.00(  0.01%)d99.99( 99.98%)
                                     0.0001  0.0078 -0.0015  0.0021  0.0006
                                    -0.0001 -0.0001  0.0001 -0.0008  0.0014
                                     0.0003  0.0002 -0.0018  0.0023  0.0008
                                    -0.0003 -0.0087 -0.0004  0.0035  0.1683
                                    -0.0016 -0.0015  0.0006 -0.6142  0.0166
                                    -0.0001 -0.0022 -0.6859  0.0122 -0.0032
                                    -0.0007  0.2661 -0.0039 -0.0001  0.0005
                                    -0.2291  0.0074 -0.0024 -0.0005
 118. (1.84825) LP ( 2)Ir  2         s(  0.05%)p 1.07(  0.05%)d99.99( 99.90%)
                                    -0.0007  0.0218  0.0025 -0.0015 -0.0006
                                     0.0004  0.0002  0.0016 -0.0117  0.0037
                                    -0.0006  0.0015 -0.0186  0.0042  0.0007
                                     0.0004  0.0005  0.0004 -0.0012  0.1309
                                     0.0067 -0.0024  0.0001  0.2829 -0.0074
                                     0.0012  0.0009  0.1304 -0.0016 -0.0005
                                     0.0000  0.9396 -0.0168  0.0004  0.0014
                                     0.0396  0.0009  0.0005 -0.0006
 119. (1.79265) LP ( 3)Ir  2         s(  0.04%)p 0.49(  0.02%)d99.99( 99.95%)
                                     0.0014  0.0153 -0.0101  0.0043  0.0002
                                     0.0004  0.0001  0.0010 -0.0101  0.0021
                                     0.0000 -0.0010  0.0069 -0.0035  0.0003
                                     0.0002 -0.0018  0.0017  0.0004 -0.4424
                                    -0.0048  0.0033  0.0013  0.3488 -0.0026
                                    -0.0016 -0.0008 -0.1450 -0.0004  0.0002
                                     0.0005  0.0105 -0.0080  0.0013 -0.0002
                                    -0.8129  0.0074 -0.0006  0.0012
1008. (0.47348) BD*( 1)Ir  1-Ir  2
              ( 50.00%)   0.7071*Ir  1 s( 27.78%)p 0.03(  0.73%)d 2.57( 71.49%)
                                    -0.0008 -0.5268  0.0142 -0.0091  0.0008
                                    -0.0013  0.0004 -0.0011  0.0598 -0.0021
                                    -0.0080 -0.0007  0.0598  0.0027 -0.0023
                                    -0.0001  0.0098  0.0000  0.0003 -0.7130
                                    -0.0423  0.0106  0.0026 -0.1618 -0.0091
                                     0.0021  0.0003 -0.1563 -0.0142  0.0048
                                     0.0006  0.1426  0.0035 -0.0066 -0.0013
                                     0.3642  0.0247 -0.0061 -0.0016
              ( 50.00%)  -0.7071*Ir  2 s( 27.77%)p 0.03(  0.74%)d 2.57( 71.49%)
                                    -0.0008 -0.5267  0.0138 -0.0092  0.0009
                                    -0.0013  0.0004  0.0011 -0.0609  0.0019
                                     0.0079  0.0007 -0.0593 -0.0020  0.0019
                                     0.0003 -0.0100 -0.0012  0.0005 -0.7224
                                    -0.0412  0.0107  0.0029 -0.1095 -0.0087
                                     0.0008 -0.0004 -0.1491 -0.0122  0.0008
                                     0.0001  0.1495  0.0040 -0.0066 -0.0013
                                     0.3654  0.0267 -0.0075 -0.0013
1009. (0.31962) BD*( 1)Ir  1- C 25
              ( 67.26%)   0.8201*Ir  1 s( 35.57%)p 0.00(  0.08%)d 1.81( 64.34%)
                                    -0.0006  0.5964  0.0016 -0.0003  0.0011
                                     0.0019  0.0000 -0.0002 -0.0026 -0.0033
                                     0.0159  0.0005 -0.0162  0.0018 -0.0133
                                     0.0002  0.0079 -0.0025  0.0077 -0.5255
```

```
                                    -0.0095 -0.0078 -0.0032  0.3891  0.0159
                                     0.0066  0.0009 -0.4304 -0.0113 -0.0083
                                    -0.0003 -0.0060 -0.0068  0.0024  0.0005
                                    -0.1719 -0.0191  0.0040  0.0002
              ( 32.74%)  -0.5722* C 25 s( 61.54%)p 0.62( 38.43%)d 0.00(  0.03%)
                                     0.0002  0.7835 -0.0388  0.0035 -0.0008
                                     0.0000 -0.3811 -0.0276  0.0110  0.0004
                                     0.3741  0.0286 -0.0096 -0.0013 -0.3109
                                    -0.0225  0.0091  0.0002 -0.0123  0.0071
                                    -0.0083 -0.0015 -0.0027
1010. (0.32210) BD*( 1)Ir  1- C 26
              ( 67.52%)   0.8217*Ir  1 s( 36.02%)p 0.00(  0.08%)d 1.77( 63.90%)
                                    -0.0004  0.6001  0.0017  0.0004  0.0022
                                     0.0018 -0.0001 -0.0002 -0.0064 -0.0039
                                     0.0106  0.0005 -0.0081 -0.0002 -0.0072
                                     0.0003 -0.0148  0.0037 -0.0180 -0.1107
                                     0.0079 -0.0008 -0.0020 -0.5054 -0.0166
                                    -0.0082 -0.0009  0.2997  0.0245 -0.0004
                                     0.0008  0.1022 -0.0032  0.0008  0.0004
                                     0.5194  0.0106  0.0116  0.0024
              ( 32.48%)  -0.5699* C 26 s( 61.68%)p 0.62( 38.29%)d 0.00(  0.03%)
                                     0.0002  0.7844 -0.0380 -0.0036 -0.0006
                                     0.0000 -0.2265 -0.0179  0.0071  0.0006
                                     0.1424  0.0111 -0.0028 -0.0008  0.5559
                                     0.0395 -0.0165 -0.0011 -0.0048 -0.0093
                                     0.0073  0.0012  0.0110
1011. (0.32164) BD*( 1)Ir  2- C 39
              ( 67.37%)   0.8208*Ir  2 s( 35.56%)p 0.00(  0.09%)d 1.81( 64.36%)
                                    -0.0006  0.5963  0.0020 -0.0002  0.0014
                                     0.0018  0.0000  0.0002  0.0070  0.0019
                                    -0.0106 -0.0005  0.0122 -0.0009  0.0107
                                     0.0001 -0.0127  0.0046 -0.0156 -0.1987
                                     0.0035 -0.0031 -0.0026  0.3961  0.0174
                                     0.0031  0.0021 -0.5433 -0.0232 -0.0062
                                    -0.0008 -0.0461 -0.0075  0.0012  0.0001
                                     0.3857  0.0030  0.0113  0.0011
              ( 32.63%)  -0.5712* C 39 s( 61.60%)p 0.62( 38.37%)d 0.00(  0.03%)
                                     0.0002  0.7839 -0.0388 -0.0034 -0.0009
                                     0.0001  0.2061  0.0154 -0.0073 -0.0007
                                    -0.2638 -0.0204  0.0067  0.0011  0.5189
                                     0.0368 -0.0158 -0.0001 -0.0060  0.0068
                                    -0.0119 -0.0015  0.0075
1012. (0.32042) BD*( 1)Ir  2- C 40
              ( 67.44%)   0.8212*Ir  2 s( 36.05%)p 0.00(  0.08%)d 1.77( 63.87%)
                                    -0.0005  0.6004  0.0012  0.0004  0.0018
                                     0.0018 -0.0001  0.0002  0.0029  0.0053
                                    -0.0146 -0.0006  0.0129 -0.0008  0.0125
                                     0.0000  0.0111 -0.0011  0.0106 -0.4389
                                    -0.0055 -0.0055 -0.0031 -0.5010 -0.0161
                                    -0.0116 -0.0004  0.4150  0.0217  0.0029
                                     0.0018  0.1422 -0.0043  0.0042 -0.0002
                                    -0.0369 -0.0158  0.0040  0.0008
              ( 32.56%)  -0.5706* C 40 s( 61.62%)p 0.62( 38.35%)d 0.00(  0.03%)
                                     0.0002  0.7840 -0.0382  0.0039 -0.0007
                                     0.0000  0.3899  0.0290 -0.0107 -0.0010
                                    -0.3077 -0.0231  0.0070  0.0009 -0.3667
                                    -0.0269  0.0102  0.0009 -0.0108 -0.0100
                                     0.0081  0.0007  0.0001
```

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
114. LP (1)Ir 1	206. RY*(4)Ir 2	0.90	1.24	0.031
114. LP (1)Ir 1	657. RY*(4) C26	2.00	1.65	0.053
114. LP (1)Ir 1	**1028. BD*(2) O11- C25**	**1.77**	**0.48**	**0.026**
114. LP (1)Ir 1	**1030. BD*(1) O12- C26**	**8.20**	**0.49**	**0.056**
114. LP (1)Ir 1	**1031. BD*(2) O12- C26**	**1.21**	**0.35**	**0.018**
114. LP (1)Ir 1	**1032. BD*(3) O12- C26**	**2.34**	**0.79**	**0.039**
115. LP (2)Ir 1	638. RY*(3) C25	1.09	2.03	0.044
115. LP (2)Ir 1	639. RY*(4) C25	0.87	1.97	0.038
115. LP (2)Ir 1	**1027. BD*(1) O11- C25**	**2.85**	**0.31**	**0.027**
115. LP (2)Ir 1	**1028. BD*(2) O11- C25**	**9.29**	**0.48**	**0.060**
115. LP (2)Ir 1	**1029. BD*(3) O11- C25**	**1.30**	**0.82**	**0.030**
115. LP (2)Ir 1	**1030. BD*(1) O12- C26**	**1.25**	**0.49**	**0.022**
116. LP (3)Ir 1	175. RY*(2)Ir 1	0.58	1.39	0.027
116. LP (3)Ir 1	638. RY*(3) C25	0.99	2.04	0.042
116. LP (3)Ir 1	639. RY*(4) C25	0.87	1.98	0.039
116. LP (3)Ir 1	641. RY*(6) C25	0.78	1.70	0.034
116. LP (3)Ir 1	656. RY*(3) C26	1.12	2.35	0.048
116. LP (3)Ir 1	658. RY*(5) C26	0.77	1.68	0.034
116. LP (3)Ir 1	659. RY*(6) C26	0.61	1.61	0.030
116. LP (3)Ir 1	**1027. BD*(1) O11- C25**	**17.80**	**0.32**	**0.069**
116. LP (3)Ir 1	**1028. BD*(2) O11- C25**	**1.15**	**0.49**	**0.022**
116. LP (3)Ir 1	**1030. BD*(1) O12- C26**	**1.46**	**0.50**	**0.025**
116. LP (3)Ir 1	**1031. BD*(2) O12- C26**	**15.53**	**0.36**	**0.068**
117. LP (1)Ir 2	806. RY*(3) C39	0.62	2.08	0.033
117. LP (1)Ir 2	807. RY*(4) C39	0.57	1.70	0.029
117. LP (1)Ir 2	825. RY*(4) C40	1.33	1.82	0.045
117. LP (1)Ir 2	**1035. BD*(1) O15- C39**	**4.38**	**0.42**	**0.038**
117. LP (1)Ir 2	**1036. BD*(2) O15- C39**	**1.32**	**0.37**	**0.020**
117. LP (1)Ir 2	**1037. BD*(3) O15- C39**	**0.85**	**0.81**	**0.024**
117. LP (1)Ir 2	**1038. BD*(1) O16- C40**	**8.19**	**0.42**	**0.053**
117. LP (1)Ir 2	**1040. BD*(3) O16- C40**	**1.33**	**0.79**	**0.029**
118. LP (2)Ir 2	177. RY*(4)Ir 1	0.63	1.29	0.026
118. LP (2)Ir 2	807. RY*(4) C39	1.18	1.70	0.042
118. LP (2)Ir 2	825. RY*(4) C40	0.84	1.82	0.036
118. LP (2)Ir 2	**1035. BD*(1) O15- C39**	**5.94**	**0.42**	**0.045**
118. LP (2)Ir 2	**1036. BD*(2) O15- C39**	**2.38**	**0.38**	**0.027**
118. LP (2)Ir 2	**1037. BD*(3) O15- C39**	**1.17**	**0.82**	**0.028**
118. LP (2)Ir 2	**1038. BD*(1) O16- C40**	**5.44**	**0.43**	**0.043**
118. LP (2)Ir 2	**1040. BD*(3) O16- C40**	**0.65**	**0.79**	**0.021**
119. LP (3)Ir 2	204. RY*(2)Ir 2	0.60	1.39	0.027
119. LP (3)Ir 2	806. RY*(3) C39	1.18	2.10	0.047
119. LP (3)Ir 2	809. RY*(6) C39	0.93	1.63	0.037
119. LP (3)Ir 2	824. RY*(3) C40	1.48	2.29	0.055
119. LP (3)Ir 2	826. RY*(5) C40	0.69	1.67	0.032
119. LP (3)Ir 2	827. RY*(6) C40	0.54	1.67	0.028
119. LP (3)Ir 2	**1035. BD*(1) O15- C39**	**4.11**	**0.43**	**0.038**
119. LP (3)Ir 2	**1036. BD*(2) O15- C39**	**12.20**	**0.39**	**0.063**
119. LP (3)Ir 2	**1038. BD*(1) O16- C40**	**1.10**	**0.44**	**0.020**
119. LP (3)Ir 2	**1039. BD*(2) O16- C40**	**12.88**	**0.42**	**0.067**
119. LP (3)Ir 2	**1040. BD*(3) O16- C40**	**0.56**	**0.80**	**0.020**