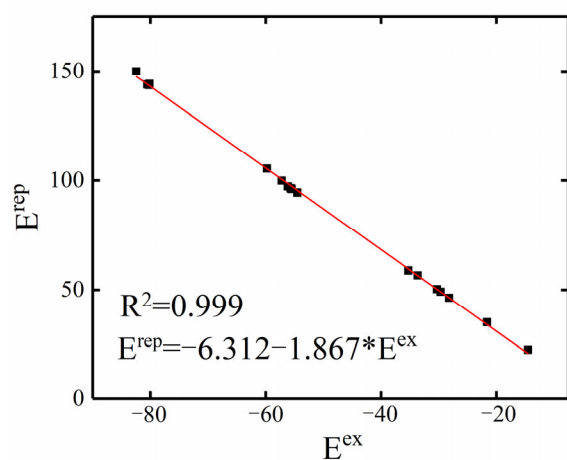


**Figure S1.** The MEP maps of the Lewis acids.



**Figure S2.** Linear relationship between the exchange energy ( $E^{\text{ex}}$ , kcal/mol) and the repulsion energy ( $E^{\text{rep}}$ , kcal/mol) in  $\text{BH}_3/\text{C}_5\text{H}_4\text{BX} \cdots \text{M}(\text{MDA})_2$ .

### Cartesian coordinates

$\text{BH}_3 \cdots \text{Ni}(\text{MDA})_2$

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.52318600 | -1.26460000 | 0.06806400  |
| H | -3.10875000 | -2.16739700 | 0.25804300  |
| C | -3.20175800 | -0.06274100 | -0.10693500 |
| H | -4.27831700 | -0.05062400 | -0.04537300 |
| C | -2.52233400 | 1.11843900  | -0.38002400 |
| H | -3.10514800 | 2.02974900  | -0.53235600 |
| O | -1.27121900 | -1.44227000 | 0.02674900  |
| O | -1.26856800 | 1.26779500  | -0.48131300 |
| C | 2.52375600  | -1.26429000 | 0.06842800  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.10956400  | -2.16705000 | 0.25791000  |
| C  | 3.20213500  | -0.06220500 | -0.10598700 |
| H  | 4.27867400  | -0.04993900 | -0.04410100 |
| C  | 2.52258000  | 1.11883600  | -0.37929000 |
| H  | 3.10523900  | 2.03029700  | -0.53132000 |
| O  | 1.27186100  | -1.44220100 | 0.02708400  |
| O  | 1.26883200  | 1.26786900  | -0.48134400 |
| Ni | 0.00010500  | -0.08697700 | -0.22563300 |
| B  | -0.00231800 | 1.01177900  | 2.39567300  |
| H  | 1.02638300  | 0.42754100  | 2.51164100  |
| H  | -0.00316500 | 2.18764800  | 2.23861600  |
| H  | -1.03022900 | 0.42606200  | 2.51135900  |

C<sub>5</sub>H<sub>4</sub>BCN...Ni(MDA)<sub>2</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.60220400  | -2.50649100 | 1.20952200  |
| H  | 1.61843200  | -3.08213000 | 2.13684100  |
| C  | 1.60808300  | -3.19050100 | 0.00003200  |
| H  | 1.62883800  | -4.26839500 | 0.00003600  |
| C  | 1.60223200  | -2.50649800 | -1.20946200 |
| H  | 1.61848000  | -3.08214300 | -2.13677700 |
| O  | 1.57940400  | -1.25043700 | 1.36815600  |
| O  | 1.57943800  | -1.25044500 | -1.36810400 |
| C  | 1.60219900  | 2.50649800  | 1.20950700  |
| H  | 1.61842000  | 3.08214200  | 2.13682300  |
| C  | 1.60808600  | 3.19050100  | 0.00001400  |
| H  | 1.62884100  | 4.26839600  | 0.00001100  |
| C  | 1.60224300  | 2.50649100  | -1.20947600 |
| H  | 1.61849900  | 3.08213000  | -2.13679500 |
| O  | 1.57939800  | 1.25044500  | 1.36814700  |
| O  | 1.57944900  | 1.25043700  | -1.36810900 |
| Ni | 1.53493300  | -0.00000100 | 0.00002200  |
| C  | -1.50113500 | -1.33040000 | 0.00001400  |
| C  | -2.89526800 | -1.23227600 | -0.00002100 |
| C  | -3.57526700 | 0.00000100  | -0.00005600 |
| C  | -2.89526500 | 1.23227700  | -0.00005600 |
| C  | -1.50113300 | 1.33039800  | -0.00002200 |
| H  | -1.03934700 | -2.30277900 | 0.00003900  |
| H  | -3.48943000 | -2.13811200 | -0.00002300 |
| B  | -0.93064700 | -0.00000200 | 0.00000900  |
| H  | -3.48942600 | 2.13811400  | -0.00008300 |
| H  | -1.03934200 | 2.30277500  | -0.00002400 |
| C  | -5.00026600 | 0.00000300  | -0.00009100 |
| N  | -6.15438100 | 0.00000400  | -0.00011900 |

C<sub>5</sub>H<sub>4</sub>BF···Ni(MDA)<sub>2</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.41332100  | -2.50714300 | 1.20968800  |
| H  | 1.42230300  | -3.08412100 | 2.13654500  |
| C  | 1.40837100  | -3.19120900 | 0.00001800  |
| H  | 1.41231400  | -4.26936000 | 0.00002000  |
| C  | 1.41335800  | -2.50714600 | -1.20965300 |
| H  | 1.42233600  | -3.08412400 | -2.13651000 |
| O  | 1.40949200  | -1.25152400 | 1.36863700  |
| O  | 1.40952600  | -1.25152700 | -1.36860200 |
| C  | 1.41332400  | 2.50714600  | 1.20968000  |
| H  | 1.42228500  | 3.08412700  | 2.13653600  |
| C  | 1.40837500  | 3.19120800  | 0.00000900  |
| H  | 1.41232100  | 4.26936000  | 0.00000800  |
| C  | 1.41336100  | 2.50714200  | -1.20966000 |
| H  | 1.42236300  | 3.08411700  | -2.13651800 |
| O  | 1.40948600  | 1.25152800  | 1.36863300  |
| O  | 1.40953300  | 1.25152200  | -1.36860500 |
| Ni | 1.37130500  | -0.00000100 | 0.00001600  |
| C  | -1.72300800 | -1.32901100 | 0.00006200  |
| C  | -3.12699500 | -1.23060800 | -0.00000100 |
| C  | -3.77015800 | 0.00000200  | -0.00006700 |
| C  | -3.12699300 | 1.23061000  | -0.00007500 |
| C  | -1.72300600 | 1.32901100  | -0.00001200 |
| H  | -1.26262600 | -2.30200500 | 0.00010900  |
| H  | -3.73831700 | -2.12477800 | -0.00000100 |
| B  | -1.15694700 | -0.00000100 | 0.00004600  |
| H  | -3.73831400 | 2.12478200  | -0.00012900 |
| H  | -1.26262200 | 2.30200400  | -0.00001900 |
| F  | -5.13642700 | 0.00000300  | -0.00012800 |

C<sub>5</sub>H<sub>5</sub>B···Ni(MDA)<sub>2</sub>

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 1.19937800 | -2.51775300 | 1.23194400  |
| H | 1.23173900 | -3.10388900 | 2.15341100  |
| C | 1.13310300 | -3.19873000 | 0.01851200  |
| H | 1.11902300 | -4.27706200 | 0.01982100  |
| C | 1.10273300 | -2.52032700 | -1.19295600 |
| H | 1.06910800 | -3.10402300 | -2.11551800 |
| O | 1.23281600 | -1.26516300 | 1.39769000  |
| O | 1.10623400 | -1.26379800 | -1.36088000 |
| C | 1.15798300 | 2.54109400  | 1.22241300  |
| H | 1.18314200 | 3.13124900  | 2.14154600  |
| C | 1.07709100 | 3.21625800  | 0.00656200  |
| H | 1.04510500 | 4.29420800  | 0.00382200  |
| C | 1.05251700 | 2.53280800  | -1.20217100 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.00439100  | 3.11221500  | -2.12676300 |
| O  | 1.21203900  | 1.28989600  | 1.39281300  |
| O  | 1.07659700  | 1.27580800  | -1.36532500 |
| Ni | 1.14272900  | 0.00896700  | 0.01941500  |
| C  | -2.10210400 | -1.35230700 | -0.29635400 |
| C  | -3.44710500 | -1.25461700 | 0.11595300  |
| C  | -4.10105100 | -0.03697600 | 0.32337300  |
| C  | -3.46857600 | 1.19573000  | 0.13965200  |
| C  | -2.12557200 | 1.32483700  | -0.27048800 |
| H  | -1.64427700 | -2.31594600 | -0.43506200 |
| H  | -4.00037200 | -2.17318800 | 0.27858700  |
| B  | -1.60770500 | -0.00791900 | -0.42459800 |
| H  | -5.13531300 | -0.04907400 | 0.63674000  |
| H  | -4.03777800 | 2.10115100  | 0.32005000  |
| H  | -1.68453000 | 2.29882600  | -0.39028200 |

C<sub>5</sub>H<sub>4</sub>BCH<sub>3</sub>...Ni(MDA)<sub>2</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.41354900  | -2.50873300 | 1.23803400  |
| H  | 1.39994300  | -3.08963200 | 2.16283900  |
| C  | 1.42183600  | -3.19157500 | 0.02595900  |
| H  | 1.41470200  | -4.26979300 | 0.02506800  |
| C  | 1.45455700  | -2.50756800 | -1.18217800 |
| H  | 1.47560200  | -3.08475200 | -2.10886500 |
| O  | 1.42390500  | -1.25508400 | 1.39929900  |
| O  | 1.46245700  | -1.25123600 | -1.34124600 |
| C  | 1.41353300  | 2.50874100  | 1.23803000  |
| H  | 1.39992500  | 3.08964100  | 2.16283400  |
| C  | 1.42181400  | 3.19158100  | 0.02595400  |
| H  | 1.41467500  | 4.26979900  | 0.02506100  |
| C  | 1.45453100  | 2.50757200  | -1.18218200 |
| H  | 1.47556700  | 3.08475500  | -2.10887000 |
| O  | 1.42389300  | 1.25509200  | 1.39929700  |
| O  | 1.46243600  | 1.25124000  | -1.34124900 |
| Ni | 1.41108900  | 0.00000300  | 0.02909700  |
| C  | -1.72469100 | -1.33019500 | -0.21420000 |
| C  | -3.11826100 | -1.21675900 | -0.04188400 |
| C  | -3.80746300 | -0.00001100 | 0.04005400  |
| C  | -3.11827500 | 1.21674500  | -0.04187300 |
| C  | -1.72470600 | 1.33019900  | -0.21418700 |
| H  | -1.26948100 | -2.30433600 | -0.26162300 |
| H  | -3.69524700 | -2.13356700 | 0.03192600  |
| B  | -1.17532500 | 0.00000500  | -0.27040400 |
| H  | -3.69527200 | 2.13354600  | 0.03194600  |
| H  | -1.26950700 | 2.30434500  | -0.26160200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -5.31014300 | -0.00002100 | 0.18338800  |
| H | -5.80900100 | -0.00002400 | -0.78982900 |
| H | -5.65749600 | -0.88014600 | 0.72506000  |
| H | -5.65750600 | 0.88010000  | 0.72506000  |

C<sub>5</sub>H<sub>4</sub>BNH<sub>2</sub>···Ni(MDA)<sub>2</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.60220400  | -2.50649100 | 1.20952200  |
| H  | 1.61843200  | -3.08213000 | 2.13684100  |
| C  | 1.60808300  | -3.19050100 | 0.00003200  |
| H  | 1.62883800  | -4.26839500 | 0.00003600  |
| C  | 1.60223200  | -2.50649800 | -1.20946200 |
| H  | 1.61848000  | -3.08214300 | -2.13677700 |
| O  | 1.57940400  | -1.25043700 | 1.36815600  |
| O  | 1.57943800  | -1.25044500 | -1.36810400 |
| C  | 1.60219900  | 2.50649800  | 1.20950700  |
| H  | 1.61842000  | 3.08214200  | 2.13682300  |
| C  | 1.60808600  | 3.19050100  | 0.00001400  |
| H  | 1.62884100  | 4.26839600  | 0.00001100  |
| C  | 1.60224300  | 2.50649100  | -1.20947600 |
| H  | 1.61849900  | 3.08213000  | -2.13679500 |
| O  | 1.57939800  | 1.25044500  | 1.36814700  |
| O  | 1.57944900  | 1.25043700  | -1.36810900 |
| Ni | 1.53493300  | -0.00000100 | 0.00002200  |
| C  | -1.50113500 | -1.33040000 | 0.00001400  |
| C  | -2.89526800 | -1.23227600 | -0.00002100 |
| C  | -3.57526700 | 0.00000100  | -0.00005600 |
| C  | -2.89526500 | 1.23227700  | -0.00005600 |
| C  | -1.50113300 | 1.33039800  | -0.00002200 |
| H  | -1.03934700 | -2.30277900 | 0.00003900  |
| H  | -3.48943000 | -2.13811200 | -0.00002300 |
| B  | -0.93064700 | -0.00000200 | 0.00000900  |
| H  | -3.48942600 | 2.13811400  | -0.00008300 |
| H  | -1.03934200 | 2.30277500  | -0.00002400 |
| C  | -5.00026600 | 0.00000300  | -0.00009100 |
| N  | -6.15438100 | 0.00000400  | -0.00011900 |

BH<sub>3</sub>···Pd(MDA)<sub>2</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.59114900 | -1.23212500 | -0.13150600 |
| H | -3.21562300 | -2.12814800 | -0.11462700 |
| C | -3.23730000 | 0.00014500  | -0.08830200 |
| H | -4.31476400 | 0.00013300  | -0.03198800 |
| C | -2.59113000 | 1.23243500  | -0.13065100 |
| H | -3.21559300 | 2.12845400  | -0.11315800 |
| O | -1.34949600 | -1.46633200 | -0.19612400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -1.34947100 | 1.46666300  | -0.19508300 |
| C  | 2.59797500  | -1.23207100 | -0.11964400 |
| H  | 3.22253200  | -2.12804300 | -0.10079900 |
| C  | 3.24305300  | 0.00012000  | -0.05761600 |
| H  | 4.31937300  | 0.00009700  | 0.01740600  |
| C  | 2.59796300  | 1.23235000  | -0.11872700 |
| H  | 3.22251400  | 2.12831200  | -0.09919900 |
| O  | 1.35770600  | -1.46558800 | -0.20656600 |
| O  | 1.35769300  | 1.46591700  | -0.20549400 |
| Pd | 0.00352700  | 0.00014700  | -0.18217300 |
| B  | -0.05186800 | -0.00223100 | 2.36169400  |
| H  | 0.53282900  | -1.03350200 | 2.45339300  |
| H  | -1.24132800 | 0.00143400  | 2.41033300  |
| H  | 0.53921700  | 1.02527500  | 2.45492800  |

C<sub>5</sub>H<sub>4</sub>BCN...Pd(MDA)<sub>2</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.42695300 | 2.59447100  | 1.23124200  |
| H  | -1.45286800 | 3.21325000  | 2.12993000  |
| C  | -1.44220300 | 3.24270900  | -0.00007000 |
| H  | -1.47588300 | 4.32085300  | -0.00009700 |
| C  | -1.42697000 | 2.59441000  | -1.23134900 |
| H  | -1.45289500 | 3.21314300  | -2.13006800 |
| O  | -1.38787100 | 1.34994300  | 1.46327700  |
| O  | -1.38789000 | 1.34987000  | -1.46332200 |
| C  | -1.42657200 | -2.59451700 | 1.23137400  |
| H  | -1.45241600 | -3.21325600 | 2.13009100  |
| C  | -1.44172100 | -3.24281800 | 0.00009300  |
| H  | -1.47525500 | -4.32096700 | 0.00012000  |
| C  | -1.42658900 | -2.59457900 | -1.23122100 |
| H  | -1.45244500 | -3.21336200 | -2.12990700 |
| O  | -1.38769200 | -1.34997200 | 1.46334800  |
| O  | -1.38771000 | -1.35004500 | -1.46325800 |
| Pd | -1.32248600 | -0.00004900 | 0.00001100  |
| C  | 1.59507900  | 1.31904000  | -0.00005300 |
| C  | 2.98500400  | 1.22950500  | -0.00005700 |
| C  | 3.66790800  | 0.00013000  | -0.00002900 |
| C  | 2.98506900  | -1.22928200 | 0.00000700  |
| C  | 1.59515000  | -1.31888700 | 0.00001600  |
| H  | 1.14354400  | 2.29738800  | -0.00007600 |
| H  | 3.57902000  | 2.13576700  | -0.00008400 |
| B  | 0.97072900  | 0.00006100  | -0.00001500 |
| H  | 3.57913200  | -2.13551300 | 0.00002700  |
| H  | 1.14365900  | -2.29725700 | 0.00004300  |
| C  | 5.09244000  | 0.00016800  | -0.00003600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N   | 6.24693600  | 0.00020400  | -0.00004200 |
| C <sub>5</sub> H <sub>4</sub> BF...Pd(MDA) <sub>2</sub> |             |             |             |
| C   | -1.25176100 | 2.59454500  | 1.23140000  |
| H   | -1.27340900 | 3.21459000  | 2.12957600  |
| C   | -1.26133800 | 3.24299800  | -0.00006900 |
| H   | -1.28515700 | 4.32146100  | -0.00009600 |
| C   | -1.25178300 | 2.59448300  | -1.23150500 |
| H   | -1.27344400 | 3.21448200  | -2.12971300 |
| O   | -1.22381900 | 1.35043700  | 1.46364600  |
| O   | -1.22384300 | 1.35036200  | -1.46368900 |
| C   | -1.25106200 | -2.59470600 | 1.23153100  |
| H   | -1.27257400 | -3.21471200 | 2.12973800  |
| C   | -1.26043800 | -3.24322200 | 0.00009400  |
| H   | -1.28397000 | -4.32169100 | 0.00012200  |
| C   | -1.25108200 | -2.59476800 | -1.23137500 |
| H   | -1.27261100 | -3.21481900 | -2.12955000 |
| O   | -1.22349500 | -1.35057800 | 1.46371600  |
| O   | -1.22351900 | -1.35065100 | -1.46362300 |
| Pd  | -1.16060500 | -0.00010100 | 0.00001200  |
| C   | 1.78253800  | 1.31743000  | -0.00005600 |
| C   | 3.18233700  | 1.22784600  | -0.00006300 |
| C   | 3.82726200  | 0.00032900  | -0.00003600 |
| C   | 3.18253000  | -1.22729000 | -0.00000200 |
| C   | 1.78274600  | -1.31709000 | 0.00000900  |
| H   | 1.33267900  | 2.29652700  | -0.00007800 |
| H   | 3.79315600  | 2.12269900  | -0.00008900 |
| B   | 1.16203700  | 0.00012200  | -0.00001900 |
| H   | 3.79348800  | -2.12204700 | 0.00001700  |
| H   | 1.33303400  | -2.29625800 | 0.00003600  |
| F   | 5.19601900  | 0.00043700  | -0.00004400 |
| C <sub>5</sub> H <sub>5</sub> B...Pd(MDA) <sub>2</sub>  |             |             |             |
| C   | 2.58265800  | 1.02359000  | 1.23173200  |
| H   | 3.20361800  | 1.05081100  | 2.12930200  |
| C   | 3.23073100  | 1.03999200  | -0.00006700 |
| H   | 4.30896300  | 1.07404900  | -0.00009500 |
| C   | 2.58259400  | 1.02361300  | -1.23183200 |
| H   | 3.20350600  | 1.05086900  | -2.12943500 |
| O   | 1.33937200  | 0.98360200  | 1.46454100  |
| O   | 1.33929600  | 0.98361500  | -1.46457700 |
| C   | -2.60662700 | 0.96112300  | 1.23185600  |
| H   | -3.22803400 | 0.97345000  | 2.12944700  |
| C   | -3.25497100 | 0.96148300  | 0.00009400  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -4.33371300 | 0.96920300  | 0.00012000  |
| C  | -2.60668700 | 0.96112000  | -1.23169900 |
| H  | -3.22813600 | 0.97343300  | -2.12926000 |
| O  | -1.36272300 | 0.95147400  | 1.46459500  |
| O  | -1.36279400 | 0.95148300  | -1.46449800 |
| Pd | -0.01100400 | 0.90685300  | 0.00001600  |
| C  | 1.34664100  | -2.03730600 | -0.00009000 |
| C  | 1.26247100  | -3.43813100 | -0.00007300 |
| C  | 0.05021500  | -4.12968500 | -0.00003200 |
| C  | -1.17861000 | -3.46800300 | -0.00000700 |
| C  | -1.29711600 | -2.06965900 | -0.00001900 |
| H  | 2.31887400  | -1.57295900 | -0.00012200 |
| H  | 2.18304500  | -4.01292400 | -0.00009200 |
| B  | 0.01738000  | -1.44917600 | -0.00005700 |
| H  | 0.06345600  | -5.21091600 | -0.00002100 |
| H  | -2.08481800 | -4.06518400 | 0.00002400  |
| H  | -2.28050000 | -1.62938600 | 0.00000300  |

C<sub>5</sub>H<sub>4</sub>BCH<sub>3</sub>...Pd(MDA)<sub>2</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.27385900  | 2.59482100  | -1.22983200 |
| H  | 1.29493000  | 3.21592700  | -2.12747400 |
| C  | 1.27693700  | 3.24324500  | 0.00181300  |
| H  | 1.29474000  | 4.32187300  | 0.00177800  |
| C  | 1.26734500  | 2.59500800  | 1.23357900  |
| H  | 1.28342000  | 3.21632100  | 2.13118500  |
| O  | 1.25305400  | 1.35104500  | -1.46250400 |
| O  | 1.24583200  | 1.35130300  | 1.46636000  |
| C  | 1.27370700  | -2.59486600 | -1.22983300 |
| H  | 1.29475100  | -3.21597400 | -2.12747500 |
| C  | 1.27675000  | -3.24328900 | 0.00181300  |
| H  | 1.29450000  | -4.32191800 | 0.00177700  |
| C  | 1.26719600  | -2.59505300 | 1.23357900  |
| H  | 1.28324400  | -3.21636800 | 2.13118300  |
| O  | 1.25297600  | -1.35108900 | -1.46250600 |
| O  | 1.24575600  | -1.35134700 | 1.46636200  |
| Pd | 1.18918900  | -0.00002200 | 0.00183100  |
| C  | -1.77529700 | 1.31744400  | -0.00940800 |
| C  | -3.17462600 | 1.21332300  | -0.01376600 |
| C  | -3.87136000 | 0.00006500  | -0.01286900 |
| C  | -3.17466300 | -1.21321200 | -0.01376400 |
| C  | -1.77533600 | -1.31737500 | -0.00940600 |
| H  | -1.32864500 | 2.29800900  | -0.01584700 |
| H  | -3.75643700 | 2.13068300  | -0.02044100 |
| B  | -1.16444400 | 0.00002500  | -0.00338400 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.75650100 | -2.13055500 | -0.02043900 |
| H | -1.32871300 | -2.29795300 | -0.01584500 |
| C | -5.38042500 | 0.00009300  | 0.02115100  |
| H | -5.78918600 | -0.88032400 | -0.47571200 |
| H | -5.76289400 | 0.00024900  | 1.04593300  |
| H | -5.78916500 | 0.88037400  | -0.47597100 |

C<sub>5</sub>H<sub>4</sub>BNH<sub>2</sub>...Pd(MDA)<sub>2</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.26006700  | -2.59535700 | 1.23201100  |
| H  | 1.27723400  | -3.21668500 | 2.12960800  |
| C  | 1.26551000  | -3.24361500 | 0.00040300  |
| H  | 1.28083900  | -4.32228100 | 0.00023400  |
| C  | 1.26221300  | -2.59487600 | -1.23124100 |
| H  | 1.28044100  | -3.21575200 | -2.12910700 |
| O  | 1.24109500  | -1.35157700 | 1.46500300  |
| O  | 1.24449800  | -1.35115000 | -1.46337600 |
| C  | 1.26140700  | 2.59479900  | 1.23213200  |
| H  | 1.27875400  | 3.21606900  | 2.12976200  |
| C  | 1.26722400  | 3.24311100  | 0.00056600  |
| H  | 1.28296900  | 4.32177200  | 0.00044700  |
| C  | 1.26377500  | 2.59443400  | -1.23110600 |
| H  | 1.28230300  | 3.21535400  | -2.12893400 |
| O  | 1.24191500  | 1.35100500  | 1.46506400  |
| O  | 1.24541200  | 1.35072900  | -1.46330600 |
| Pd | 1.18243700  | -0.00021900 | 0.00091600  |
| C  | -1.78385800 | -1.31271200 | 0.00164700  |
| C  | -3.18368400 | -1.21625800 | -0.00666800 |
| C  | -3.87295600 | 0.00077800  | -0.00952300 |
| C  | -3.18351800 | 1.21738900  | -0.00691000 |
| C  | -1.78338000 | 1.31384900  | 0.00124700  |
| H  | -1.33886900 | -2.29425000 | 0.00573300  |
| H  | -3.76905400 | -2.13130400 | -0.01746800 |
| B  | -1.16310100 | 0.00055100  | 0.00143300  |
| H  | -3.76840500 | 2.13275700  | -0.01776300 |
| H  | -1.33906100 | 2.29563900  | 0.00511400  |
| N  | -5.29269700 | 0.00051900  | -0.08579600 |
| H  | -5.70730200 | -0.82226400 | 0.32585500  |
| H  | -5.70772700 | 0.82334400  | 0.32534100  |

BH<sub>3</sub>...Pt(MDA)<sub>2</sub>

|   |            |            |             |
|---|------------|------------|-------------|
| C | 2.59017500 | 1.23481300 | -0.08838200 |
| H | 3.21152200 | 2.13062000 | -0.07076200 |
| C | 3.22919000 | 0.00002500 | -0.04838900 |
| H | 4.30673100 | 0.00002300 | 0.00840500  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.59018000  | -1.23476100 | -0.08855100 |
| H  | 3.21152900  | -2.13056900 | -0.07105000 |
| O  | 1.34514900  | 1.47424000  | -0.15268500 |
| O  | 1.34515600  | -1.47418300 | -0.15289700 |
| C  | -2.59304300 | 1.23481900  | -0.08148700 |
| H  | -3.21458700 | 2.13049600  | -0.06327500 |
| C  | -3.23077100 | 0.00002100  | -0.02022100 |
| H  | -4.30706200 | 0.00001700  | 0.05667900  |
| C  | -2.59304900 | -1.23477100 | -0.08168400 |
| H  | -3.21459500 | -2.13045000 | -0.06361700 |
| O  | -1.34951900 | 1.47346100  | -0.16971700 |
| O  | -1.34952500 | -1.47340200 | -0.16994900 |
| Pt | -0.00201200 | 0.00002500  | -0.14138800 |
| B  | 0.03255400  | -0.00048000 | 2.30554300  |
| H  | -0.55466200 | 1.02657000  | 2.45185400  |
| H  | -0.55230200 | -1.02893100 | 2.45141700  |
| H  | 1.22138500  | 0.00086400  | 2.41515800  |

C<sub>5</sub>H<sub>4</sub>BCN...Pt(MDA)<sub>2</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.20942100  | -2.59546400 | 1.23379500  |
| H  | 1.23431900  | -3.21159800 | 2.13204400  |
| C  | 1.22184300  | -3.23630100 | 0.00000200  |
| H  | 1.24848100  | -4.31474200 | -0.00000300 |
| C  | 1.20950500  | -2.59545100 | -1.23378400 |
| H  | 1.23443900  | -3.21157500 | -2.13203800 |
| O  | 1.17731600  | -1.34716200 | 1.47136400  |
| O  | 1.17740100  | -1.34714700 | -1.47134100 |
| C  | 1.20945200  | 2.59545300  | 1.23382100  |
| H  | 1.23435400  | 3.21157800  | 2.13207500  |
| C  | 1.22182700  | 3.23630300  | 0.00003500  |
| H  | 1.24845900  | 4.31474400  | 0.00004100  |
| C  | 1.20944800  | 2.59546600  | -1.23375800 |
| H  | 1.23437200  | 3.21160100  | -2.13200600 |
| O  | 1.17734700  | 1.34714900  | 1.47137800  |
| O  | 1.17735600  | 1.34716400  | -1.47132900 |
| Pt | 1.11087800  | 0.00000200  | 0.00001700  |
| C  | -1.78982400 | -1.30919300 | 0.00008100  |
| C  | -3.17771200 | -1.22748500 | 0.00005100  |
| C  | -3.86309400 | -0.00000500 | -0.00006000 |
| C  | -3.17771600 | 1.22747800  | -0.00014600 |
| C  | -1.78982900 | 1.30919200  | -0.00012800 |
| H  | -1.34595600 | -2.29247600 | 0.00017100  |
| H  | -3.77068700 | -2.13454300 | 0.00011300  |
| B  | -1.12173700 | 0.00000100  | -0.00001200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.77069500 | 2.13453400  | -0.00022900 |
| H | -1.34596400 | 2.29247600  | -0.00020200 |
| C | -5.28708500 | -0.00000700 | -0.00008500 |
| N | -6.44195200 | -0.00001000 | -0.00010600 |

C<sub>5</sub>H<sub>4</sub>BF···Pt(MDA)<sub>2</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.05425400  | -2.59471600 | 1.23393200  |
| H  | 1.07514400  | -3.21201400 | 2.13169200  |
| C  | 1.06124400  | -3.23576000 | -0.00001000 |
| H  | 1.07816700  | -4.31444300 | -0.00001600 |
| C  | 1.05437300  | -2.59469800 | -1.23394300 |
| H  | 1.07531200  | -3.21198300 | -2.13171100 |
| O  | 1.03333300  | -1.34687000 | 1.47166600  |
| O  | 1.03344100  | -1.34684900 | -1.47166400 |
| C  | 1.05432800  | 2.59469500  | 1.23397700  |
| H  | 1.07523700  | 3.21197500  | 2.13174900  |
| C  | 1.06123600  | 3.23576300  | 0.00004700  |
| H  | 1.07815900  | 4.31444500  | 0.00006000  |
| C  | 1.05428000  | 2.59472300  | -1.23389800 |
| H  | 1.07519400  | 3.21202600  | -2.13165400 |
| O  | 1.03339000  | 1.34684500  | 1.47168900  |
| O  | 1.03336600  | 1.34687900  | -1.47164100 |
| Pt | 0.96910000  | 0.00000100  | 0.00000900  |
| C  | -1.94927900 | -1.30752500 | 0.00012400  |
| C  | -3.34732600 | -1.22589400 | 0.00009000  |
| C  | -3.99320300 | -0.00000700 | -0.00005400 |
| C  | -3.34733600 | 1.22588600  | -0.00017100 |
| C  | -1.94929000 | 1.30753000  | -0.00015100 |
| H  | -1.50758600 | -2.29178800 | 0.00024300  |
| H  | -3.95815700 | -2.12087000 | 0.00017300  |
| B  | -1.28530200 | 0.00000500  | -0.00000300 |
| H  | -3.95817500 | 2.12085700  | -0.00027800 |
| H  | -1.50760600 | 2.29179600  | -0.00025200 |
| F  | -5.36410500 | -0.00001200 | -0.00008100 |

C<sub>3</sub>H<sub>5</sub>B···Pt(MDA)<sub>2</sub>

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 0.83251500 | -2.59398400 | 1.23422600  |
| H | 0.85299700 | -3.21190300 | 2.13166400  |
| C | 0.84084800 | -3.23482300 | 0.00015300  |
| H | 0.85820400 | -4.31353500 | 0.00020000  |
| C | 0.83255700 | -2.59409600 | -1.23397800 |
| H | 0.85318100 | -3.21209700 | -2.13135700 |
| O | 0.81054900 | -1.34653700 | 1.47240200  |
| O | 0.81055900 | -1.34667000 | -1.47227500 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.83029400  | 2.59477800  | 1.23399200  |
| H  | 0.85034400  | 3.21279300  | 2.13137400  |
| C  | 0.83811100  | 3.23551500  | -0.00013700 |
| H  | 0.85455600  | 4.31424200  | -0.00018100 |
| C  | 0.83038300  | 2.59467300  | -1.23421100 |
| H  | 0.85039100  | 3.21261400  | -2.13164500 |
| O  | 0.80933900  | 1.34733500  | 1.47228200  |
| O  | 0.80948300  | 1.34720900  | -1.47239400 |
| Pt | 0.74657200  | 0.00030800  | 0.00000000  |
| C  | -2.17699500 | -1.31206500 | -0.00028400 |
| C  | -3.57430500 | -1.21998300 | -0.00031500 |
| C  | -4.25429600 | -0.00177700 | -0.00005600 |
| C  | -3.57535100 | 1.21701100  | 0.00025100  |
| C  | -2.17811900 | 1.31029800  | 0.00031800  |
| H  | -1.73283400 | -2.29532800 | -0.00052100 |
| H  | -4.15922700 | -2.13449000 | -0.00054700 |
| B  | -1.52433700 | -0.00060300 | 0.00003400  |
| H  | -5.33597600 | -0.00224000 | -0.00009400 |
| H  | -4.16105700 | 2.13101600  | 0.00044500  |
| H  | -1.73481100 | 2.29394600  | 0.00059000  |

C<sub>5</sub>H<sub>4</sub>BCH<sub>3</sub>...Pt(MDA)<sub>2</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.07174300 | -2.59438100 | -1.23271100 |
| H  | -1.09257500 | -3.21243900 | -2.13007600 |
| C  | -1.07457700 | -3.23540500 | 0.00132800  |
| H  | -1.08782600 | -4.31416800 | 0.00128600  |
| C  | -1.06637000 | -2.59454500 | 1.23544700  |
| H  | -1.08327100 | -3.21276200 | 2.13278600  |
| O  | -1.05487900 | -1.34689900 | -1.47081600 |
| O  | -1.04873800 | -1.34710900 | 1.47368300  |
| C  | -1.07171500 | 2.59439900  | -1.23268400 |
| H  | -1.09255400 | 3.21246500  | -2.13004300 |
| C  | -1.07455300 | 3.23541100  | 0.00136200  |
| H  | -1.08779600 | 4.31417400  | 0.00133000  |
| C  | -1.06635800 | 2.59453700  | 1.23547400  |
| H  | -1.08324200 | 3.21274500  | 2.13281900  |
| O  | -1.05486000 | 1.34692000  | -1.47080100 |
| O  | -1.04873400 | 1.34709800  | 1.47369600  |
| Pt | -0.98887400 | 0.00000200  | 0.00135200  |
| C  | 1.93953100  | -1.30638300 | -0.00856700 |
| C  | 3.33649400  | -1.21100800 | -0.01358300 |
| C  | 4.03576000  | -0.00001100 | -0.01289200 |
| C  | 3.33650600  | 1.21099200  | -0.01364700 |
| C  | 1.93954400  | 1.30638300  | -0.00863500 |

|  |             |             |             |
|--|-------------|-------------|-------------|
| H  | 1.50135900  | -2.29240500 | -0.01458400 |
| H  | 3.91766100  | -2.12919100 | -0.02065800 |
| B  | 1.27995400  | 0.00000300  | -0.00291700 |
| H  | 3.91768200  | 2.12917000  | -0.02077100 |
| H  | 1.50138200  | 2.29240800  | -0.01470700 |
| C  | 5.54466400  | -0.00001800 | 0.02104600  |
| H  | 5.92837400  | 0.00000800  | 1.04577600  |
| H  | 5.95389300  | -0.88059700 | -0.47586000 |
| H  | 5.95390200  | 0.88053100  | -0.47590700 |
| C <sub>5</sub> H <sub>4</sub> BNH <sub>2</sub> ...Pt(MDA) <sub>2</sub> |             |             |             |
| C  | -1.06065600 | -2.59402200 | -1.23372600 |
| H  | -1.07891100 | -3.21188000 | -2.13128700 |
| C  | -1.06205300 | -3.23537500 | 0.00030700  |
| H  | -1.07101000 | -4.31418700 | 0.00011900  |
| C  | -1.05981300 | -2.59449700 | 1.23431200  |
| H  | -1.07791800 | -3.21278300 | 2.13160000  |
| O  | -1.04937200 | -1.34651500 | -1.47126800 |
| O  | -1.04768800 | -1.34691800 | 1.47271000  |
| C  | -1.05964200 | 2.59425400  | -1.23377700 |
| H  | -1.07768100 | 3.21210600  | -2.13134700 |
| C  | -1.06085000 | 3.23562700  | 0.00024600  |
| H  | -1.06946900 | 4.31444200  | 0.00004000  |
| C  | -1.05879600 | 2.59477600  | 1.23426600  |
| H  | -1.07666000 | 3.21309000  | 2.13153900  |
| O  | -1.04877700 | 1.34674200  | -1.47130100 |
| O  | -1.04707800 | 1.34720100  | 1.47269600  |
| Pt   | -0.98449200 | 0.00011300  | 0.00084200  |
| C  | 1.94718800  | -1.30288300 | -0.00044100 |
| C  | 3.34498000  | -1.21490400 | -0.00723100 |
| C  | 4.03651700  | -0.00053900 | -0.00945800 |
| C  | 3.34534000  | 1.21410700  | -0.00712700 |
| C  | 1.94764200  | 1.30251200  | -0.00028300 |
| H  | 1.51071200  | -2.28976800 | 0.00309300  |
| H  | 3.92962800  | -2.13088900 | -0.01706600 |
| B  | 1.28017000  | -0.00009400 | -0.00020200 |
| H  | 3.93033000  | 2.12987100  | -0.01696200 |
| H  | 1.51140800  | 2.28951200  | 0.00332100  |
| N  | 5.45771700  | -0.00068600 | -0.08384200 |
| H  | 5.86971100  | 0.82162300  | 0.33198400  |
| H  | 5.86952300  | -0.82312000 | 0.33194800  |