

Supporting Information

Probing hyperconjugative aromaticity in 2*H*-pyrrolium and cyclopentadiene containing Group 9 transition metal substituent: Bridged carbonyl ligands can enhance aromaticity

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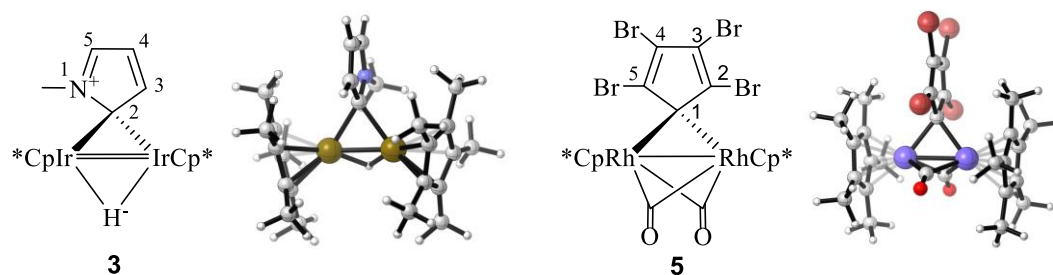


Figure S1. Structures of **3** ($C_{25}H_{37}Ir_2N$) and **5** ($C_{27}H_{30}Br_4O_2Rh_2$).

Table S1. Comparison of bond lengths (Å) and relative deriviations (RD) of $C_{25}H_{37}Ir_2N$.

	Exp.	B3LYP	B3PW91	M06	M06L	TPSS	PBE0	PBE0/def2-TZVP
N1-C2	1.362	1.415	1.411	1.405	1.409	1.426	1.406	1.400
C2-C3	1.442	1.418	1.417	1.409	1.414	1.427	1.414	1.406
C3-C4	1.383	1.406	1.403	1.405	1.402	1.407	1.403	1.398
C4-C5	1.363	1.394	1.393	1.389	1.390	1.401	1.391	1.384
C5-N1	1.352	1.359	1.354	1.357	1.360	1.364	1.352	1.349
RD(%) ^[a]	0.00	2.00	1.83	1.86	1.87	2.23	1.73	1.63

$$^{[a]} RD (\%) = \frac{1}{n} \sum \frac{|BL_{func.} - BL_{exp.}|}{BL_{exp.}} \times 100\%$$

Table S2. Comparison of bond lengths (Å) and relative deriviations (RD) of $C_{27}H_{30}Br_4O_2Rh_2$.

	Exp.	B3LYP	B3PW91	M06	M06L	TPSS	PBE0	PBE0/def2-TZVP
C1-C2	1.454	1.470	1.465	1.456	1.454	1.470	1.462	1.457
C2-C3	1.362	1.374	1.372	1.372	1.375	1.381	1.370	1.365
C3-C4	1.457	1.452	1.446	1.444	1.443	1.453	1.444	1.441
C4-C5	1.325	1.374	1.374	1.374	1.377	1.382	1.372	1.363
C5-C1	1.506	1.469	1.466	1.458	1.456	1.471	1.464	1.455
RD (%) ^[a]	0.00	1.70	1.72	1.73	1.83	1.88	1.67	1.53

$$^{[a]} RD (\%) = \frac{1}{n} \sum \frac{|BL_{func.} - BL_{exp.}|}{BL_{exp.}} \times 100\%$$

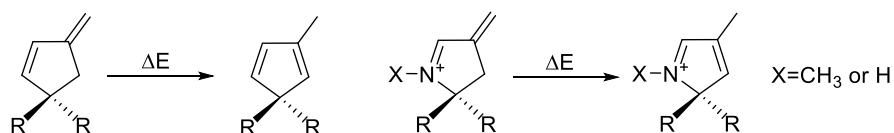


Figure S2. Isomerization stabilization energy (ISE) methods calculated by the electronic energy differences between the reactants and products.

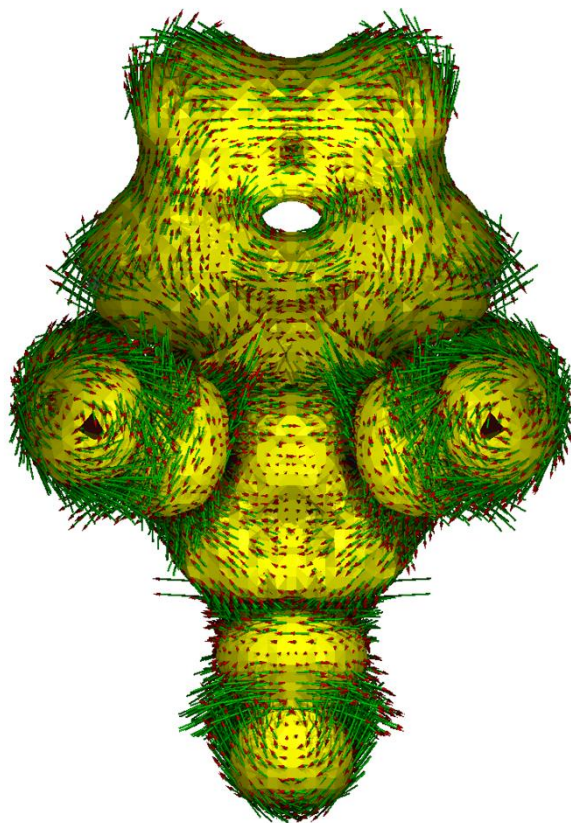


Figure S3. ACID graph for compound **11**. The isovalue of AICD surface is 0.02 a.u.

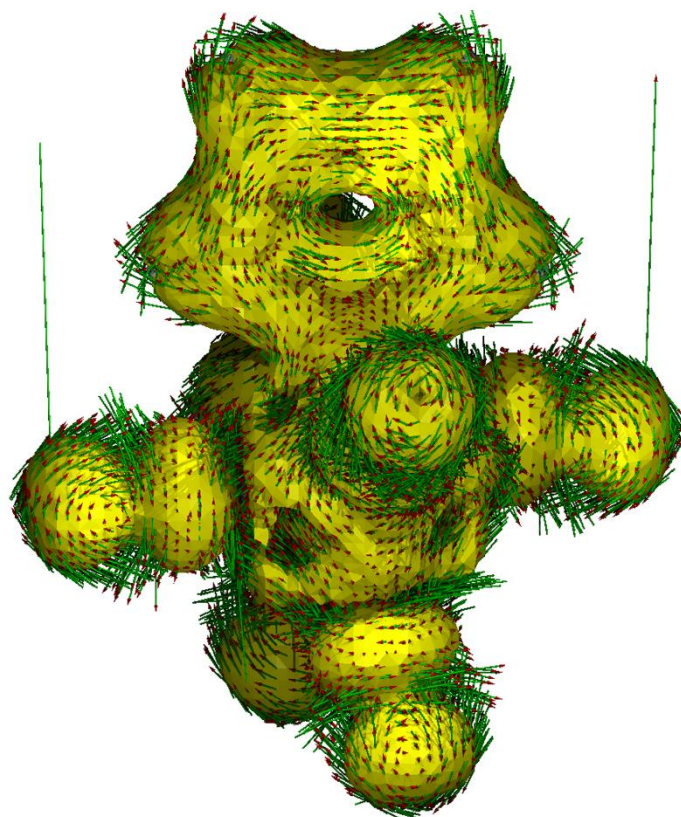


Figure S4. ACID graph for compound **12**. The isovalue of AICD surface is 0.02 a.u.

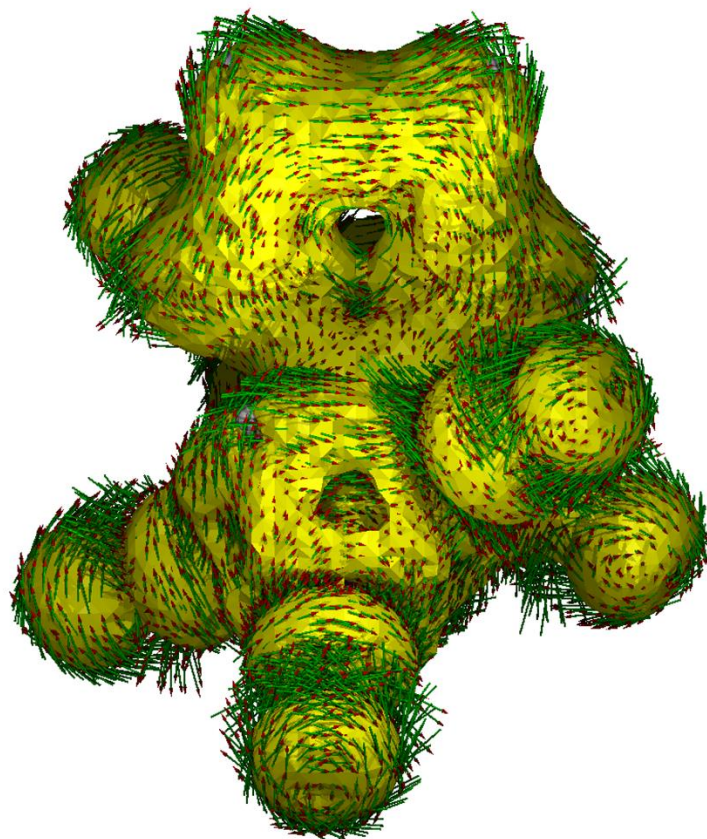


Figure S5. ACID graph for compound **13**. The isovalue of AICD surface is 0.02 a.u.

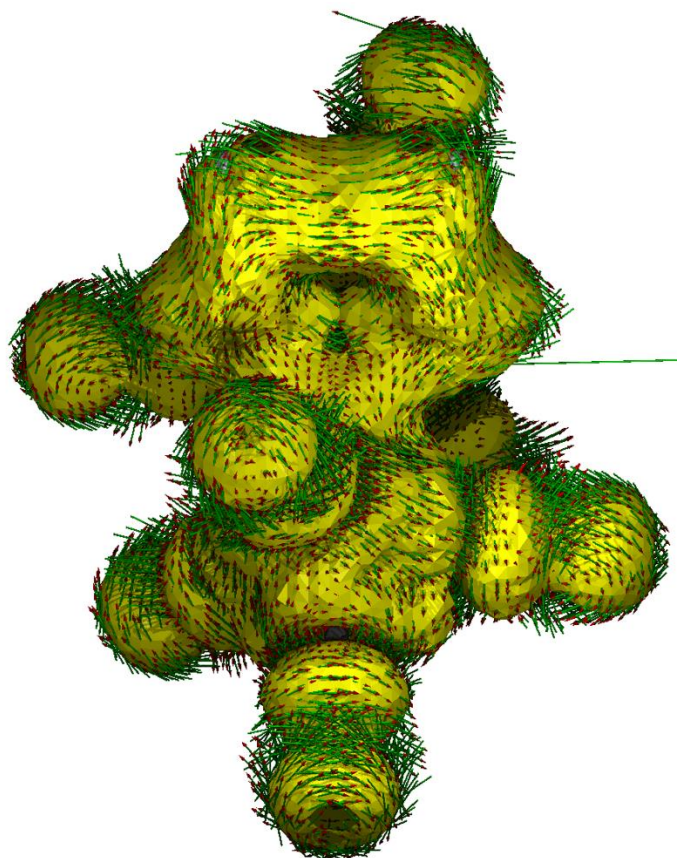


Figure S6. ACID graph for compound **14** The isovalue of AICD surface is 0.02 a.u.

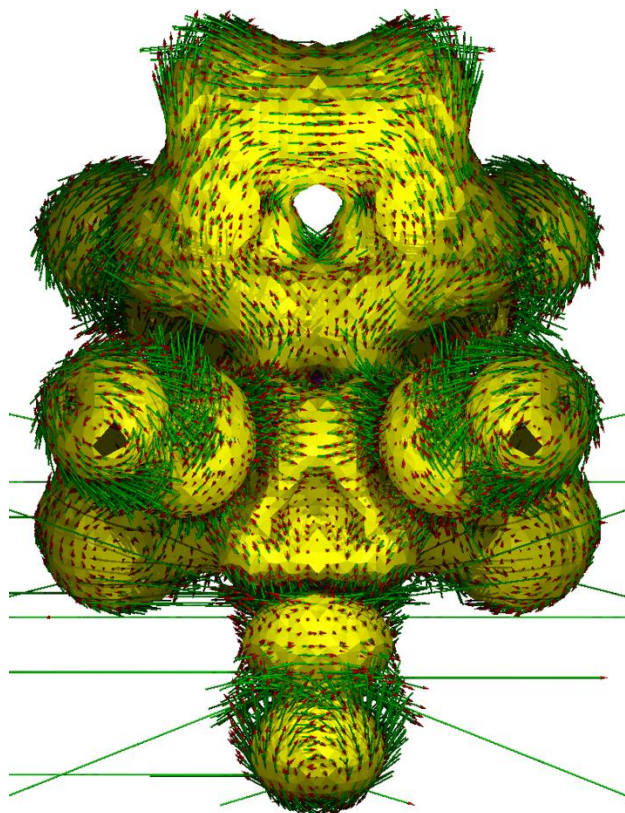


Figure S7. ACID graph for compound **15**. The isovalue of AICD surface is 0.02 a.u.

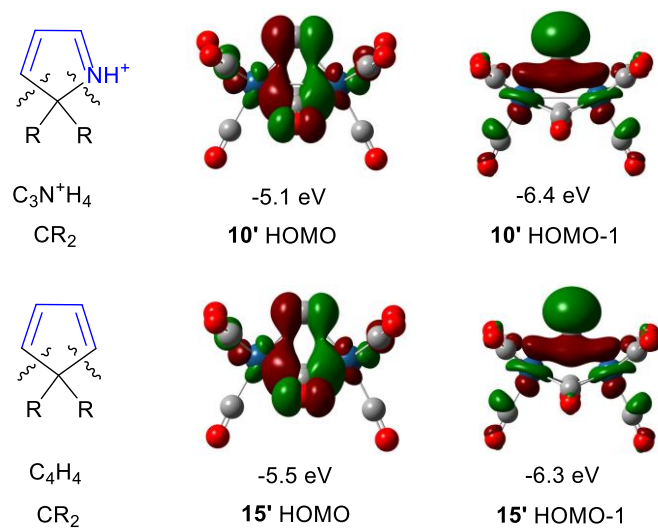


Figure S8. The HOMO and HOMO-1 orbitals of CR_2 fragments of compounds **10** and **15**.

Cartesian coordinates together with the electronic energies (a.u.) for all the complexes calculated in this study

1-Methyl-2H-pyrrolium

E = -249.363794

1 1

C	-0.17676200	-1.14000900	-0.00008600
C	-0.11748900	1.11108800	-0.00007900
H	0.30825200	2.11865900	-0.00020700
C	-1.50674100	0.74810900	-0.00002600
H	-2.33643100	1.45391800	-0.00015100
C	-1.55738600	-0.60609000	0.00013200
H	-2.44910500	-1.23541400	0.00044500
N	0.64828500	0.05432300	0.00040600
H	0.04535100	-1.76126700	0.88713200
H	0.04454500	-1.75909200	-0.88914200
C	2.09900800	0.01705400	-0.00002100
H	2.49095000	1.04108300	0.00070900
H	2.45761800	-0.51028300	0.89557700
H	2.45705200	-0.50878100	-0.89672700

1

E = -3792.566924

0 1

N	-0.00095800	2.49095600	-0.74815300
C	3.02634800	0.46601900	-0.09803100
C	2.86374400	-0.51432200	-1.11402600
C	2.27262200	-1.48648000	0.91528000
C	2.64704700	-0.12700300	1.15666600
C	3.44922600	1.88611400	-0.27890900
H	4.49689500	2.03756000	0.03094900
H	2.81723700	2.56327100	0.31565900
H	3.36515700	2.19819600	-1.32931700
C	3.12202500	-0.34108300	-2.57391800
H	4.11580800	-0.73032300	-2.85417800
H	3.08710800	0.71756300	-2.86746700
H	2.37591800	-0.87644900	-3.17899100
C	2.05715000	-2.99662900	-1.19655000
H	2.95023500	-3.63932800	-1.27888000
H	1.68279400	-2.81234800	-2.21347800
H	1.28276800	-3.56455000	-0.66203400
C	1.89002800	-2.48220200	1.95664700
H	2.78398800	-2.96775400	2.38555400
H	1.24811700	-3.27268400	1.54550200
H	1.34243400	-2.00668600	2.78269300

C	2.74346300	0.52565200	2.49475300
H	3.72066200	0.31163400	2.96115800
H	1.96389600	0.16107800	3.17918600
H	2.63574300	1.61573700	2.42018700
C	-3.00963800	0.48659900	0.10552000
C	-2.93554300	-0.36359900	-1.03179300
C	-2.42859600	-1.63859800	-0.59353600
C	-2.23319900	-1.58425700	0.82199000
C	-2.56256900	-0.25837100	1.25180800
C	-3.43195400	1.91829900	0.12814700
H	-4.44255400	2.02924300	0.55565600
H	-3.45205700	2.34863000	-0.88272600
H	-2.73824000	2.52504800	0.72924500
C	-3.29747800	-0.01334300	-2.43678600
H	-4.31890000	-0.35010600	-2.68443000
H	-2.61346900	-0.48412700	-3.15809800
H	-3.25939400	1.07205200	-2.60605800
C	-2.18989200	-2.82352100	-1.46962700
H	-3.10617100	-3.42719000	-1.58452700
H	-1.40798300	-3.47530600	-1.05562200
H	-1.86232100	-2.51852500	-2.47368100
C	-1.79963200	-2.70371500	1.70565700
H	-2.66951000	-3.20749300	2.16215500
H	-1.15639600	-2.34293300	2.51998100
H	-1.23356800	-3.46233900	1.14770400
C	-2.54745800	0.22767400	2.66237100
H	-3.46773100	-0.07694100	3.19015500
H	-2.48115500	1.32253900	2.70967900
H	-1.69434700	-0.18372600	3.22176300
C	-0.00276100	1.46319600	0.20565100
C	0.02151500	2.13593500	1.44094800
H	0.03157600	1.62834900	2.40305100
C	0.03816500	3.52507700	1.22793600
H	0.06263400	4.31872800	1.97348600
C	0.02178400	3.70462000	-0.15120000
H	0.02538200	4.62252500	-0.73895100
C	-0.04920800	2.29889400	-2.17433100
H	-1.01001100	2.64083500	-2.59209300
H	0.05917000	1.22603100	-2.37266100
H	0.76746400	2.84528200	-2.67125500
H	-0.00395600	-0.63873100	-1.25972300
C	2.36956100	-1.71788800	-0.49244400
Co	1.07012800	-0.20774100	-0.13813800
Co	-1.07379500	-0.20358700	-0.13245000

2

E = -1248.883265

O 1

N	0.01191600	2.62563300	-0.74571300
C	3.30926500	0.48394200	0.17216700
C	3.29458600	-0.35176000	-0.98236100
C	2.51250700	-1.61070600	0.82579800
C	2.81848800	-0.28403900	1.29291600
C	3.79039900	1.89611800	0.24278200
H	4.82126500	1.94526400	0.63423100
H	3.15163100	2.50567800	0.89780400
H	3.79068500	2.37047500	-0.74847700
C	3.77766300	0.00505400	-2.34886800
H	4.83153600	-0.29364300	-2.49175400
H	3.71721000	1.08756500	-2.53072300
H	3.18734300	-0.49543400	-3.12965500
C	2.63763900	-2.82889800	-1.47920800
H	3.58734000	-3.38975300	-1.52891300
H	2.37059100	-2.53640700	-2.50445000
H	1.86071900	-3.51812500	-1.12068500
C	2.09019100	-2.76346300	1.67341200
H	2.96540100	-3.28376200	2.10213600
H	1.51805000	-3.49988800	1.09256200
H	1.45491000	-2.43554300	2.50810500
C	2.79436800	0.17114000	2.71431000
H	3.75423900	-0.05188400	3.21334800
H	2.00094000	-0.33006100	3.28672300
H	2.62623800	1.25411000	2.78747400
C	-3.31330000	0.50167400	0.14955900
C	-3.29143800	-0.33790900	-1.00178800
C	-2.77194300	-1.62512100	-0.59742300
C	-2.53375700	-1.59509100	0.81850300
C	-2.83685400	-0.26522700	1.27762900
C	-3.78492700	1.91743200	0.20968700
H	-4.81970000	1.97579000	0.58939900
H	-3.76959100	2.38799500	-0.78323000
H	-3.14857700	2.52426200	0.86958500
C	-3.75859900	0.01776000	-2.37426200
H	-4.81217000	-0.27670300	-2.52750000
H	-3.16262300	-0.48741300	-3.14782400
H	-3.69065900	1.09949000	-2.55766100
C	-2.64402500	-2.82107100	-1.48294800
H	-3.59574500	-3.37809600	-1.53674400

H	-1.87247400	-3.51198700	-1.11616300
H	-2.36891300	-2.53396300	-2.50756400
C	-2.12494700	-2.74682600	1.67412600
H	-3.00652400	-3.26250200	2.09536500
H	-1.49724000	-2.41874900	2.51452300
H	-1.54950400	-3.48724600	1.10162700
C	-2.82556500	0.19305200	2.69826700
H	-3.78629700	-0.03871400	3.19162500
H	-2.66907500	1.27776100	2.77067200
H	-2.03097300	-0.29940300	3.27673600
C	0.00490700	1.56651900	0.17700400
C	-0.00653900	2.20853200	1.43647000
H	-0.02377500	1.67145100	2.38382600
C	-0.00265800	3.60082300	1.26490100
H	-0.01761700	4.37434800	2.03151800
C	0.01185500	3.81785600	-0.10986700
H	0.01987000	4.75420300	-0.66820400
C	0.08752500	2.48227500	-2.17843400
H	-0.31501800	3.38442200	-2.66074600
H	-0.50119500	1.60892900	-2.48710400
H	1.12620400	2.33028400	-2.51388400
H	-0.00223200	-0.72355400	-1.27726300
C	2.76428900	-1.63712500	-0.58785200
Rh	1.21995700	-0.16538100	-0.16714300
Rh	-1.22490100	-0.16013700	-0.17054200

3

E = -1236.521878

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Ir	1.23782700	-0.18762900	-0.09198300
Ir	-1.23563900	-0.18916200	-0.09024800
N	-0.00413300	2.61840400	-0.70655700
C	3.29238500	0.61033400	0.20156600
C	3.30591500	-0.15784800	-1.00416300
C	2.68361200	-1.57629500	0.75457900
C	2.91528000	-0.25677200	1.29496200
C	3.65088100	2.05398600	0.33255400
H	4.69340700	2.17378600	0.67387000
H	2.99464500	2.56466000	1.05152100
H	3.55259600	2.57853000	-0.62786800
C	3.71387500	0.32050700	-2.35733800
H	4.79666700	0.17731000	-2.52252700
H	3.49946100	1.39069300	-2.48853400
H	3.18588900	-0.22289100	-3.15364500

C	2.82299000	-2.64966400	-1.62246200
H	3.80864300	-3.13616100	-1.72376800
H	2.50750400	-2.32249700	-2.62319700
H	2.10638000	-3.40953900	-1.28210800
C	2.40029800	-2.81070200	1.54396000
H	3.33837300	-3.30454400	1.85441400
H	1.81759600	-3.53576100	0.95956200
H	1.82531500	-2.58163300	2.45181300
C	2.91744100	0.11005400	2.74181500
H	3.90752800	-0.07907100	3.19328400
H	2.17630500	-0.47397100	3.30536400
H	2.68377400	1.17357000	2.88576200
C	-3.29078800	0.60603200	0.20759300
C	-3.30828000	-0.16501900	-0.99633400
C	-2.88847600	-1.50672000	-0.66095100
C	-2.67665400	-1.57846700	0.76286500
C	-2.90854500	-0.25808700	1.30144400
C	-3.64855300	2.05008000	0.33705100
H	-4.69079000	2.17150700	0.67863300
H	-3.55001200	2.57371000	-0.62398000
H	-2.99136300	2.56096100	1.05503500
C	-3.72693500	0.30676200	-2.34839200
H	-4.80472300	0.13188500	-2.51598700
H	-3.18160200	-0.21611600	-3.14685300
H	-3.54615800	1.38374400	-2.47370700
C	-2.82371300	-2.65650000	-1.61198900
H	-3.80894300	-3.14489900	-1.70839300
H	-2.10432300	-3.41473000	-1.27380600
H	-2.51323000	-2.32999100	-2.61451100
C	-2.38831500	-2.81063600	1.55390100
H	-3.32441600	-3.30301900	1.87250500
H	-1.80665300	-2.57921500	2.45690700
H	-1.81026100	-3.53777900	0.96748600
C	-2.90554900	0.11188200	2.74747700
H	-3.89531400	-0.07196500	3.20182800
H	-2.66675700	1.17465100	2.88861600
H	-2.16559000	-0.47419700	3.31040400
C	-0.00260200	1.56813200	0.22789400
C	0.00413800	2.21805200	1.48324400
H	0.01185500	1.68392700	2.43194800
C	0.00510300	3.60864900	1.29739100
H	0.01393200	4.38777500	2.05846200
C	-0.00127800	3.81573600	-0.07801100
H	-0.00300200	4.74712400	-0.64434100

C	-0.04087600	2.46964800	-2.13900600
H	0.74564400	3.07840700	-2.61147500
H	-1.01741000	2.77538800	-2.54921700
H	0.12733900	1.41259400	-2.37890200
H	0.00036600	-0.84963000	-1.15503300
C	2.88994800	-1.50123500	-0.66995700

4

E = -1418.716899

O 1

Rh	-0.36541000	-1.24009300	-0.16804500
Rh	0.36541000	1.24009300	-0.16804500
O	-2.48827100	0.72963200	-0.89071000
O	2.48827100	-0.72963200	-0.89071000
C	-1.40536300	0.40327900	-0.57802100
C	1.40536300	-0.40327900	-0.57802100
C	0.00000000	0.00000000	1.49860800
C	-1.11038100	0.34233400	2.38349400
C	-0.69326600	0.21575700	3.68160100
C	0.69326600	-0.21575700	3.68160100
C	1.11038100	-0.34233400	2.38349400
C	-0.15553500	3.37883600	0.19478600
C	1.11825800	3.07790400	0.80974400
C	2.04736800	2.74551700	-0.23059500
C	1.34752500	2.82354800	-1.48758400
C	0.00000000	3.23556200	-1.22368900
C	-1.37310400	3.87276600	0.90371900
C	1.40833500	3.19701000	2.26839200
C	3.49770300	2.42693400	-0.07724900
C	1.97651400	2.62092600	-2.82668300
C	-1.06157600	3.51491100	-2.23486300
C	0.15553500	-3.37883600	0.19478600
C	0.00000000	-3.23556200	-1.22368900
C	-1.34752500	-2.82354800	-1.48758400
C	-2.04736800	-2.74551700	-0.23059500
C	-1.11825800	-3.07790400	0.80974400
C	1.37310400	-3.87276600	0.90371900
C	1.06157600	-3.51491100	-2.23486300
C	-1.97651400	-2.62092600	-2.82668300
C	-3.49770300	-2.42693400	-0.07724900
C	-1.40833500	-3.19701000	2.26839200
H	-1.38351700	4.97558400	0.95553900
H	-2.29276500	3.55631400	0.39041700
H	-1.41639000	3.48825900	1.93212400

H	2.38325300	2.76241000	2.52249100
H	1.41832300	4.25806100	2.56947900
H	0.65222100	2.67590000	2.87558800
H	4.12446300	3.25757500	-0.44311900
H	3.77525600	1.52370400	-0.64220100
H	3.75898100	2.24863200	0.97433800
H	2.70135000	1.79431100	-2.80836000
H	1.22814100	2.39340900	-3.59819800
H	2.51881700	3.52717000	-3.14736900
H	-1.19753400	4.60154800	-2.36582600
H	-0.80790700	3.09087200	-3.21590100
H	-2.02927300	3.09114800	-1.92837100
H	1.38351700	-4.97558400	0.95553900
H	2.29276500	-3.55631400	0.39041700
H	1.41639000	-3.48825900	1.93212400
H	1.19753400	-4.60154800	-2.36582600
H	0.80790700	-3.09087200	-3.21590100
H	2.02927300	-3.09114800	-1.92837100
H	-2.51881700	-3.52717000	-3.14736900
H	-2.70135000	-1.79431100	-2.80836000
H	-1.22814100	-2.39340900	-3.59819800
H	-4.12446300	-3.25757500	-0.44311900
H	-3.75898100	-2.24863200	0.97433800
H	-3.77525600	-1.52370400	-0.64220100
H	-1.41832300	-4.25806100	2.56947900
H	-0.65222100	-2.67590000	2.87558800
H	-2.38325300	-2.76241000	2.52249100
H	-2.10434500	0.64239800	2.04859800
H	-1.29503200	0.39848600	4.57433800
H	1.29503200	-0.39848600	4.57433800
H	2.10434500	-0.64239800	2.04859800

5

E = -11710.602243

O 1

Rh	1.28515100	0.03959300	-1.27859400
Rh	-1.28515100	-0.03959300	-1.27859400
O	0.06312800	-2.39337400	-2.54351600
O	-0.06312800	2.39337400	-2.54351600
C	0.00000000	-1.39683100	-1.93561000
C	0.00000000	1.39683100	-1.93561000
C	0.00000000	0.00000000	0.39100400
C	0.03094900	-1.14421600	1.29729800
C	0.01741700	-0.72290000	2.60356400

C	-0.01741700	0.72290000	2.60356400
C	-0.03094900	1.14421600	1.29729800
C	-3.21328300	-0.99237500	-0.72383400
C	-3.21222500	0.39143800	-0.27821500
C	-3.15515000	1.23397000	-1.42837200
C	-3.06043100	0.38237500	-2.58935100
C	-3.13947300	-0.98487500	-2.15079600
C	-3.39530900	-2.18421700	0.15339300
C	-3.33721100	0.82131000	1.14344400
C	-3.20360100	2.72288300	-1.46144600
C	-3.02040000	0.87092300	-3.99831400
C	-3.16062300	-2.19366700	-3.02372100
C	3.21328300	0.99237500	-0.72383400
C	3.13947300	0.98487500	-2.15079600
C	3.06043100	-0.38237500	-2.58935100
C	3.15515000	-1.23397000	-1.42837200
C	3.21222500	-0.39143800	-0.27821500
C	3.39530900	2.18421700	0.15339300
C	3.16062300	2.19366700	-3.02372100
C	3.02040000	-0.87092300	-3.99831400
C	3.20360100	-2.72288300	-1.46144600
C	3.33721100	-0.82131000	1.14344400
H	-4.46756100	-2.39431400	0.30968700
H	-2.93437600	-3.08000000	-0.28388000
H	-2.93597100	-2.03023100	1.13950800
H	-2.97227800	1.84627500	1.28982800
H	-4.39188100	0.77937400	1.46294600
H	-2.75512800	0.16811700	1.80951100
H	-4.18757400	3.07065000	-1.81759800
H	-2.43711600	3.13234000	-2.13669100
H	-3.02786500	3.15026600	-0.46603100
H	-2.38033200	1.76031900	-4.08901200
H	-2.63024900	0.10427900	-4.68126300
H	-4.02954900	1.14898100	-4.34671000
H	-4.19377100	-2.55474200	-3.15574200
H	-2.74834200	-1.98024500	-4.01872500
H	-2.56697900	-3.01107400	-2.59157000
H	4.46756100	2.39431400	0.30968700
H	2.93437600	3.08000000	-0.28388000
H	2.93597100	2.03023100	1.13950800
H	4.19377100	2.55474200	-3.15574200
H	2.74834200	1.98024500	-4.01872500
H	2.56697900	3.01107400	-2.59157000
H	4.02954900	-1.14898100	-4.34671000

H	2.38033200	-1.76031900	-4.08901200
H	2.63024900	-0.10427900	-4.68126300
H	4.18757400	-3.07065000	-1.81759800
H	3.02786500	-3.15026600	-0.46603100
H	2.43711600	-3.13234000	-2.13669100
H	4.39188100	-0.77937400	1.46294600
H	2.75512800	-0.16811700	1.80951100
H	2.97227800	-1.84627500	1.28982800
Br	-0.14204500	2.94268900	0.79656000
Br	-0.06676200	1.78218100	4.13599300
Br	0.06676200	-1.78218100	4.13599300
Br	0.14204500	-2.94268900	0.79656000

6

E= -1096.531677

1 1

C	0.00003300	1.49077400	0.01747800
C	0.00015000	2.40407300	1.13738800
H	0.00012700	2.07889500	2.17799600
C	0.00028200	3.70815700	0.68834800
H	0.00039500	4.62309000	1.27791800
H	0.00004000	2.05247900	-2.06135000
C	0.00025800	3.64034100	-0.71988900
H	0.00034100	4.45587700	-1.44539000
Ir	-1.24892800	-0.24133700	-0.00702500
Ir	1.24890000	-0.24143800	-0.00702700
C	-2.44295400	0.14499200	1.47129500
C	-1.50294000	-2.16497300	-0.07126900
C	-2.57297000	0.22865200	-1.34911500
C	1.50267500	-2.16509600	-0.07129100
C	2.57298700	0.22842900	-1.34911500
C	2.44298900	0.14476000	1.47127700
O	-3.06288600	0.36228900	2.39570800
O	-3.26897100	0.51554200	-2.19817800
O	-1.65479700	-3.28909900	-0.10580600
O	1.65437000	-3.28924400	-0.10584100
O	3.26901300	0.51524100	-2.19818400
O	3.06295800	0.36196900	2.39568600
N	0.00009800	2.36986800	-1.09784600

7

E = -1097.756007

1 1

Ir	1.34645000	-0.23789900	0.07179000
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Ir	-1.35807500	-0.20676900	-0.07295600
C	0.00015500	1.45628700	0.02135900
C	0.03868400	2.36247100	1.14870500
H	0.04266900	2.03524000	2.18797000
C	0.08776400	3.66818500	0.71153500
H	0.13181300	4.57600200	1.31012600
C	0.07260300	3.61228200	-0.69693300
H	0.09193200	4.43275400	-1.41648100
H	-0.03927500	2.04752600	-2.05153500
C	-1.86066000	-2.03392400	-0.46225700
O	-2.10450200	-3.10259700	-0.74971300
C	-1.48515700	-0.38760000	1.92593600
O	-1.56497800	-0.50500800	3.04800800
C	1.50942400	-0.35173100	-1.92660100
O	1.60159100	-0.42716200	-3.05253200
C	1.80413200	-2.08393000	0.40719800
O	2.02606000	-3.16708900	0.65611400
C	-3.07561400	0.64239500	-0.38490400
O	-4.05632800	1.16351800	-0.60899800
C	3.06652600	0.57385100	0.47167100
O	4.04660000	1.06702600	0.75310700
H	-1.12820700	-0.09004600	-1.66754200
H	1.08988000	-0.17587400	1.66222300
N	0.02451400	2.34780400	-1.08530300

8

E = -1098.881495

1 1

Ir	1.91556300	-0.20828900	-0.13891100
Ir	-1.92727900	-0.16983600	0.12394100
C	-0.00836100	0.95733900	0.03878600
H	0.01487400	1.50606000	2.12321700
C	0.09997300	3.10860200	0.80645600
H	0.13435400	3.91172200	1.54497600
C	0.09158200	3.19694600	-0.59928500
H	0.13561200	4.11621600	-1.18018000
C	0.02126000	1.89807700	-1.06459300
H	-0.01182300	1.58776900	-2.10893800
H	-2.27320400	0.56348200	1.58107700
H	2.21256200	0.41588200	-1.65386900
C	-2.77802300	1.34047700	-0.77213100
O	-3.31529000	2.20265900	-1.26678400
C	-3.58722100	-1.15207200	0.07667100
O	-4.55723200	-1.73234100	0.03341500

C	-1.12086200	-1.57171500	1.20326400
O	-0.72522200	-2.39470700	1.87005900
C	1.06192400	-1.64686700	-1.13795300
O	0.66032400	-2.49246900	-1.77127000
C	3.53965500	-1.23613300	-0.06543800
O	4.48994800	-1.84465300	0.01470800
C	2.82667700	1.36079800	0.55656800
O	3.36555600	2.28602500	0.91977300
H	-1.49317600	-0.81114300	-1.34357900
H	1.52218200	-0.75417100	1.38449000
N	0.06234800	1.83585600	1.16459900

9

E = -1322.779162

1 1

C	0.00774400	0.97556600	-0.00638900
C	-0.00523700	1.87904000	1.12964600
H	-0.01779000	1.54022800	2.16588800
C	-0.02410700	3.19484100	0.71645300
H	-0.04531900	4.09170500	1.33247100
H	0.03312100	1.62252400	-2.07259400
C	-0.02386900	3.16034700	-0.69143400
H	-0.03235100	3.99154700	-1.39905200
Ir	-1.94150900	-0.18285800	0.01031400
Ir	1.94680100	-0.18112400	-0.01614200
C	1.16617400	-1.45768600	-1.27759200
C	2.82743800	1.50264500	-0.53580500
C	3.62305600	-1.13596100	-0.08731000
C	1.81415900	-0.45364600	1.93498000
C	-3.60635300	-1.15654800	0.01373900
C	-1.79228200	-0.34601800	-1.93702400
C	-2.84778200	1.43237700	0.71056100
C	-1.17038400	-1.48822700	1.25628100
O	3.33627300	2.47556700	-0.82915400
O	1.78147900	-0.60685500	3.06005400
O	0.76212900	-2.23044300	-2.00908400
O	4.60635200	-1.69423600	-0.13938700
O	-4.58276600	-1.72917100	0.00878600
O	-0.77646600	-2.27632000	1.97536900
O	-1.71108300	-0.41082700	-3.07090700
O	-3.43218800	2.32547900	1.09801000
N	-0.00376500	1.90209500	-1.09772500

10

E = -1322.777646

1 1

O	0.00020500	-1.32668400	-2.40654900
O	0.00016500	-1.51256900	2.31552900
C	0.00013700	-0.88100300	-1.31549700
C	0.00010800	-0.97621700	1.26887800
C	0.00012600	1.46618600	0.04065900
C	-0.00092700	3.61926900	-0.66251900
C	-0.00114300	3.65673700	0.73021200
C	-0.00045400	2.32917700	1.16465500
H	-0.00037400	1.99521300	2.20324800
H	-0.00172100	4.55533700	1.34402300
H	-0.00127000	4.43655600	-1.38348900
H	0.00011900	2.03729800	-2.02603800
Ir	1.49508400	-0.24460000	-0.00255000
Ir	-1.49496400	-0.24491600	-0.00257600
C	2.58734000	0.54793900	1.53629900
C	2.40619100	-1.95555400	-0.04722300
C	2.61266300	0.63105100	-1.45882200
C	-2.40568500	-1.95599800	-0.04737900
C	-2.58748100	0.54737800	1.53621800
C	-2.61258200	0.63072800	-1.45885100
O	3.15638700	0.95910500	2.41908700
O	3.22529200	1.07398100	-2.29750600
O	2.91738700	-2.96375600	-0.07997800
O	-2.91669500	-2.96429500	-0.08022400
O	-3.22524800	1.07357800	-2.29755100
O	-3.15678800	0.95827400	2.41896500
N	-0.00019500	2.33272600	-1.05671300

11

E = -1080.107544

0 1

C	-0.00024000	1.43796800	0.00006500
C	-0.00059200	2.34657000	-1.16338000
H	-0.00040000	2.01088000	-2.20154300
C	-0.00120300	3.63823200	-0.72480700
H	-0.00162300	4.53287500	-1.35039100
C	-0.00065500	2.34645700	1.16359600
H	-0.00052500	2.01066700	2.20172700
C	-0.00124000	3.63816200	0.72514800
H	-0.00169500	4.53274500	1.35081900
Ir	1.26193100	-0.25652400	0.00001300
Ir	-1.26179100	-0.25705500	-0.00003900

C	2.44696800	0.27961800	-1.41251900
C	1.51224300	-2.19144100	-0.00007600
C	2.44688700	0.27954300	1.41264700
C	-1.51076100	-2.19213100	-0.00014000
C	-2.44718800	0.27832900	1.41246300
C	-2.44711300	0.27856800	-1.41252200
O	3.09151500	0.58919900	-2.30086600
O	3.09137700	0.58908300	2.30105000
O	1.64583600	-3.32517400	-0.00012900
O	-1.64360000	-3.32595400	-0.00020000
O	-3.09195000	0.58742100	2.30082700
O	-3.09182600	0.58782200	-2.30086300

12

E = -1081.328237

O 1

Ir	1.36169300	-0.24073400	0.06467500
Ir	-1.36169200	-0.24071300	-0.06467100
C	0.00000300	1.41107200	-0.00001800
C	-0.01552700	2.33085300	1.16409100
H	-0.00808800	2.00424000	2.20479000
C	-0.00957400	3.61602300	0.72806200
H	-0.01248400	4.50964000	1.35496400
C	0.00968100	3.61600800	-0.72814000
H	0.01265400	4.50961300	-1.35505800
C	0.01551500	2.33083000	-1.16414400
H	0.00803900	2.00419900	-2.20483700
C	-1.86126900	-2.08550800	-0.41635400
O	-2.10359900	-3.16289900	-0.69820600
C	-1.46845500	-0.33212800	1.92111000
O	-1.54075700	-0.39867500	3.05320300
C	1.46844000	-0.33219300	-1.92110300
O	1.54076800	-0.39887000	-3.05318700
C	1.86130300	-2.08551400	0.41640000
O	2.10352100	-3.16292200	0.69828200
C	-2.96657400	0.74344900	-0.43883400
O	-3.89246600	1.35057900	-0.70384200
C	2.96656400	0.74346000	0.43879400
O	3.89242200	1.35062700	0.70383500
H	-1.10668200	-0.15855300	-1.65933100
H	1.10667700	-0.15851700	1.65933200

13

E = -1082.451833

O 1

Ir	1.91491400	-0.20035100	-0.17045100
Ir	-1.91489400	-0.20029600	0.17050400
C	0.00002400	0.94044400	-0.00011400
C	0.07580500	1.87175100	1.15288200
H	0.09068800	1.55265100	2.19711200
C	0.05043100	3.16487000	0.71838600
H	0.08489700	4.05455500	1.34971100
C	-0.05034900	3.16471700	-0.71907200
H	-0.08481200	4.05426800	-1.35058700
C	-0.07574600	1.87150800	-1.15330000
H	-0.09062700	1.55219600	-2.19746500
H	-2.42893800	1.03393300	1.16219100
H	2.42897600	1.03370700	-1.16234600
C	-2.57124900	0.84930600	-1.32938500
O	-3.05042100	1.41952000	-2.18676600
C	-3.56103200	-1.19583100	0.29704300
O	-4.52124100	-1.80273100	0.36754900
C	-1.15798500	-1.01433100	1.75095200
O	-0.74835500	-1.45906700	2.71148700
C	1.15802200	-1.01473300	-1.75073400
O	0.74829200	-1.45974400	-2.71109800
C	3.56108100	-1.19584500	-0.29688100
O	4.52129800	-1.80273300	-0.36739000
C	2.57121300	0.84954700	1.32924300
O	3.05005000	1.42010400	2.18658400
H	-1.27037200	-1.35143400	-0.84226800
H	1.27038200	-1.35127900	0.84254400

14

E = -1306.354781

O 1

C	0.00000000	0.94529300	0.00001800
C	-0.00702600	1.87667400	1.15913600
H	-0.04272100	1.55634000	2.20154200
C	-0.00299300	3.16616400	0.72419200
H	-0.01906300	4.05631000	1.35556200
C	0.00698800	1.87671800	-1.15906600
H	0.04268700	1.55642300	-2.20148400
C	0.00292200	3.16619100	-0.72407300
H	0.01896100	4.05636200	-1.35540800
Ir	-1.94245800	-0.19362600	0.01827400
Ir	1.94245700	-0.19361000	-0.01828100
C	1.15253700	-1.41232400	-1.30594900

C	2.77053200	1.49119000	-0.63675800
C	3.61755400	-1.16431200	-0.04908100
C	1.80676200	-0.33484100	1.92524700
C	-3.61753100	-1.16436400	0.04904200
C	-1.80676100	-0.33476400	-1.92525800
C	-2.77055900	1.49115700	0.63677400
C	-1.15250300	-1.41234700	1.30591200
O	3.34356900	2.41463900	-0.97534700
O	1.77118100	-0.41844300	3.06308700
O	0.73457100	-2.16086100	-2.06226400
O	4.59667200	-1.74478900	-0.06717700
O	-4.59663100	-1.74487400	0.06714300
O	-0.73450300	-2.16085500	2.06223700
O	-1.77118100	-0.41828100	-3.06310500
O	-3.34358600	2.41461200	0.97536300

15

E = -1306.343924

O 1

O	0.00043400	-1.39457700	-2.33387000
O	0.00019300	-1.39501000	2.33368400
C	0.00029400	-0.89382900	-1.25684300
C	0.00016500	-0.89374800	1.25689600
C	0.00001400	1.35155800	0.00000800
C	-0.00057600	2.24332000	-1.15974800
C	-0.00163800	3.54118000	-0.72064100
C	-0.00167100	3.54118300	0.72064800
C	-0.00069100	2.24332400	1.15976100
H	-0.00043400	1.91438500	2.20147600
H	-0.00241100	4.43174900	1.35174600
H	-0.00234100	4.43174400	-1.35174300
H	-0.00021700	1.91437800	-2.20146200
Ir	1.54317700	-0.23822900	0.00008300
Ir	-1.54293000	-0.23871900	-0.00007600
C	2.57668400	0.63374500	1.50000600
C	2.45429300	-1.95039900	0.00013500
C	2.57683800	0.63377800	-1.49971100
C	-2.45333300	-1.95120200	-0.00013300
C	-2.57700200	0.63288400	1.49969600
C	-2.57685600	0.63292900	-1.49992400
O	3.08097700	1.11040800	2.39577300
O	3.08120700	1.11037500	-2.39547100
O	2.92817000	-2.98399300	0.00016000
O	-2.92675000	-2.98501200	-0.00016300

O	-3.08154700	1.10917800	-2.39568600
O	-3.08177900	1.10917800	2.39538600

16

E = -806.455610

1 1

Ir	-1.28781800	-0.18100400	0.37235600
Ir	1.28489800	-0.19406500	-0.37326400
C	-2.94305300	-0.08504500	-1.30444500
C	-3.48042200	0.00004300	0.01525000
C	-2.40955300	-2.03811700	-0.19527000
C	-2.28715300	-1.33358300	-1.43660000
C	2.93141200	-0.05592200	1.29868000
C	2.29505500	-1.31296600	1.45172000
C	2.43124900	-2.03474200	0.22390700
C	3.18354900	-1.22699600	-0.68468800
C	3.47263300	0.01574700	-0.02079000
C	0.01499500	1.41626000	0.02129100
H	-0.56517600	2.00073000	-1.96452000
C	-0.19731800	3.57462800	-0.65964200
H	-0.40283500	4.39835000	-1.34530500
C	0.22037500	3.62768300	0.68775200
H	0.38830300	4.53639000	1.26234700
C	-3.17499100	-1.22842600	0.69906400
C	0.34927200	2.32078300	1.10199100
H	0.63610500	1.97995800	2.09545600
H	-1.44493000	0.57713600	1.73520300
H	-0.40054600	-0.81557000	1.50728300
H	1.39898500	0.53011900	-1.75863300
H	0.39868800	-0.90244000	-1.46761100
H	-3.04721600	0.67129800	-2.08166100
H	-1.78748900	-1.70477400	-2.33061200
H	-4.08013500	0.81833300	0.41167700
H	-3.50488100	-1.50758200	1.69847600
H	-2.03642200	-3.04036100	0.00990200
H	3.51803900	-1.51832600	-1.67911800
H	4.06197500	0.83630700	-0.42769900
H	3.01206400	0.71919900	2.05966400
H	1.79746000	-1.67457400	2.35069800
H	2.07303200	-3.04541500	0.03346500
N	-0.31806100	2.31220700	-1.03262400

17

E = -807.603584

1 1

Ir	-1.85323700	-0.46058100	-0.02291900
Ir	1.85323900	-0.46056400	-0.02296400
C	-3.39054400	1.30194800	0.15958800
C	-3.56308500	0.40899300	1.25157300
C	-3.93603200	-0.76571100	-0.70947300
C	-3.61493800	0.59054700	-1.05089600
C	3.39056100	1.30192200	0.15982300
C	3.56308800	0.40880300	1.25167100
C	3.90267300	-0.87721600	0.71743700
C	3.93603500	-0.76561600	-0.70954500
C	3.61494900	0.59069700	-1.05076700
C	-0.00000600	0.68011400	-0.01637700
H	-0.00002600	1.30387600	-2.07550400
C	-0.00002500	2.86344100	-0.70152900
H	-0.00003900	3.69486200	-1.40875000
C	-0.00000900	2.89743400	0.70582400
H	-0.00001100	3.79532000	1.32105500
C	-3.90267900	-0.87709900	0.71752800
C	0.00001300	1.57687000	1.11958100
H	0.00002700	1.22280900	2.15008400
H	1.16581900	-0.89505700	-1.37549100
H	-1.27347100	-1.91684000	-0.11993800
H	1.27338700	-1.91678400	-0.12006200
H	-1.10003100	-1.05150000	1.23131700
H	-1.16575000	-0.89518900	-1.37537400
H	1.10004200	-1.05155900	1.23124300
N	-0.00002000	1.60366600	-1.10727900
H	-3.11652500	2.35367800	0.23974700
H	-3.59600300	1.01014500	-2.05561600
H	-4.20884700	-1.55706400	-1.40633100
H	-4.13910800	-1.77027600	1.29418400
H	-3.48395400	0.66445600	2.30723200
H	3.59602700	1.01044700	-2.05542400
H	3.11655000	2.35364200	0.24013600
H	3.48395000	0.66410700	2.30736900
H	4.13908700	-1.77048100	1.29396200
H	4.20884700	-1.55686700	-1.40651800

18

E = -804.862788

0 1

Ir	1.22971400	-0.27143600	-0.09625100
Ir	-1.22969500	-0.27146900	-0.09624400

C	3.37474700	0.36850500	0.07065500
C	3.29348300	-0.61266100	-0.94805800
C	2.54873100	-1.58135000	1.02799800
C	2.89989000	-0.21295700	1.29389600
C	-3.37468400	0.36849100	0.07090100
C	-3.29351900	-0.61246200	-0.94802800
C	-2.76311900	-1.81700100	-0.36489000
C	-2.54869000	-1.58159200	1.02779500
C	-2.89980000	-0.21324800	1.29400000
C	-0.00000300	1.48613000	0.04490700
C	-0.00008400	2.33987700	1.17489400
H	-0.00009400	1.97514800	2.20048700
C	-0.00010000	3.67553200	0.75461800
H	-0.00013300	4.57084000	1.37426200
C	-0.00005400	3.65313300	-0.64017600
H	-0.00005400	4.47741400	-1.35266600
H	0.00000900	-0.80686100	-1.25192000
C	2.76309400	-1.81707100	-0.36464100
H	-0.00009700	2.04796200	-1.99774600
H	3.70653900	1.39785800	-0.05529600
H	2.85908000	0.28357800	2.26198200
H	2.18956900	-2.30629400	1.75624900
H	2.59236400	-2.75698800	-0.88700200
H	3.56156900	-0.47484000	-1.99405000
H	-2.18952600	-2.30670700	1.75587400
H	-2.85893800	0.28308100	2.26218900
H	-3.70643500	1.39788700	-0.05481700
H	-3.56166000	-0.47441500	-1.99397500
H	-2.59242600	-2.75680700	-0.88746100
N	-0.00008500	2.37040500	-1.03960200

19

E = -1080.155493

O 1

O	0.59021000	-1.40304900	2.42825300
O	-0.59015900	-1.40304000	-2.42830300
C	0.21447200	-0.91932900	1.44763300
C	-0.21439500	-0.91929400	-1.44770900
C	-0.00006200	1.44631300	-0.00005000
C	0.11283500	2.32827000	1.15801400
C	0.06216500	3.62898800	0.71546900
C	-0.06245100	3.62896200	-0.71563000
C	-0.11302700	2.32822700	-1.15813600
H	-0.23346600	1.99117200	-2.18849200

H	-0.12391000	4.52079100	-1.34158100
H	0.12355800	4.52084000	1.34139400
H	0.23329000	1.99125400	2.18838100
Ir	-1.35505000	-0.21080400	0.22307400
Ir	1.35503200	-0.21074200	-0.22309300
C	2.70950700	0.85818100	0.58652600
O	3.53546900	1.51444000	1.01461600
C	2.49845800	-1.71377400	-0.58207500
O	3.20416100	-2.57513800	-0.83033000
C	-2.70958900	0.85801900	-0.58654500
O	-3.53595600	1.51425300	-1.01389200
C	-2.49836300	-1.71394400	0.58198200
O	-3.20314600	-2.57605400	0.83026900

20

E = -2470.311865

O 1

O	0.81184000	-1.10262100	2.33640000
O	-0.81175900	-1.10273400	-2.33637900
C	0.38065300	-0.61765700	1.34764400
C	-0.38062600	-0.61768200	-1.34765300
C	0.00007600	1.73914500	0.00005100
C	0.00368600	2.61229400	1.15067900
C	-0.01384600	3.93243500	0.71468600
C	0.01378100	3.93251000	-0.71435400
C	-0.00362500	2.61241400	-1.15048500
H	0.01367400	2.27278600	-2.18815300
H	0.04054300	4.82092400	-1.34935600
H	-0.04068900	4.82078600	1.34977300
H	-0.01355700	2.27254500	2.18830900
Ir	-1.32760600	0.01310600	0.32157500
Ir	1.32765100	0.01310500	-0.32156900
P	-3.08693500	1.16777800	-0.67978600
P	-2.45190000	-1.92841000	0.85802200
P	3.08706400	1.16781700	0.67957000
P	2.45170200	-1.92860300	-0.85785800
C	-3.29483900	2.85039800	-0.00897700
H	-2.33624200	3.38549400	-0.08301500
H	-4.07940000	3.39398800	-0.55790900
H	-3.56944700	2.77772800	1.05293000
C	-2.98173700	1.42391100	-2.48906900
H	-3.89071000	1.91105200	-2.87360200
H	-2.10913200	2.05746800	-2.69300400
H	-2.82920600	0.45297700	-2.98120000

C	-4.80869400	0.53931500	-0.51865000
H	-4.91457000	-0.45576400	-0.97139700
H	-5.08028700	0.48042800	0.54445100
H	-5.50555200	1.22850500	-1.01967900
C	-3.84737700	-1.87549800	2.04987100
H	-4.25585600	-2.88153200	2.23400000
H	-3.48023200	-1.45264500	2.99643200
H	-4.64556500	-1.22506100	1.66984800
C	-3.15352500	-2.84158600	-0.56987300
H	-2.36611200	-2.93830400	-1.33138800
H	-3.52470200	-3.83513400	-0.27530500
H	-3.97504500	-2.26732800	-1.01758400
C	-1.41194800	-3.23203600	1.62258100
H	-2.00021100	-4.13847500	1.83141700
H	-0.59134600	-3.47906800	0.93406600
H	-0.96213700	-2.84811100	2.54811100
C	1.41144500	-3.23217600	-1.62208400
H	1.99944800	-4.13889900	-1.83043200
H	0.59051400	-3.47866700	-0.93377500
H	0.96206600	-2.84841500	-2.54789800
C	3.84699300	-1.87634000	-2.04998400
H	4.64547000	-1.22603300	-1.67034000
H	4.25511300	-2.88258200	-2.23379100
H	3.47981400	-1.45374300	-2.99664300
C	3.15348000	-2.84162400	0.57006300
H	3.52455000	-3.83524100	0.27560300
H	3.97514500	-2.26731400	1.01742600
H	2.36625800	-2.93814700	1.33179900
C	4.80880200	0.53938000	0.51801000
H	5.50579700	1.22841400	1.01905500
H	4.91465200	-0.45577800	0.97057400
H	5.08021100	0.48061800	-0.54514600
C	3.29472700	2.85048200	0.00881700
H	2.33616300	3.38556200	0.08340300
H	4.07956300	3.39401000	0.55741600
H	3.56877200	2.77794400	-1.05324200
C	2.98227600	1.42389300	2.48890000
H	3.89146400	1.91077600	2.87324900
H	2.10987100	2.05765000	2.69307300
H	2.82962900	0.45295600	2.98099200