

# Supporting Information

## Sensing and extraction of hazardous metals by di-phosphonates of heterocycles: combined experimental and theoretical study

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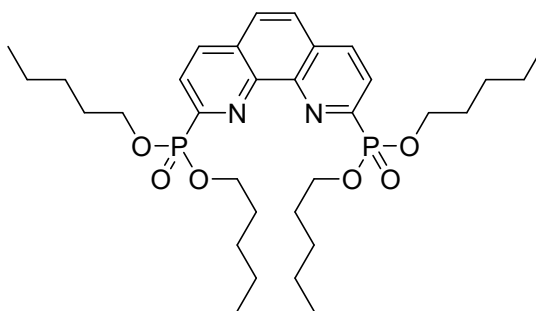
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### 1. Spectral information for Phen-PO-C5 (Tetrapentyl 1,10-phenanthroline-2,9-diylbis(phosphonate))

Tetrapentyl 1,10-phenanthroline-2,9-diylbis(phosphonate)



Yield 10%, colorless oil.

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.37 (dd, *J* = 8.1, 5.5 Hz, 2H), 8.29 (dd, *J* = 8.1, 4.9 Hz, 2H), 7.90 (s, 2H), 4.42 (dq, *J* = 10.0, 6.7 Hz, 4H), 4.36 (dq, *J* = 10.1, 6.8 Hz, 4H), 1.76 (dq, *J* = 13.6, 6.6 Hz, 1H), 1.38 (pd, *J* = 7.4, 2.0 Hz, 8H), 1.32 (hd, *J* = 7.0, 1.9 Hz, 8H), 0.85 (t, *J* = 7.2 Hz, 12H).

$^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ )  $\delta$  152.71 (d,  $J = 227.4$  Hz), 145.62 (d,  $J = 25.9$  Hz), 135.52 (d,  $J = 11.8$  Hz), 129.21 (s), 127.68 (s), 125.86 (d,  $J = 26.3$  Hz), 67.38 (d,  $J = 6.7$  Hz), 29.84 (d,  $J = 5.9$  Hz), 27.15 (s), 21.74 (s), 13.41 (s).

$^{31}\text{P}$  NMR (243 MHz,  $\text{CDCl}_3$ )  $\delta$  12.49.

**HR-ESI-MS:** calc.  $m/z = 621,3217$ ; found  $m/z = 621,3191$

**FT-IR:**  $1263\text{ cm}^{-1}$  (P=O)

## 2. Solvent Extraction

Table S1 Distribution ratio for the d-metal cations for the pyridine ligands Organic phase:  $c(\text{L}) = 0.05\text{ mol L}^{-1}$  in F-3, Aqueous phase:  $c(\text{HNO}_3) = 3\text{ mol L}^{-1}$ ,  $c(\text{M(II)}) = 1 \cdot 10^{-4}\text{ mol L}^{-1}$ .  
Temperature:  $25\text{ }^\circ\text{C}$ .

|              | D(Co)           | D(Ni)           | D(Cu)           | D(Zn)           | D(Cd)           | D(Pb)           |
|--------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Py-PO-iPr    | $0.03 \pm 0.01$ | $0.02 \pm 0.01$ | <0.01           | $0.01 \pm 0.01$ | $0.04 \pm 0.01$ | $0.8 \pm 0.2$   |
| Py-PO-cHex   | $0.03 \pm 0.01$ | $0.02 \pm 0.01$ | $0.01 \pm 0.01$ | $0.21 \pm 0.1$  | $0.04 \pm 0.01$ | $0.2 \pm 0.1$   |
| Py-PO-C5     | $0.01 \pm 0.01$ | $0.01 \pm 0.01$ | <0.01           | $0.02 \pm 0.01$ | <0.01           | $0.3 \pm 0.1$   |
| Py-PO-2EtHex | $0.01 \pm 0.01$ | <0.01           | $0.01 \pm 0.01$ | <0.01           | <0.01           | $0.03 \pm 0.01$ |

**Table S2** Distribution ratio for the d-metal cations for the ligand PO-Phen-C5 Organic phase:  $c(\text{PO-Phen-C5}) = 0.05\text{ mol L}^{-1}$  in F-3, Aqueous phase:  $c(\text{HNO}_3) = 3\text{ mol L}^{-1}$ ,  $c(\text{M(II)}) = 1 \cdot 10^{-4}\text{ mol L}^{-1}$ . Temperature:  $25\text{ }^\circ\text{C}$ .

|  | D(Co) | D(Ni) | D(Cu)           | D(Zn)           | D(Cd) | D(Pb) |
|--|-------|-------|-----------------|-----------------|-------|-------|
| Phen-PO-C5, $c(\text{HNO}_3) = 0.05\text{ mol L}^{-1}$ | <0.01 | <0.01 | $0.6 \pm 0.2$   | <0.01           | >90   | >90   |
| Phen-PO-C5, $c(\text{HNO}_3) = 1\text{ mol L}^{-1}$    | <0.01 | <0.01 | $0.11 \pm 0.04$ | <0.01           | >90   | >90   |
| Phen-PO-C5, $c(\text{HNO}_3) = 3\text{ mol L}^{-1}$    | <0.01 | <0.01 | $1.27 \pm 0.5$  | $0.03 \pm 0.01$ | >90   | >90   |

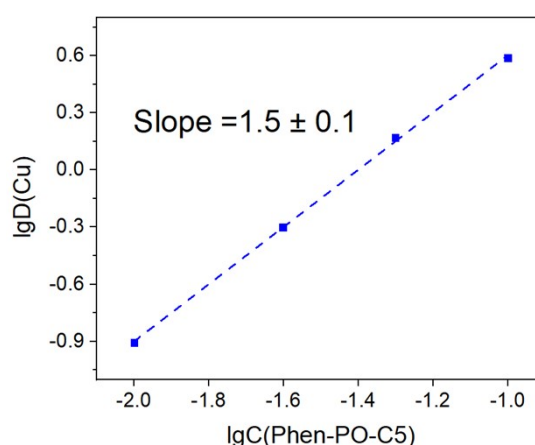
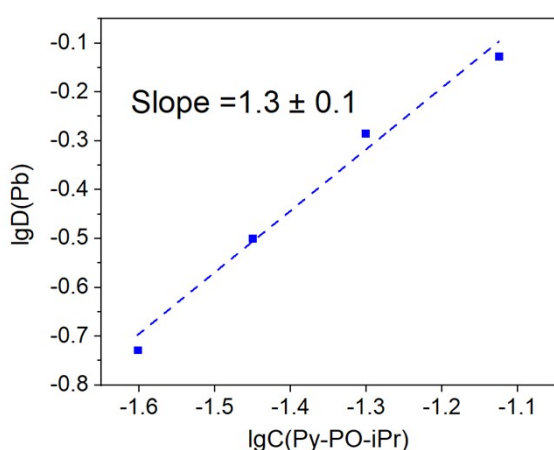


Figure S1 Dependence of Pb(II) and Cu(II) extraction on ligand concentration, Organic phase:  $c(\text{L}) = 0.025 - 0.1\text{ mol L}^{-1}$  in F-3, Aqueous phase:  $c(\text{HNO}_3) = 3\text{ mol L}^{-1}$  with  $c(\text{M(II)}) = 1 \cdot 10^{-4}\text{ mol L}^{-1}$ . Temperature:  $25\text{ }^\circ\text{C}$ .

a)

b)

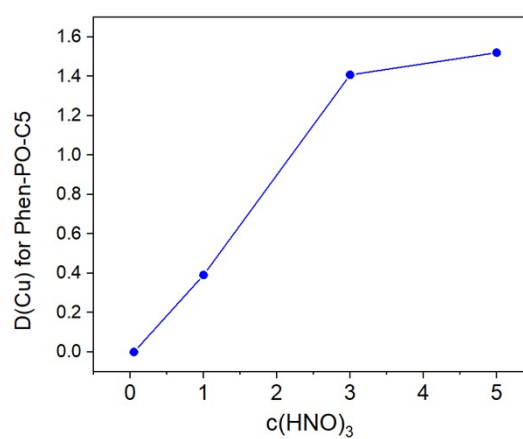
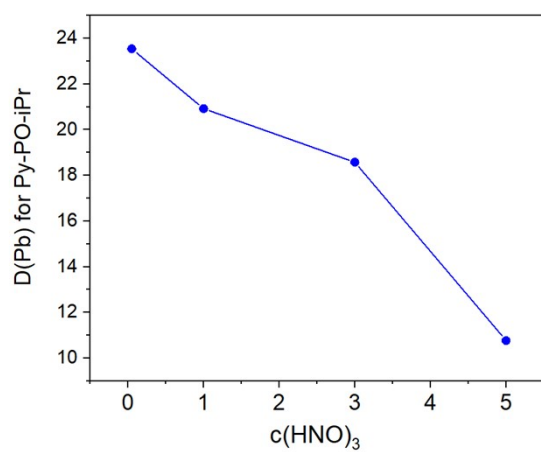


Figure S2 The dependence of extraction of Pb(II) (a) and Cu(II) (b) on nitric acid concentration for Py-PO-iPr and Phen-PO-C5 ligands. Organic phase:  $c(\text{Py-PO-iPr}) = 0.1 \text{ mol L}^{-1}$ ,  $c(\text{Phen-PO-C5}) = 0.05 \text{ mol L}^{-1}$  in F-3, Aqueous phase:  $c(\text{HNO}_3) = 0.05\text{-}5 \text{ mol L}^{-1}$   $c(\text{M(II)}) = 1 \cdot 10^{-4} \text{ mol L}^{-1}$ .  
Temperature:  $25 \pm 1^\circ\text{C}$ .

### 3. Sensor experiments

Membrane Composition: membrane mass = 300 mg,  $c(\text{Ligand}) = 50 \text{ mmol}\cdot\text{kg}^{-1}$ ,  $c(\text{CCD}) = 10 \text{ mmol}\cdot\text{kg}^{-1}$ ,  $m(\text{PVC}) : m(\text{NPOE}) = 1:2$ .

Table S3 Membranes composition.

| Ligand       | Ligand mass, mg | CCD mass, mg | PVC mass, mg | NPOE mass, mg |
|--------------|-----------------|--------------|--------------|---------------|
| Py-PO-iPr    | 6.1             | 1.5          | 97.5         | 194.9         |
| Py-PO-cHex   | 8.5             | 1.5          | 96.7         | 193.3         |
| Py-PO-C5     | 7.8             | 1.5          | 96.9         | 193.8         |
| Py-PO-2EtHex | 10.3            | 1.5          | 96.1         | 192.1         |
| Phen-PO-C5   | 9.3             | 1.5          | 96.4         | 192.8         |

Table S4 Slopes ( $\pm 2 \text{ mV/dec}$ ) of electrode functions for various cations. Inner electrolyte solution is  $0.01 \text{ mol}\cdot\text{L}^{-1} \text{ NaCl}$ .

| Sensor type/Cation | Py-PO-iPr | Py-PO-cHex | Py-PO-C5  | Py-PO-2EtHex | Phen-PO-C5 |
|--------------------|-----------|------------|-----------|--------------|------------|
| Zn(II)             | 24        | 19         | 4         | 25           | <b>58</b>  |
| Cu(II)             | 30        | 22         | 12        | <b>37</b>    | <b>76</b>  |
| Ni(II)             | 7         | 9          | 4         | 15           | <b>31</b>  |
| Co(II)             | 11        | 12         | 4         | 19           | <b>44</b>  |
| Cd(II)             | 21        | 20         | 10        | 28           | <b>49</b>  |
| Pb(II)             | <b>35</b> | <b>31</b>  | <b>46</b> | <b>40</b>    | <b>55</b>  |

Table S5 Slopes ( $\pm 2 \text{ mV/dec}$ ) of electrode functions for various cations. Inner electrolyte solution is  $0.01 \text{ mol}\cdot\text{L}^{-1} \text{ CuCl}_2$  or  $\text{ZnCl}_2$ .

| Sensor type | Sensor filler   | Py-PO-iPr | Py-PO-cHex | Py-PO-C5 | Py-PO-2EtHex | Phen-PO-C5 |
|-------------|-----------------|-----------|------------|----------|--------------|------------|
| Cation      |                 |           |            |          |              |            |
| Cu(II)      | $\text{CuCl}_2$ | 19        | 20         | 14       | <b>27</b>    | <b>32</b>  |
| Zn(II)      | $\text{ZnCl}_2$ | 14        | 16         | 8        | 22           | 22         |

Table S6 Lower detection limits (LOD) and linear response ranges (LR) for potentiometric sensors (mol/L). Inner electrolyte solution is 0.01 mol·L<sup>-1</sup> NaCl.

| Sensor type/Cation | Parameter | Py-PO-iPr                           | Py-PO-cHex                          | Py-PO-C5                            | Py-PO-2EtHex                        | Phen-PO-C5                          |
|--------------------|-----------|-------------------------------------|-------------------------------------|-------------------------------------|-------------------------------------|-------------------------------------|
| Zn(II)             | LOD       | 6*10 <sup>-6</sup>                  | 3*10 <sup>-6</sup>                  | -                                   | 4*10 <sup>-6</sup>                  | 10 <sup>-6</sup>                    |
|                    | LR        | 10 <sup>-5</sup> – 10 <sup>-3</sup> | 10 <sup>-5</sup> – 10 <sup>-3</sup> | -                                   | 10 <sup>-5</sup> – 10 <sup>-3</sup> | 10 <sup>-6</sup> – 10 <sup>-3</sup> |
| Cu(II)             | LOD       | 3*10 <sup>-6</sup>                  | 2*10 <sup>-6</sup>                  | -                                   | 10 <sup>-6</sup>                    | 10 <sup>-6</sup>                    |
|                    | LR        | 10 <sup>-5</sup> – 10 <sup>-3</sup> | 10 <sup>-5</sup> – 10 <sup>-3</sup> | -                                   | 10 <sup>-6</sup> – 10 <sup>-3</sup> | 10 <sup>-6</sup> – 10 <sup>-3</sup> |
| Ni(II)             | LOD       | 3*10 <sup>-5</sup>                  | 10 <sup>-5</sup>                    | -                                   | 3*10 <sup>-6</sup>                  | 10 <sup>-6</sup>                    |
|                    | LR        | 10 <sup>-4</sup> – 10 <sup>-3</sup> | 10 <sup>-5</sup> – 10 <sup>-3</sup> | -                                   | 10 <sup>-5</sup> – 10 <sup>-3</sup> | 10 <sup>-6</sup> – 10 <sup>-3</sup> |
| Co(II)             | LOD       | 10 <sup>-5</sup>                    | 3*10 <sup>-6</sup>                  | -                                   | 10 <sup>-6</sup>                    | 10 <sup>-6</sup>                    |
|                    | LR        | 10 <sup>-5</sup> – 10 <sup>-3</sup> | 10 <sup>-5</sup> – 10 <sup>-3</sup> | -                                   | 10 <sup>-6</sup> – 10 <sup>-3</sup> | 10 <sup>-6</sup> – 10 <sup>-3</sup> |
| Cd(II)             | LOD       | 3*10 <sup>-6</sup>                  | 3*10 <sup>-6</sup>                  | -                                   | 10 <sup>-5</sup>                    | 10 <sup>-6</sup>                    |
|                    | LR        | 10 <sup>-5</sup> – 10 <sup>-3</sup> | 10 <sup>-5</sup> – 10 <sup>-3</sup> | -                                   | 10 <sup>-5</sup> – 10 <sup>-3</sup> | 10 <sup>-6</sup> – 10 <sup>-3</sup> |
| Pb(II)             | LOD       | 4*10 <sup>-6</sup>                  | 10 <sup>-7</sup>                    | 10 <sup>-6</sup>                    | 2*10 <sup>-6</sup>                  | 10 <sup>-6</sup>                    |
|                    | LR        | 10 <sup>-5</sup> – 10 <sup>-3</sup> | 10 <sup>-7</sup> – 10 <sup>-3</sup> | 10 <sup>-5</sup> – 10 <sup>-3</sup> | 10 <sup>-5</sup> – 10 <sup>-3</sup> | 10 <sup>-6</sup> – 10 <sup>-3</sup> |

#### 4. X-ray diffraction data

Table S7 Crystallographic details for CdCl<sub>2</sub>Py-PO-iPr , Pb(NO<sub>3</sub>)<sub>2</sub>Py-PO-cHex and Cd(NO<sub>3</sub>)<sub>2</sub>Py-PO-iPr structures.

|  | CdCl <sub>2</sub> Py-PO-iPr   | Pb(NO <sub>3</sub> ) <sub>2</sub> Py-PO-cHex                                     | Cd(NO <sub>3</sub> ) <sub>2</sub> Py-PO-iPr                                      |
|--|---|--|--|
| Empirical formula                      | C <sub>34</sub> H <sub>62</sub> Cd <sub>2</sub> Cl <sub>3.6</sub> N <sub>2.4</sub> O <sub>13.2</sub> P <sub>4</sub> | C <sub>58</sub> H <sub>94</sub> N <sub>4</sub> O <sub>18</sub> P <sub>4</sub> Pb | C <sub>17</sub> H <sub>31</sub> CdN <sub>3</sub> O <sub>12</sub> P <sub>24</sub> |
| Mw                                     | 1191.96   | 1466.44  | 643.79   |
| T (K)                                  | 150(2)  | 150(2)   | 100(2)   |
| Crystal size (mm <sup>3</sup> )        | 0.35 × 0.25 × 0.1   | 0.32 × 0.1 × 0.08  | 0.17 × 0.13 × 0.01   |
| Crystal system                         | monoclinic  | monoclinic   | monoclinic   |
| Space group                            | P21/n   | P21/c  | P21/c  |
| <i>a</i> (Å)                           | 12.8333(9)  | 12.9451(13)  | 22.4562(14)  |
| <i>b</i> (Å)                           | 16.1328(11)   | 35.541(3)  | 13.6538(9)   |
| <i>c</i> (Å)                           | 13.2377(9)  | 15.6372(14)  | 18.4024(11)  |
| <i>α</i> (°)                           | 90  | 90   | 90   |
| <i>β</i> (°)                           | 110.798(2)  | 108.592(4)   | 108.491(2)   |
| <i>γ</i> (°)                           | 90  | 90   | 90   |
| V (Å <sup>3</sup> )                    | 2562.1(3)   | 6819.0(11)   | 5351.1(6)  |
| Z                                      | 2   | 4  | 8  |
| ρ <sub>calc</sub> (g/cm <sup>3</sup> ) | 1.545   | 1.428  | 1.598  |
| μ (mm <sup>-1</sup> )                  | 1.198   | 2.636  | 0.996  |

|  |                                    |                                    |                                    |
|--|------------------------------------|------------------------------------|------------------------------------|
| F(000)   | 1211                               | 3024                               | 2624                               |
| $\theta$ range for data collection ( $^\circ$ )        | $2.28 < \theta < 27.79$            | $2.02 < \theta < 25.05$            | $1.77 < \theta < 26.43$            |
| Reflections collected                                  | 43896                              | 49253                              | 61083                              |
| Independent reflections                                | 5817                               | 12064                              | 10953                              |
| Data/<br>restraints/<br>parameters                     | 5817/4/286                         | 12064/290/530                      | 10953/0/647                        |
| Goodness-of-fit<br>on $F^2$                            | 1.149                              | 1.039                              | 1.092                              |
| Final R indexes<br>[ $I \geq 2\sigma(I)$ ]             | $R_1 = 0.0355,$<br>$wR_2 = 0.0785$ | $R_1 = 0.0747,$<br>$wR_2 = 0.1991$ | $R_1 = 0.0449,$<br>$wR_2 = 0.0830$ |
| Final R indexes<br>[all data]                          | $R_1 = 0.0395,$<br>$wR_2 = 0.0801$ | $R_1 = 0.1143,$<br>$wR_2 = 0.2263$ | $R_1 = 0.0814,$<br>$wR_2 = 0.0955$ |
| Largest diff.<br>peak/hole<br>( $e \text{ \AA}^{-3}$ ) | 1.05 / -0.77                       | 1.25 / -1.69                       | 1.19 / -1.12                       |

Table S8 Distances in the coordination sphere of Cadmium in Cd(NO<sub>3</sub>)<sub>2</sub>Py-PO-iPr

| Bond    | Å        | Bond    | Å        |
|---------|----------|---------|----------|
| Cd1 N1  | 2.369(3) | Cd2 N4  | 2.351(3) |
| Cd1 O1  | 2.295(3) | Cd2 O13 | 2.292(3) |
| Cd1 O2  | 2.292(3) | Cd2 O14 | 2.313(3) |
| Cd1 O7  | 2.522(3) | Cd2 O23 | 2.528(3) |
| Cd1 O8  | 2.264(3) | Cd2 O22 | 2.273(3) |
| Cd1 O10 | 2.296(3) | Cd2 O20 | 2.293(3) |
| Cd1 O11 | 2.452(3) | Cd2 O19 | 2.446(3) |

Table S9 Torsion angles in the ligands in Cd(NO<sub>3</sub>)<sub>2</sub>Py-PO-iPr

| Torsion angle | Cd1       | Torsion angle | Cd2      |
|---------------|-----------|---------------|----------|
| O1 P1 C1 N1   | 17.3(4)°  | O13 P3 C18 N4 | 7.4(4)°  |
| O2 P2 C5 N1   | -13.0(3)° | O14 P4 C22 N4 | -4.8(4)° |

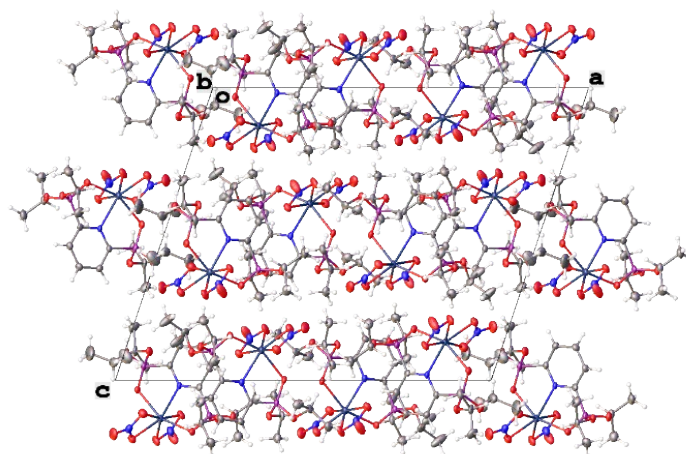
Figure S3 Fragment of the crystal packing of Cd(NO<sub>3</sub>)<sub>2</sub>Py-PO-iPr



Table S10 Distances in the coordination sphere of Pb and torsion angles for the chelating and bridging ligands in  $\text{Pb}(\text{NO}_3)_2\text{Py-PO-cHex}$ .

| Bond       | Å                  | Torsion angle   | °                  |
|------------|--------------------|-----------------|--------------------|
| Pb1 O1     | 2.690(8)           | N1 C1 P2a/P2 O1 | -13.7(14)/23.5(15) |
| Pb1 O2     | 2.549(8)           | N1 C5 P1 O2     | 3.9(13)            |
| Pb1 O3     | 2.573(6)           | N2 C6 P3 O3     | -174.4(10)         |
| Pb1 O4'    | 2.626(7)           | N2 C10 P4 O4    | 176.9(9)           |
| Pb1 O5/O5a | 2.73 (4) / 2.61(4) |                 |                    |
| Pb1 O6/O6a | 2.54(3) / 2.61(3)  |                 |                    |
| Pb1 O8     | 2.783(11)          |                 |                    |
| Pb1 O9     | 2.763(9)           |                 |                    |
| Pb1 N1     | 2.826(8)           |                 |                    |

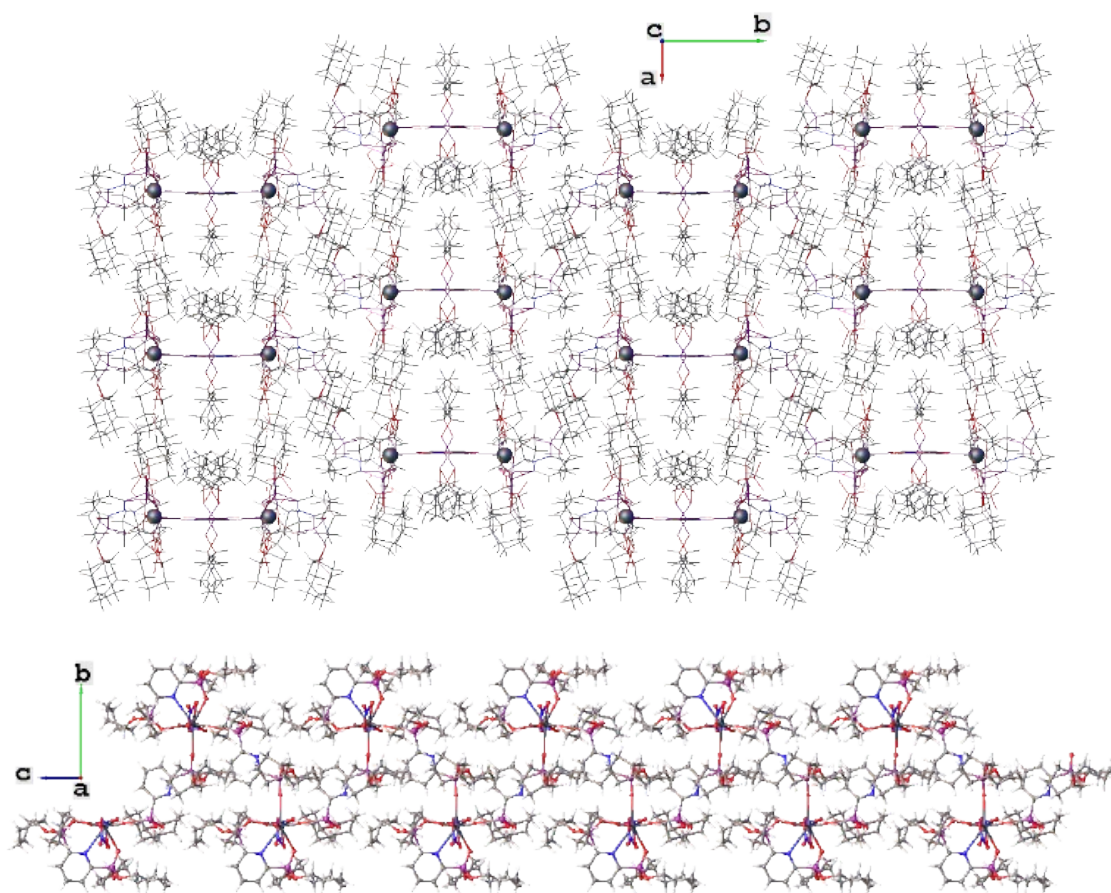


Figure S4 Polymeric chains (side and top views) in  $\text{Pb}(\text{NO}_3)_2\text{Py-PO-cHex}$ .

Table S11 Distances in the coordination sphere of Cd in CdCl<sub>2</sub>Py-PO-iPr.

| Bond     | Å          | Average bond lengths<br>in Cadmium complexes, Å |              |
|----------|------------|---|--------------|
| Bond     | Å          | Cd Cl(bridging)                                 | 2.635(0.089) |
| Cd1 Cl2  | 2.4436(7)  |   |              |
| Cd1 Cl2' | 2.8910(8)  | Cd Cl(terminal)                                 | 2.473(0.068) |
| Cd1 Cl1  | 2.5315(13) | Cd O  | 2.358(0.099) |
| Cd1 O2   | 2.367(2)   |   |              |
| Cd1 O1   | 2.349(2)   |   |              |
|          |            |   |              |

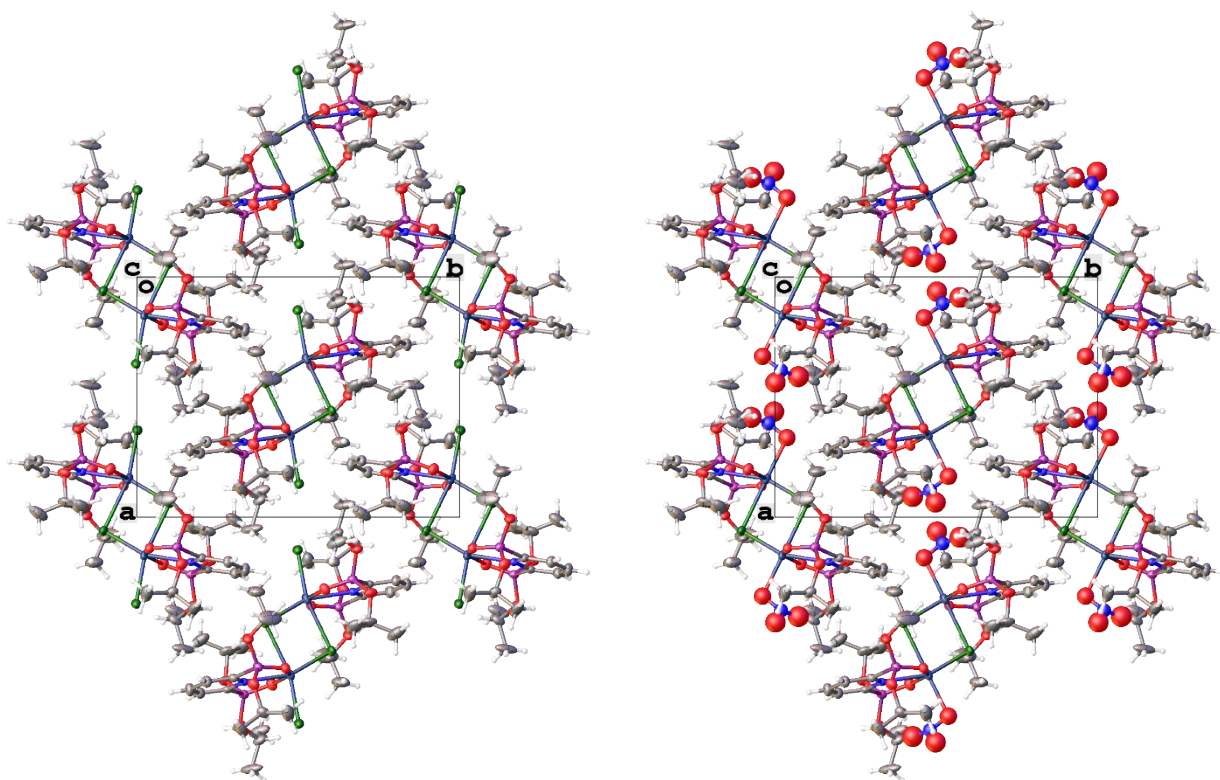


Figure S5 Fragment of the crystal packing of CdCl<sub>2</sub>Py-PO-iPr (with chloride – left and with nitrate – right).

## 5. DFT calculations

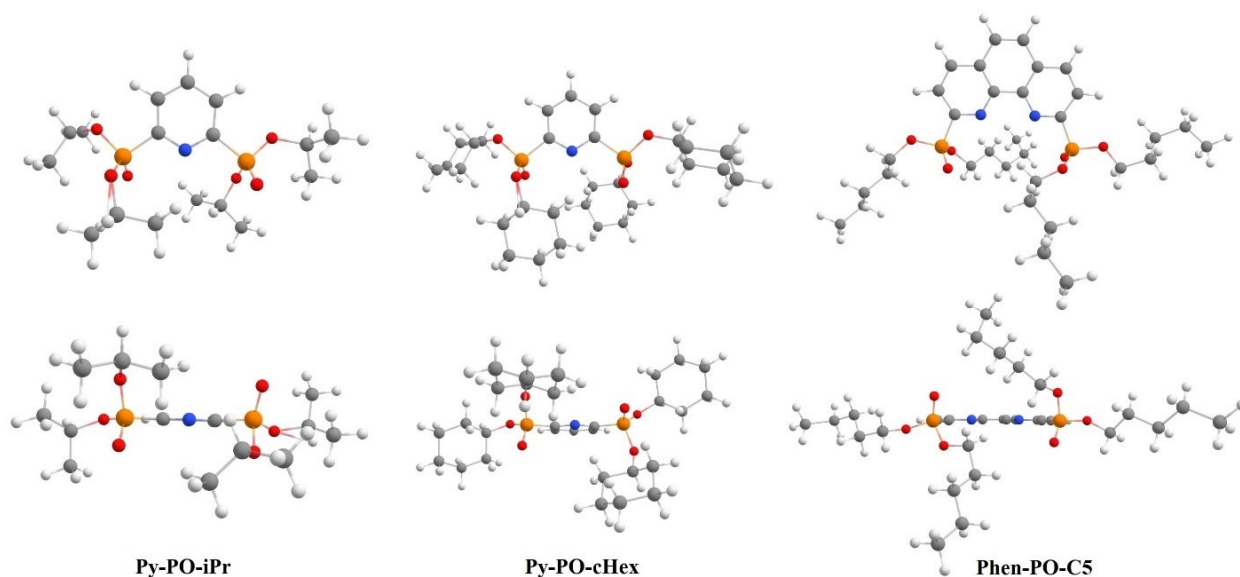


Figure S6 Optimized structures of the ligands in two projections at B97M-V/def2-TZVP level of theory.

Table S12 The energy difference between the classical and non-classical structures of Py-PO-iPr\*Pb(NO<sub>3</sub>)<sub>2</sub> complex depending on chosen functional. def2-TZVP basis set, solvent effects at CPCM(acetone) level.

| Level of theory | ( $E_{\text{classical}} - E_{\text{non-classical}}$ ), kcal/mol |
|-----------------|---|
| revPBE0-D3      | 4.8   |
| B3LYP           | -3.7  |
| wB97M-V         | -1.1  |
| B2PLYP          | 1.8   |

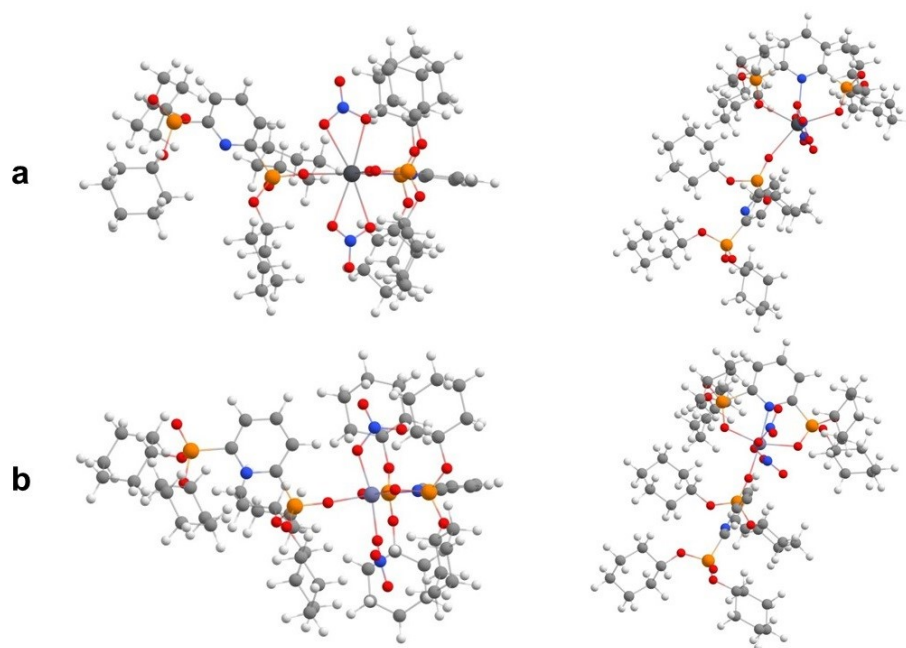


Figure S7 Structure of the (a)  $\text{Pb}(\text{NO}_3)_2 \cdot 2\text{Py-PO-cHex}$  complex, (b)  $\text{Zn}(\text{NO}_3)_2 \cdot 2\text{Py-PO-cHex}$  complexes.

Table S13 The energy of complex formation for Py-PO-iPr\*M(NO<sub>3</sub>)<sub>2</sub> complex (M=Pb, Cd, Zn, Cu) with def2-TZVP basis set (CPCM model) depending on chosen functional, kcal/mol.

| DFT functional | M  | Initial state                                     |  |
|----------------|----|---|--|
|                |    | [M(H <sub>2</sub> O) <sub>6</sub> ] <sup>2+</sup> | [M(NO <sub>3</sub> )(H <sub>2</sub> O) <sub>5</sub> ] <sup>+</sup> |
| revPBE0-D3     | Pb | -11.6   | -5.1   |
|                | Cd | -6.9  | -1.2   |
|                | Zn | -3.1  | 2.6  |
|                | Cu | -7.9  | -0.1   |
| B3LYP          | Pb | -8.8  | -1.6   |
|                | Cd | -6.9  | -1.4   |
|                | Zn | -0.7  | 5.4  |
|                | Cu | -6.3  | 2.1  |
| wB97M-V        | Pb | -20.1   | -8.6   |
|                | Cd | -18.4   | -6.9   |
|                | Zn | -15.0   | -4.4   |
|                | Cu | -16.0   | -3.7   |
| B2PLYP         | Pb | -15.0   | -6.8   |
|                | Cd | -12.2   | -5.0   |
|                | Zn | -6.4  | 0.6  |
|                | Cu | -8.7  | -0.3   |

Table S14 DFT energies of complex formation at wB97M-V/def2-TZVP theoretical level.

| Complex                                       | Energy of complex formation (including solvents at CPCM level), kcal/mol |  | Preorganization energy (gas phase), kcal/mol |
|---|--|--|--|
|   | [M(H <sub>2</sub> O) <sub>6</sub> ] <sup>2+</sup> initial state          | [M(NO <sub>3</sub> )(H <sub>2</sub> O) <sub>5</sub> ] <sup>+</sup> initial state |  |
| Pb(NO <sub>3</sub> ) <sub>2</sub> *Py-PO-iPr  | -20.1  | -8.6   | 9.7  |
| Cd(NO <sub>3</sub> ) <sub>2</sub> *Py-PO-iPr  | -18.4  | -6.9   | 11.4   |
| Cu(NO <sub>3</sub> ) <sub>2</sub> *Py-PO-iPr  | -16.0  | -3.7   | 12.0   |
| Zn(NO <sub>3</sub> ) <sub>2</sub> *Py-PO-iPr  | -15.0  | -4.4   | 16.4   |
| Pb(NO <sub>3</sub> ) <sub>2</sub> *Py-PO-cHex | -24.7  | -13.2  | 9.8  |
| Cd(NO <sub>3</sub> ) <sub>2</sub> *Py-PO-cHex | -22.7  | -11.2  | 12.0   |
| Cu(NO <sub>3</sub> ) <sub>2</sub> *Py-PO-cHex | -19.1  | -6.7   | 13.8   |
| Zn(NO <sub>3</sub> ) <sub>2</sub> *Py-PO-cHex | -20.9  | -10.3  | 15.4   |
| Pb(NO <sub>3</sub> ) <sub>2</sub> *Phen-PO-C5 | -33.5  | -22.0  | 12.7   |
| Cd(NO <sub>3</sub> ) <sub>2</sub> *Phen-PO-C5 | -32.8  | -21.2  | 13.7   |
| Cu(NO <sub>3</sub> ) <sub>2</sub> *Phen-PO-C5 | -27.8  | -15.5  | 13.8   |
| Zn(NO <sub>3</sub> ) <sub>2</sub> *Phen-PO-C5 | -22.3  | -11.7  | 16.8   |

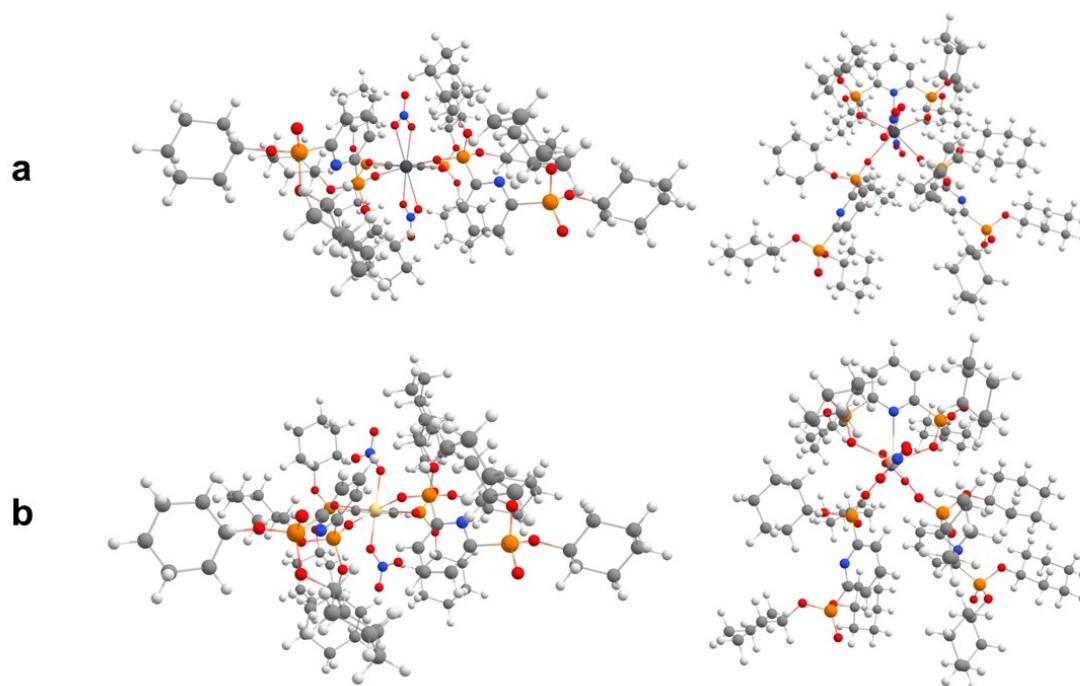


Figure S8 Structure of the (a)  $\text{Pb}(\text{NO}_3)_2 \cdot 3\text{Py-PO-cHex}$  complex, (b)  $\text{Cd}(\text{NO}_3)_2 \cdot 3\text{Py-PO-cHex}$  complexes.

Table S15 DFT energies of complex formation in the at PBE/def2-SVP theoretical level.

| Complex   | Energy of complex formation according to reactions (1) and (2), kcal/mol |
|---|--|
| $\text{Pb}(\text{NO}_3)_2 \cdot 2\text{Py-PO-cHex}$ | -39.5  |
| $\text{Cd}(\text{NO}_3)_2 \cdot 2\text{Py-PO-cHex}$ | -22.0  |
| $\text{Zn}(\text{NO}_3)_2 \cdot 2\text{Py-PO-cHex}$ | -26.4  |
| $\text{Cu}(\text{NO}_3)_2 \cdot 2\text{Py-PO-cHex}$ | -23.0  |
| $\text{Pb}(\text{NO}_3)_2 \cdot 3\text{Py-PO-cHex}$ | -29.2  |
| $\text{Cd}(\text{NO}_3)_2 \cdot 3\text{Py-PO-cHex}$ | -13.5  |

#### Cartesian coordinates of the optimized geometries

| Structure | XYZ coordinates |              |              |              |
|-----------|-----------------|--------------|--------------|--------------|
| Py-PO-iPr | 6               | -1.648374000 | -0.821804000 | 0.238477000  |
|           | 6               | -2.398787000 | -1.735002000 | 0.969691000  |
|           | 6               | -1.758246000 | -2.490662000 | 1.935012000  |
|           | 6               | -0.401794000 | -2.315325000 | 2.139994000  |
|           | 6               | 0.265007000  | -1.379717000 | 1.361428000  |
|           | 7               | -0.343294000 | -0.647002000 | 0.430461000  |
|           | 1               | -2.311140000 | -3.207419000 | 2.522112000  |
|           | 1               | -3.452878000 | -1.839473000 | 0.779907000  |
|           | 1               | 0.134846000  | -2.878674000 | 2.884534000  |
|           | 15              | 2.035233000  | -1.058018000 | 1.439541000  |
|           | 15              | -2.335068000 | 0.253378000  | -1.040765000 |
|           | 8               | 2.159625000  | 0.496542000  | 1.686594000  |
|           | 8               | -3.855710000 | -0.156791000 | -0.937805000 |

|            |   |              |              |              |
|------------|---|--------------|--------------|--------------|
|            | 8 | -2.007559000 | 1.672935000  | -0.882022000 |
|            | 8 | 2.381425000  | -1.670210000 | 2.850393000  |
|            | 8 | 2.777235000  | -1.556536000 | 0.277786000  |
|            | 6 | -4.972804000 | 0.679852000  | -1.343191000 |
|            | 6 | -5.206276000 | 1.749096000  | -0.306392000 |
|            | 6 | -4.780893000 | 1.232260000  | -2.732508000 |
|            | 1 | -5.803730000 | -0.022947000 | -1.344291000 |
|            | 1 | -4.371653000 | 2.443481000  | -0.284331000 |
|            | 1 | -5.319513000 | 1.309807000  | 0.680904000  |
|            | 1 | -3.979938000 | 1.966990000  | -2.745785000 |
|            | 1 | -4.545661000 | 0.441925000  | -3.439360000 |
|            | 6 | 3.686559000  | 1.960823000  | 0.576144000  |
|            | 6 | 1.219195000  | 2.462967000  | 0.707666000  |
|            | 6 | 2.284494000  | 1.413571000  | 0.556887000  |
|            | 1 | 3.875997000  | 2.487998000  | 1.509415000  |
|            | 1 | 4.412442000  | 1.159170000  | 0.473522000  |
|            | 1 | 0.226953000  | 2.024899000  | 0.660726000  |
|            | 1 | 1.337556000  | 2.988074000  | 1.653748000  |
|            | 1 | 2.126215000  | 0.840087000  | -0.353614000 |
|            | 8 | -1.892325000 | -0.401363000 | -2.410584000 |
|            | 6 | -0.844707000 | 0.088099000  | -3.299653000 |
|            | 6 | -1.324773000 | 1.312005000  | -4.037595000 |
|            | 6 | 0.457464000  | 0.311070000  | -2.577553000 |
|            | 1 | -0.736539000 | -0.740387000 | -3.996653000 |
|            | 1 | -1.458843000 | 2.142130000  | -3.349527000 |
|            | 1 | -2.265078000 | 1.118092000  | -4.546316000 |
|            | 1 | 0.360330000  | 1.121172000  | -1.859163000 |
|            | 1 | 0.786710000  | -0.578741000 | -2.049979000 |
|            | 6 | 4.746794000  | -1.019108000 | 2.924705000  |
|            | 6 | 4.039261000  | -3.419353000 | 2.656423000  |
|            | 6 | 3.720097000  | -2.073057000 | 3.254897000  |
|            | 1 | 4.883528000  | -0.939222000 | 1.849037000  |
|            | 1 | 4.455155000  | -0.048507000 | 3.314549000  |
|            | 1 | 3.278799000  | -4.149451000 | 2.920100000  |
|            | 1 | 4.092817000  | -3.347229000 | 1.574056000  |
|            | 1 | 3.624444000  | -2.159466000 | 4.335346000  |
|            | 1 | 1.222720000  | 0.581446000  | -3.302551000 |
|            | 1 | -0.588151000 | 1.596774000  | -4.785701000 |
|            | 1 | -5.696094000 | 1.722356000  | -3.056276000 |
|            | 1 | -6.115738000 | 2.297839000  | -0.541203000 |
|            | 1 | 1.299753000  | 3.190841000  | -0.097186000 |
|            | 1 | 3.828268000  | 2.658728000  | -0.245969000 |
|            | 1 | 5.700578000  | -1.295021000 | 3.368485000  |
|            | 1 | 4.996065000  | -3.773922000 | 3.033432000  |
| Py-PO-cHex | 6 | -2.160751000 | -0.864994000 | 0.726532000  |
|            | 6 | -3.022220000 | -1.913067000 | 1.029400000  |
|            | 6 | -2.487675000 | -3.181033000 | 1.168080000  |
|            | 6 | -1.126983000 | -3.366495000 | 0.993649000  |
|            | 6 | -0.345879000 | -2.259045000 | 0.690249000  |
|            | 7 | -0.853020000 | -1.036316000 | 0.565914000  |
|            | 1 | -3.125237000 | -4.017690000 | 1.408386000  |
|            | 1 | -4.075484000 | -1.727931000 | 1.156285000  |

|  |    |              |              |              |
|--|----|--------------|--------------|--------------|
|  | 1  | -0.673404000 | -4.337785000 | 1.091576000  |
|  | 15 | 1.423502000  | -2.321373000 | 0.334897000  |
|  | 15 | -2.696364000 | 0.846114000  | 0.494966000  |
|  | 8  | -1.731290000 | 1.837043000  | 0.976997000  |
|  | 8  | 1.731645000  | -3.792962000 | 0.820354000  |
|  | 8  | 1.762746000  | -1.989268000 | -1.053031000 |
|  | 6  | 4.154296000  | -3.896786000 | 0.390394000  |
|  | 6  | 5.263745000  | -4.839088000 | -0.050429000 |
|  | 6  | 4.987031000  | -5.396474000 | -1.436315000 |
|  | 6  | 3.636778000  | -6.091541000 | -1.479498000 |
|  | 6  | 2.525073000  | -5.155080000 | -1.033525000 |
|  | 6  | 2.824694000  | -4.613293000 | 0.345867000  |
|  | 1  | 4.114022000  | -3.041102000 | -0.285429000 |
|  | 1  | 4.335041000  | -3.513403000 | 1.393641000  |
|  | 1  | 5.341029000  | -5.666887000 | 0.660199000  |
|  | 1  | 6.221465000  | -4.321911000 | -0.025344000 |
|  | 1  | 5.778311000  | -6.082984000 | -1.734665000 |
|  | 1  | 4.992293000  | -4.577857000 | -2.160044000 |
|  | 1  | 3.663629000  | -6.964879000 | -0.821156000 |
|  | 1  | 3.427617000  | -6.467035000 | -2.479690000 |
|  | 1  | 1.562767000  | -5.666158000 | -1.021245000 |
|  | 1  | 2.436414000  | -4.313618000 | -1.720514000 |
|  | 1  | 2.843934000  | -5.437952000 | 1.061011000  |
|  | 8  | 2.105013000  | -1.426718000 | 1.441629000  |
|  | 6  | 1.751436000  | 0.874402000  | 0.598554000  |
|  | 6  | 2.407450000  | 2.243546000  | 0.517804000  |
|  | 6  | 3.728375000  | 2.175459000  | -0.227216000 |
|  | 6  | 4.658543000  | 1.167943000  | 0.426979000  |
|  | 6  | 4.006351000  | -0.203448000 | 0.517393000  |
|  | 6  | 2.691044000  | -0.106708000 | 1.256263000  |
|  | 1  | 1.533998000  | 0.514562000  | -0.408578000 |
|  | 1  | 0.805724000  | 0.923239000  | 1.130718000  |
|  | 1  | 2.582062000  | 2.625117000  | 1.528038000  |
|  | 1  | 1.724447000  | 2.945818000  | 0.041274000  |
|  | 1  | 4.199287000  | 3.157213000  | -0.268155000 |
|  | 1  | 3.540792000  | 1.872389000  | -1.261115000 |
|  | 1  | 4.909941000  | 1.516794000  | 1.432806000  |
|  | 1  | 5.598930000  | 1.095376000  | -0.117638000 |
|  | 1  | 4.660755000  | -0.912993000 | 1.022887000  |
|  | 1  | 3.808046000  | -0.590679000 | -0.482883000 |
|  | 1  | 2.878799000  | 0.213257000  | 2.282633000  |
|  | 8  | -3.116410000 | 0.976532000  | -1.029030000 |
|  | 6  | -0.944787000 | 0.670764000  | -2.135990000 |
|  | 6  | -0.065992000 | 1.154247000  | -3.277289000 |
|  | 6  | 0.175046000  | 2.650359000  | -3.182902000 |
|  | 6  | -1.142792000 | 3.405541000  | -3.151066000 |
|  | 6  | -2.015422000 | 2.932521000  | -1.998705000 |
|  | 6  | -2.242037000 | 1.440072000  | -2.094034000 |
|  | 1  | -0.424261000 | 0.815595000  | -1.190006000 |
|  | 1  | -1.142302000 | -0.396543000 | -2.224677000 |
|  | 1  | -0.546105000 | 0.926739000  | -4.233726000 |
|  | 1  | 0.873705000  | 0.604537000  | -3.265109000 |



|          |    |              |              |              |
|----------|----|--------------|--------------|--------------|
|          | 1  | 0.790886000  | 2.992577000  | -4.013937000 |
|          | 1  | 0.734845000  | 2.865311000  | -2.268012000 |
|          | 1  | -1.668231000 | 3.245697000  | -4.097393000 |
|          | 1  | -0.973928000 | 4.478386000  | -3.070838000 |
|          | 1  | -2.977198000 | 3.445838000  | -1.999325000 |
|          | 1  | -1.531629000 | 3.149812000  | -1.046662000 |
|          | 1  | -2.821288000 | 1.223438000  | -2.993373000 |
|          | 8  | -4.105990000 | 0.786181000  | 1.202562000  |
|          | 6  | -4.893238000 | 3.061983000  | 0.665066000  |
|          | 6  | -5.707009000 | 4.220790000  | 1.221435000  |
|          | 6  | -5.122066000 | 4.718020000  | 2.532134000  |
|          | 6  | -5.031568000 | 3.590031000  | 3.545426000  |
|          | 6  | -4.223866000 | 2.425257000  | 2.994741000  |
|          | 6  | -4.818795000 | 1.951227000  | 1.688191000  |
|          | 1  | -3.881547000 | 3.405454000  | 0.441664000  |
|          | 1  | -5.321286000 | 2.685014000  | -0.262131000 |
|          | 1  | -6.737934000 | 3.895141000  | 1.386510000  |
|          | 1  | -5.751828000 | 5.024793000  | 0.488636000  |
|          | 1  | -5.718424000 | 5.539271000  | 2.927458000  |
|          | 1  | -4.121008000 | 5.115467000  | 2.347986000  |
|          | 1  | -6.041226000 | 3.249282000  | 3.792460000  |
|          | 1  | -4.588459000 | 3.940140000  | 4.476024000  |
|          | 1  | -4.197967000 | 1.596691000  | 3.701392000  |
|          | 1  | -3.193056000 | 2.730100000  | 2.815122000  |
|          | 1  | -5.825548000 | 1.570017000  | 1.868493000  |
| Py-PO-C5 | 6  | -4.763458000 | -0.615449000 | 1.255768000  |
|          | 6  | -5.416170000 | 0.040074000  | 0.242500000  |
|          | 6  | -4.679160000 | 0.700015000  | -0.750205000 |
|          | 6  | -3.272215000 | 0.655867000  | -0.644680000 |
|          | 7  | -2.642057000 | 0.020470000  | 0.346191000  |
|          | 6  | -3.362064000 | -0.597327000 | 1.261533000  |
|          | 6  | -5.279210000 | 1.399694000  | -1.834216000 |
|          | 6  | -2.470663000 | 1.326874000  | -1.632684000 |
|          | 6  | -3.102517000 | 2.023733000  | -2.684555000 |
|          | 6  | -4.523013000 | 2.034482000  | -2.762704000 |
|          | 6  | -2.274187000 | 2.690250000  | -3.598969000 |
|          | 1  | -2.720602000 | 3.235028000  | -4.418218000 |
|          | 6  | -0.912523000 | 2.660558000  | -3.435206000 |
|          | 6  | -0.391214000 | 1.938834000  | -2.352699000 |
|          | 7  | -1.144634000 | 1.282450000  | -1.493145000 |
|          | 1  | -6.357215000 | 1.417486000  | -1.899440000 |
|          | 1  | -5.299072000 | -1.138092000 | 2.029864000  |
|          | 1  | -6.495498000 | 0.052562000  | 0.196740000  |
|          | 15 | -2.298397000 | -1.420063000 | 2.459784000  |
|          | 1  | -4.988552000 | 2.568623000  | -3.577940000 |
|          | 1  | -0.250001000 | 3.181272000  | -4.106787000 |
|          | 15 | 1.352329000  | 1.761945000  | -1.938759000 |
|          | 8  | 1.947080000  | 3.072133000  | -2.592828000 |
|          | 8  | 1.956930000  | 0.490828000  | -2.341912000 |
|          | 8  | -1.334717000 | -0.547445000 | 3.130545000  |
|          | 8  | -1.646092000 | -2.634386000 | 1.677988000  |
|          | 6  | 3.375211000  | 3.269154000  | -2.590296000 |

|  |   |              |              |              |
|--|---|--------------|--------------|--------------|
|  | 1 | 3.697466000  | 3.433899000  | -1.563275000 |
|  | 6 | 3.684823000  | 4.454787000  | -3.460087000 |
|  | 1 | 3.852858000  | 2.363468000  | -2.962814000 |
|  | 1 | 3.154121000  | 5.326423000  | -3.071064000 |
|  | 6 | 3.323688000  | 4.239697000  | -4.918043000 |
|  | 1 | 4.749338000  | 4.666008000  | -3.355362000 |
|  | 1 | 2.278292000  | 3.937636000  | -4.978321000 |
|  | 1 | 3.905230000  | 3.401219000  | -5.311022000 |
|  | 6 | 3.545029000  | 5.463514000  | -5.790653000 |
|  | 6 | 4.998628000  | 5.880853000  | -5.903935000 |
|  | 1 | 2.954291000  | 6.293677000  | -5.396717000 |
|  | 1 | 3.151303000  | 5.261662000  | -6.786991000 |
|  | 6 | -0.372686000 | -2.506508000 | 1.001727000  |
|  | 1 | 0.221250000  | -3.357032000 | 1.332117000  |
|  | 1 | 0.119405000  | -1.596390000 | 1.338389000  |
|  | 6 | -0.563801000 | -2.523653000 | -0.490213000 |
|  | 6 | 0.760422000  | -2.563912000 | -1.230323000 |
|  | 1 | -1.115967000 | -1.630984000 | -0.784890000 |
|  | 1 | -1.177736000 | -3.387436000 | -0.747533000 |
|  | 1 | 1.384957000  | -1.730859000 | -0.906025000 |
|  | 6 | 0.610202000  | -2.479350000 | -2.739502000 |
|  | 1 | 1.298759000  | -3.480722000 | -0.968551000 |
|  | 6 | -0.138354000 | -3.648936000 | -3.348598000 |
|  | 1 | 1.601654000  | -2.404707000 | -3.183638000 |
|  | 1 | 0.113002000  | -1.540796000 | -2.988474000 |
|  | 8 | 1.437806000  | 2.089115000  | -0.397539000 |
|  | 6 | 1.192828000  | 1.062620000  | 0.602035000  |
|  | 1 | 0.130721000  | 0.835254000  | 0.600583000  |
|  | 6 | 1.649573000  | 1.584124000  | 1.932151000  |
|  | 1 | 1.748332000  | 0.171065000  | 0.310859000  |
|  | 1 | 1.115231000  | 2.511006000  | 2.149550000  |
|  | 6 | 3.144788000  | 1.812052000  | 2.019313000  |
|  | 1 | 1.325547000  | 0.865399000  | 2.687332000  |
|  | 1 | 3.451839000  | 2.510836000  | 1.238049000  |
|  | 1 | 3.666154000  | 0.874247000  | 1.805066000  |
|  | 6 | 3.588704000  | 2.339805000  | 3.368103000  |
|  | 1 | 3.276209000  | 1.642313000  | 4.148035000  |
|  | 1 | 3.063064000  | 3.273988000  | 3.577417000  |
|  | 6 | 5.084307000  | 2.565583000  | 3.449238000  |
|  | 8 | -3.375451000 | -2.142473000 | 3.362735000  |
|  | 6 | -2.942649000 | -2.852036000 | 4.541168000  |
|  | 1 | -3.647976000 | -2.585311000 | 5.324675000  |
|  | 1 | -1.960138000 | -2.488294000 | 4.839704000  |
|  | 6 | -2.934458000 | -4.337082000 | 4.296739000  |
|  | 6 | -2.538960000 | -5.107745000 | 5.540286000  |
|  | 1 | -2.248463000 | -4.559535000 | 3.479396000  |
|  | 1 | -3.926326000 | -4.646705000 | 3.963251000  |
|  | 1 | -1.547016000 | -4.787637000 | 5.870088000  |
|  | 6 | -2.534686000 | -6.609433000 | 5.331860000  |
|  | 1 | -3.220071000 | -4.859961000 | 6.359275000  |
|  | 1 | -3.525890000 | -6.927113000 | 5.002360000  |
|  | 6 | -2.137105000 | -7.373153000 | 6.577504000  |

|  |    |              |              |              |
|--|----|--------------|--------------|--------------|
|  | 1  | -1.854921000 | -6.854448000 | 4.513634000  |
|  | 1  | 5.383998000  | 2.952416000  | 4.420247000  |
|  | 1  | 5.413383000  | 3.278266000  | 2.694223000  |
|  | 1  | 5.630789000  | 1.639013000  | 3.279928000  |
|  | 1  | 5.608422000  | 5.065516000  | -6.291319000 |
|  | 1  | 5.415015000  | 6.170827000  | -4.941928000 |
|  | 1  | 5.118025000  | 6.727852000  | -6.574752000 |
|  | 1  | -2.139681000 | -8.447305000 | 6.411269000  |
|  | 1  | -2.819939000 | -7.165238000 | 7.399764000  |
|  | 1  | -1.137928000 | -7.093100000 | 6.907099000  |
|  | 1  | -0.162754000 | -3.581903000 | -4.433986000 |
|  | 1  | -1.170020000 | -3.697689000 | -3.005576000 |
|  | 1  | 0.335204000  | -4.596265000 | -3.089708000 |
| Py-PO-iPr*Pb(NO <sub>3</sub> ) <sub>2</sub><br>(classical structure) | 6  | -1.483648000 | -0.638073000 | -0.034160000 |
|  | 6  | -2.355151000 | -1.168972000 | 0.904988000  |
|  | 6  | -1.866289000 | -1.481711000 | 2.160139000  |
|  | 6  | -0.530463000 | -1.249950000 | 2.432991000  |
|  | 6  | 0.271384000  | -0.720993000 | 1.431924000  |
|  | 7  | -0.196918000 | -0.425175000 | 0.223894000  |
|  | 1  | -2.515242000 | -1.897455000 | 2.914112000  |
|  | 1  | -3.390441000 | -1.326187000 | 0.648805000  |
|  | 1  | -0.105527000 | -1.476698000 | 3.397409000  |
|  | 15 | 2.025835000  | -0.382279000 | 1.668416000  |
|  | 15 | -2.022020000 | -0.149527000 | -1.682312000 |
|  | 8  | -3.304376000 | 0.735280000  | -1.516405000 |
|  | 8  | -0.912530000 | 0.487972000  | -2.430581000 |
|  | 8  | 2.618071000  | -1.588317000 | 2.482839000  |
|  | 8  | 2.693893000  | -0.098126000 | 0.380475000  |
|  | 6  | -3.359019000 | 2.166824000  | -1.169392000 |
|  | 6  | -2.780263000 | 2.402685000  | 0.198587000  |
|  | 6  | -2.734255000 | 3.007544000  | -2.249855000 |
|  | 1  | -4.433057000 | 2.335062000  | -1.149398000 |
|  | 1  | -1.707735000 | 2.221028000  | 0.222552000  |
|  | 1  | -3.267230000 | 1.778004000  | 0.944045000  |
|  | 1  | -1.661222000 | 2.860781000  | -2.311486000 |
|  | 1  | -3.170731000 | 2.780977000  | -3.219108000 |
|  | 8  | -2.597135000 | -1.480313000 | -2.246702000 |
|  | 6  | -2.799913000 | -1.789748000 | -3.671752000 |
|  | 6  | -3.405602000 | -0.622832000 | -4.406554000 |
|  | 6  | -1.500441000 | -2.267359000 | -4.255424000 |
|  | 1  | -3.515510000 | -2.606445000 | -3.622488000 |
|  | 1  | -2.703965000 | 0.206649000  | -4.467629000 |
|  | 1  | -4.318184000 | -0.280077000 | -3.928550000 |
|  | 1  | -0.774204000 | -1.460302000 | -4.302448000 |
|  | 1  | -1.082386000 | -3.078306000 | -3.667740000 |
|  | 6  | 4.404836000  | -2.618855000 | 1.180205000  |
|  | 6  | 2.052172000  | -3.511763000 | 1.061926000  |
|  | 6  | 3.106250000  | -2.848986000 | 1.907069000  |
|  | 1  | 4.247711000  | -2.041851000 | 0.274916000  |
|  | 1  | 5.115715000  | -2.093649000 | 1.812568000  |
|  | 1  | 1.136154000  | -3.670627000 | 1.625949000  |
|  | 1  | 1.819964000  | -2.941285000 | 0.163908000  |

|  |    |              |              |              |
|--|----|--------------|--------------|--------------|
|  | 1  | 3.286553000  | -3.438664000 | 2.802816000  |
|  | 1  | -1.669360000 | -2.631430000 | -5.266228000 |
|  | 1  | -3.644131000 | -0.931885000 | -5.421136000 |
|  | 1  | -2.918414000 | 4.056061000  | -2.029422000 |
|  | 1  | -2.930730000 | 3.442680000  | 0.476202000  |
|  | 1  | 4.837413000  | -3.578715000 | 0.908631000  |
|  | 1  | 2.414865000  | -4.484640000 | 0.739176000  |
|  | 82 | 1.415763000  | 0.510718000  | -1.756596000 |
|  | 7  | 0.523533000  | 3.296740000  | -0.818390000 |
|  | 8  | 0.549995000  | 2.210911000  | -0.132913000 |
|  | 8  | 0.135824000  | 4.326008000  | -0.299737000 |
|  | 8  | 0.888394000  | 3.233727000  | -2.010620000 |
|  | 7  | 1.418853000  | -2.342590000 | -2.871962000 |
|  | 8  | 1.814981000  | -1.470283000 | -3.672259000 |
|  | 8  | 1.460348000  | -3.531098000 | -3.115452000 |
|  | 8  | 0.939275000  | -1.938349000 | -1.748377000 |
|  | 8  | 1.980602000  | 0.757804000  | 2.730696000  |
|  | 6  | 3.047534000  | 1.735131000  | 2.982002000  |
|  | 6  | 4.388870000  | 1.057445000  | 3.087873000  |
|  | 6  | 2.993887000  | 2.816519000  | 1.937777000  |
|  | 1  | 2.760279000  | 2.137013000  | 3.950264000  |
|  | 1  | 4.689181000  | 0.640371000  | 2.128710000  |
|  | 1  | 4.376518000  | 0.263353000  | 3.828584000  |
|  | 1  | 3.297088000  | 2.429172000  | 0.968945000  |
|  | 1  | 1.991329000  | 3.220241000  | 1.841641000  |
|  | 1  | 3.671762000  | 3.619823000  | 2.217602000  |
|  | 1  | 5.136530000  | 1.789850000  | 3.381829000  |
| Py-PO-iPr*Pb(NO <sub>3</sub> ) <sub>2</sub><br>(non-classical structure) | 6  | -1.513069000 | 0.172156000  | 0.310691000  |
|  | 6  | -2.440702000 | -0.671234000 | 0.907064000  |
|  | 6  | -1.994365000 | -1.616975000 | 1.814062000  |
|  | 6  | -0.643669000 | -1.684155000 | 2.098907000  |
|  | 6  | 0.209343000  | -0.784611000 | 1.472920000  |
|  | 7  | -0.212908000 | 0.123217000  | 0.598763000  |
|  | 1  | -2.690068000 | -2.288482000 | 2.291427000  |
|  | 1  | -3.486998000 | -0.577713000 | 0.666149000  |
|  | 1  | -0.249493000 | -2.407092000 | 2.794833000  |
|  | 15 | 1.981837000  | -0.743509000 | 1.794058000  |
|  | 15 | -1.947785000 | 1.422909000  | -0.916428000 |
|  | 8  | -2.136500000 | 0.746488000  | -2.319191000 |
|  | 8  | 2.003428000  | -0.469881000 | 3.339478000  |
|  | 8  | -3.395362000 | 1.806870000  | -0.411179000 |
|  | 8  | -0.960719000 | 2.504071000  | -0.999843000 |
|  | 8  | 2.521684000  | -2.212420000 | 1.714675000  |
|  | 8  | 2.662622000  | 0.253660000  | 0.947780000  |
|  | 6  | -4.116516000 | 2.872832000  | -1.105877000 |
|  | 6  | -5.553337000 | 2.437302000  | -1.177162000 |
|  | 6  | -3.902216000 | 4.155058000  | -0.349543000 |
|  | 1  | -3.700168000 | 2.956675000  | -2.111045000 |
|  | 1  | -5.950039000 | 2.286184000  | -0.175642000 |
|  | 1  | -5.655104000 | 1.509061000  | -1.733567000 |
|  | 1  | -4.284920000 | 4.061576000  | 0.664490000  |
|  | 1  | -2.845645000 | 4.398442000  | -0.304697000 |

|   |    |              |              |              |
|---|----|--------------|--------------|--------------|
|   | 6  | -2.317648000 | -1.636535000 | -2.629070000 |
|   | 6  | -3.069843000 | -0.332179000 | -2.605692000 |
|   | 6  | -3.695982000 | 0.007951000  | -3.930944000 |
|   | 1  | -3.002279000 | -2.448638000 | -2.865555000 |
|   | 1  | -1.852678000 | -1.849349000 | -1.670352000 |
|   | 1  | -3.830908000 | -0.334873000 | -1.821068000 |
|   | 1  | -4.216500000 | 0.961381000  | -3.885974000 |
|   | 1  | -4.407722000 | -0.761024000 | -4.220190000 |
|   | 6  | 4.457655000  | -2.366846000 | 0.245857000  |
|   | 6  | 2.130022000  | -2.717315000 | -0.655547000 |
|   | 6  | 3.066342000  | -2.870182000 | 0.510884000  |
|   | 1  | 4.447517000  | -1.335546000 | -0.088348000 |
|   | 1  | 5.077437000  | -2.456556000 | 1.134550000  |
|   | 1  | 1.129579000  | -3.068363000 | -0.410813000 |
|   | 1  | 2.079485000  | -1.688606000 | -1.001315000 |
|   | 1  | 3.096964000  | -3.908349000 | 0.833481000  |
|   | 6  | 3.200840000  | -0.929590000 | 5.339234000  |
|   | 6  | 3.540793000  | 1.227608000  | 4.078108000  |
|   | 6  | 3.294488000  | -0.254009000 | 4.000848000  |
|   | 1  | 2.396450000  | -0.491412000 | 5.925701000  |
|   | 1  | 3.010371000  | -1.992754000 | 5.228159000  |
|   | 1  | 3.568832000  | 1.665457000  | 3.085584000  |
|   | 1  | 2.754545000  | 1.708827000  | 4.655690000  |
|   | 1  | 4.062361000  | -0.733174000 | 3.392094000  |
|   | 82 | 1.762112000  | 1.746958000  | -0.971876000 |
|   | 7  | 4.514122000  | 0.967908000  | -1.558412000 |
|   | 8  | 5.605031000  | 0.454559000  | -1.650634000 |
|   | 8  | 4.347564000  | 2.152494000  | -1.176718000 |
|   | 8  | 3.457108000  | 0.296653000  | -1.844788000 |
|   | 7  | 0.668186000  | 0.428052000  | -3.303584000 |
|   | 8  | 0.213632000  | -0.173283000 | -4.248680000 |
|   | 8  | 1.168629000  | 1.575992000  | -3.410595000 |
|   | 8  | 0.648552000  | -0.085544000 | -2.129584000 |
|   | 1  | -6.152524000 | 3.197732000  | -1.670867000 |
|   | 1  | -4.426434000 | 4.971205000  | -0.840626000 |
|   | 1  | -2.923315000 | 0.070816000  | -4.692793000 |
|   | 1  | -1.533177000 | -1.597530000 | -3.378476000 |
|   | 1  | 4.910466000  | -2.962912000 | -0.542698000 |
|   | 1  | 2.497138000  | -3.310825000 | -1.488959000 |
|   | 1  | 4.130912000  | -0.801001000 | 5.886553000  |
|   | 1  | 4.492549000  | 1.422372000  | 4.566292000  |
| Py-PO-iPr*Cd(NO <sub>3</sub> ) <sub>2</sub> | 6  | -1.511001000 | -0.547706000 | 0.316577000  |
|   | 6  | -2.387464000 | -1.039510000 | 1.272266000  |
|   | 6  | -1.883106000 | -1.391515000 | 2.512485000  |
|   | 6  | -0.527850000 | -1.248623000 | 2.754605000  |
|   | 6  | 0.282170000  | -0.758999000 | 1.739539000  |
|   | 7  | -0.209341000 | -0.412350000 | 0.552667000  |
|   | 1  | -2.537331000 | -1.772767000 | 3.280256000  |
|   | 1  | -3.436601000 | -1.135207000 | 1.044118000  |
|   | 1  | -0.096052000 | -1.513238000 | 3.706750000  |
|   | 15 | 2.075511000  | -0.560620000 | 1.915612000  |
|   | 15 | -2.014049000 | -0.030443000 | -1.340042000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 8  | 2.282957000  | 0.326709000  | 3.185816000  |
| 8  | -3.373526000 | 0.739345000  | -1.179903000 |
| 8  | -0.932959000 | 0.721018000  | -2.010111000 |
| 8  | 2.636450000  | -1.905283000 | 2.472132000  |
| 8  | 2.634420000  | -0.060264000 | 0.644454000  |
| 6  | -3.510809000 | 2.181078000  | -0.933855000 |
| 6  | -2.722622000 | 2.607076000  | 0.275549000  |
| 6  | -3.167412000 | 2.951102000  | -2.181250000 |
| 1  | -4.575645000 | 2.265080000  | -0.730074000 |
| 1  | -1.649716000 | 2.529438000  | 0.110717000  |
| 1  | -2.996119000 | 2.022003000  | 1.150867000  |
| 1  | -2.107875000 | 2.878686000  | -2.404980000 |
| 1  | -3.732980000 | 2.579869000  | -3.031540000 |
| 6  | 3.054300000  | 2.557238000  | 2.639084000  |
| 6  | 1.446493000  | 2.098245000  | 4.524023000  |
| 6  | 1.889177000  | 1.747255000  | 3.132790000  |
| 1  | 3.891966000  | 2.478430000  | 3.329004000  |
| 1  | 3.375137000  | 2.219026000  | 1.658675000  |
| 1  | 0.612871000  | 1.477663000  | 4.842568000  |
| 1  | 2.265402000  | 1.964325000  | 5.227042000  |
| 1  | 1.059167000  | 1.840329000  | 2.432920000  |
| 8  | -2.451743000 | -1.389623000 | -1.963034000 |
| 6  | -2.578692000 | -1.664674000 | -3.404523000 |
| 6  | -3.373085000 | -0.586361000 | -4.092580000 |
| 6  | -1.215110000 | -1.882182000 | -3.998728000 |
| 1  | -3.140745000 | -2.594853000 | -3.401493000 |
| 1  | -2.819391000 | 0.350356000  | -4.113964000 |
| 1  | -4.329329000 | -0.420253000 | -3.605632000 |
| 1  | -0.652206000 | -0.952679000 | -4.027547000 |
| 1  | -0.647853000 | -2.613348000 | -3.432668000 |
| 6  | 4.138416000  | -2.809639000 | 0.763897000  |
| 6  | 1.761511000  | -3.615125000 | 0.950729000  |
| 6  | 2.973842000  | -3.093428000 | 1.674216000  |
| 1  | 3.856220000  | -2.127973000 | -0.031610000 |
| 1  | 4.968867000  | -2.380677000 | 1.316664000  |
| 1  | 0.927189000  | -3.764023000 | 1.632101000  |
| 1  | 1.461701000  | -2.952833000 | 0.141114000  |
| 1  | 3.272169000  | -3.791039000 | 2.452434000  |
| 1  | -1.321467000 | -2.244795000 | -5.018485000 |
| 1  | -3.557217000 | -0.885050000 | -5.121483000 |
| 1  | -3.420457000 | 3.998867000  | -2.038277000 |
| 1  | -2.939452000 | 3.650075000  | 0.493216000  |
| 1  | 1.131878000  | 3.137704000  | 4.556750000  |
| 1  | 2.762510000  | 3.600631000  | 2.554145000  |
| 1  | 4.470829000  | -3.742558000 | 0.315137000  |
| 1  | 2.002440000  | -4.575257000 | 0.500894000  |
| 48 | 1.271469000  | 0.590394000  | -1.153397000 |
| 7  | 1.512357000  | 3.217572000  | -0.341312000 |
| 8  | 0.654336000  | 2.465882000  | 0.222236000  |
| 8  | 1.684105000  | 4.361935000  | 0.009498000  |
| 8  | 2.181803000  | 2.699528000  | -1.287246000 |
| 7  | 1.828971000  | -1.473249000 | -2.884249000 |

|   |    |              |              |              |
|---|----|--------------|--------------|--------------|
|   | 8  | 2.132506000  | -0.256557000 | -3.100162000 |
|   | 8  | 2.068488000  | -2.339080000 | -3.693349000 |
|   | 8  | 1.251577000  | -1.725085000 | -1.782053000 |
| Py-PO-iPr*Cu(NO <sub>3</sub> ) <sub>2</sub> | 6  | -1.452014000 | -0.415724000 | 0.269342000  |
|   | 6  | -2.347101000 | -0.794437000 | 1.257405000  |
|   | 6  | -1.861743000 | -1.099490000 | 2.516400000  |
|   | 6  | -0.498687000 | -1.029643000 | 2.740785000  |
|   | 6  | 0.334610000  | -0.650026000 | 1.699653000  |
|   | 7  | -0.140429000 | -0.339496000 | 0.493223000  |
|   | 1  | -2.534064000 | -1.389821000 | 3.307868000  |
|   | 1  | -3.400378000 | -0.840641000 | 1.033688000  |
|   | 1  | -0.073768000 | -1.267565000 | 3.703000000  |
|   | 15 | 2.136625000  | -0.569313000 | 1.869411000  |
|   | 15 | -1.949257000 | 0.009033000  | -1.414848000 |
|   | 8  | 2.416658000  | 0.271926000  | 3.157949000  |
|   | 8  | -3.344449000 | 0.723721000  | -1.316414000 |
|   | 8  | -0.871506000 | 0.741045000  | -2.098617000 |
|   | 8  | 2.602701000  | -1.958577000 | 2.419985000  |
|   | 8  | 2.700329000  | -0.106835000 | 0.591063000  |
|   | 6  | -3.587285000 | 2.160530000  | -1.135872000 |
|   | 6  | -3.109941000 | 2.607869000  | 0.218097000  |
|   | 6  | -3.005213000 | 2.959122000  | -2.272220000 |
|   | 1  | -4.673356000 | 2.199656000  | -1.178805000 |
|   | 1  | -2.026025000 | 2.560828000  | 0.297805000  |
|   | 1  | -3.550961000 | 2.006873000  | 1.009951000  |
|   | 1  | -1.920894000 | 2.962016000  | -2.240638000 |
|   | 1  | -3.321561000 | 2.559348000  | -3.231869000 |
|   | 6  | 3.119362000  | 2.515494000  | 2.541833000  |
|   | 6  | 1.896550000  | 2.002659000  | 4.682396000  |
|   | 6  | 2.055835000  | 1.696949000  | 3.220602000  |
|   | 1  | 4.073323000  | 2.397439000  | 3.051992000  |
|   | 1  | 3.240980000  | 2.221630000  | 1.504044000  |
|   | 1  | 1.127549000  | 1.380642000  | 5.132700000  |
|   | 1  | 2.831927000  | 1.831862000  | 5.210444000  |
|   | 1  | 1.107971000  | 1.822156000  | 2.700397000  |
|   | 8  | -2.334114000 | -1.406404000 | -1.960459000 |
|   | 6  | -2.479380000 | -1.750475000 | -3.379371000 |
|   | 6  | -3.375067000 | -0.768417000 | -4.088692000 |
|   | 6  | -1.122327000 | -1.886488000 | -4.015509000 |
|   | 1  | -2.966754000 | -2.720774000 | -3.325566000 |
|   | 1  | -2.895544000 | 0.205258000  | -4.169865000 |
|   | 1  | -4.323655000 | -0.649745000 | -3.574357000 |
|   | 1  | -0.630532000 | -0.919572000 | -4.079612000 |
|   | 1  | -0.487039000 | -2.561302000 | -3.451406000 |
|   | 6  | 4.070939000  | -2.927149000 | 0.720652000  |
|   | 6  | 1.648152000  | -3.593621000 | 0.871512000  |
|   | 6  | 2.880409000  | -3.149796000 | 1.615264000  |
|   | 1  | 3.839308000  | -2.222976000 | -0.071722000 |
|   | 1  | 4.916119000  | -2.547957000 | 1.287310000  |
|   | 1  | 0.799841000  | -3.705087000 | 1.542705000  |
|   | 1  | 1.394672000  | -2.897341000 | 0.075798000  |
|   | 1  | 3.128664000  | -3.876210000 | 2.385066000  |

|   |    |              |              |              |
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|   | 1  | -1.235572000 | -2.280644000 | -5.022882000 |
|   | 1  | -3.569578000 | -1.127280000 | -5.096294000 |
|   | 1  | -3.358826000 | 3.984834000  | -2.199333000 |
|   | 1  | -3.405076000 | 3.642022000  | 0.379199000  |
|   | 1  | 1.613886000  | 3.043917000  | 4.810467000  |
|   | 1  | 2.838035000  | 3.565236000  | 2.565369000  |
|   | 1  | 4.358267000  | -3.874251000 | 0.270012000  |
|   | 1  | 1.838935000  | -4.557814000 | 0.406503000  |
|   | 29 | 1.186527000  | 0.384791000  | -1.048132000 |
|   | 7  | 0.938377000  | 2.982621000  | -0.032614000 |
|   | 8  | 0.159078000  | 2.422234000  | 0.749973000  |
|   | 8  | 1.184576000  | 4.168738000  | -0.004773000 |
|   | 8  | 1.528633000  | 2.262106000  | -0.927251000 |
|   | 7  | 1.991793000  | -1.124080000 | -2.781163000 |
|   | 8  | 2.265092000  | 0.106226000  | -2.801021000 |
|   | 8  | 2.345086000  | -1.906352000 | -3.618543000 |
|   | 8  | 1.281285000  | -1.483485000 | -1.772014000 |
| Py-PO-iPr*Zn(NO <sub>3</sub> ) <sub>2</sub> | 6  | -1.608168000 | -0.671579000 | 0.045664000  |
|   | 6  | -2.473850000 | -1.192827000 | 0.993298000  |
|   | 6  | -1.979235000 | -1.479064000 | 2.254367000  |
|   | 6  | -0.644436000 | -1.234337000 | 2.530511000  |
|   | 6  | 0.154025000  | -0.714983000 | 1.524709000  |
|   | 7  | -0.326314000 | -0.446829000 | 0.314894000  |
|   | 1  | -2.625891000 | -1.887564000 | 3.014255000  |
|   | 1  | -3.508030000 | -1.364933000 | 0.742987000  |
|   | 1  | -0.223707000 | -1.444731000 | 3.500330000  |
|   | 15 | 1.915434000  | -0.349799000 | 1.650973000  |
|   | 15 | -2.052203000 | -0.187425000 | -1.633919000 |
|   | 8  | -3.351767000 | 0.684743000  | -1.555204000 |
|   | 8  | -0.880775000 | 0.459202000  | -2.264653000 |
|   | 8  | 2.610823000  | -1.538303000 | 2.399167000  |
|   | 8  | 2.429833000  | -0.055569000 | 0.294840000  |
|   | 6  | -3.446413000 | 2.116555000  | -1.237453000 |
|   | 6  | -3.004267000 | 2.374465000  | 0.177469000  |
|   | 6  | -2.717444000 | 2.950565000  | -2.256885000 |
|   | 1  | -4.517601000 | 2.281003000  | -1.326513000 |
|   | 1  | -1.929224000 | 2.250265000  | 0.286384000  |
|   | 1  | -3.523317000 | 1.722876000  | 0.876584000  |
|   | 1  | -1.642847000 | 2.822284000  | -2.183999000 |
|   | 1  | -3.030731000 | 2.695537000  | -3.265569000 |
|   | 8  | -2.575659000 | -1.517723000 | -2.246929000 |
|   | 6  | -2.655644000 | -1.813878000 | -3.687974000 |
|   | 6  | -3.295556000 | -0.674910000 | -4.437473000 |
|   | 6  | -1.293128000 | -2.185234000 | -4.202599000 |
|   | 1  | -3.313076000 | -2.679254000 | -3.697783000 |
|   | 1  | -2.649923000 | 0.201336000  | -4.436607000 |
|   | 1  | -4.257681000 | -0.406457000 | -4.011959000 |
|   | 1  | -0.633070000 | -1.321510000 | -4.212040000 |
|   | 1  | -0.838564000 | -2.959811000 | -3.594559000 |
|   | 6  | 4.246474000  | -2.526863000 | 0.872067000  |
|   | 6  | 1.951393000  | -3.531008000 | 1.137238000  |
|   | 6  | 3.085420000  | -2.791765000 | 1.792927000  |



|   |    |              |              |              |
|---|----|--------------|--------------|--------------|
|   | 1  | 3.929565000  | -2.003123000 | -0.023805000 |
|   | 1  | 5.009976000  | -1.935734000 | 1.370545000  |
|   | 1  | 1.124807000  | -3.678978000 | 1.828313000  |
|   | 1  | 1.589974000  | -3.012145000 | 0.251496000  |
|   | 1  | 3.427158000  | -3.335153000 | 2.670465000  |
|   | 1  | -1.384732000 | -2.553117000 | -5.222082000 |
|   | 1  | -3.446954000 | -0.973032000 | -5.471864000 |
|   | 1  | -2.950495000 | 3.998538000  | -2.084633000 |
|   | 1  | -3.235879000 | 3.403255000  | 0.442649000  |
|   | 1  | 4.690552000  | -3.475341000 | 0.579747000  |
|   | 1  | 2.299325000  | -4.510155000 | 0.817340000  |
|   | 30 | 0.998559000  | 0.319338000  | -1.252614000 |
|   | 7  | 1.023583000  | 2.914057000  | -0.769831000 |
|   | 8  | 0.312772000  | 2.297812000  | 0.060485000  |
|   | 8  | 1.178208000  | 4.113946000  | -0.742878000 |
|   | 8  | 1.603018000  | 2.202852000  | -1.666390000 |
|   | 7  | 1.532645000  | -1.933986000 | -2.571331000 |
|   | 8  | 1.940734000  | -0.720866000 | -2.686960000 |
|   | 8  | 1.925613000  | -2.782325000 | -3.340238000 |
|   | 8  | 0.721685000  | -2.171665000 | -1.647552000 |
|   | 8  | 1.946171000  | 0.789791000  | 2.709877000  |
|   | 6  | 3.048545000  | 1.748466000  | 2.898483000  |
|   | 6  | 4.379789000  | 1.044930000  | 2.926748000  |
|   | 6  | 2.960464000  | 2.827431000  | 1.855288000  |
|   | 1  | 2.821645000  | 2.153975000  | 3.880950000  |
|   | 1  | 4.624920000  | 0.639557000  | 1.946705000  |
|   | 1  | 4.392768000  | 0.240368000  | 3.655695000  |
|   | 1  | 3.203778000  | 2.435294000  | 0.871005000  |
|   | 1  | 1.966693000  | 3.260260000  | 1.818788000  |
|   | 1  | 3.672156000  | 3.614466000  | 2.093969000  |
|   | 1  | 5.153346000  | 1.761668000  | 3.190471000  |
| Py-PO-cHex*Pb(NO <sub>3</sub> ) <sub>2</sub><br>(classical structure) | 6  | -1.096147000 | -0.740868000 | 0.904824000  |
|   | 6  | -1.706177000 | -1.715732000 | 1.679395000  |
|   | 6  | -0.913502000 | -2.674015000 | 2.284592000  |
|   | 6  | 0.454404000  | -2.620503000 | 2.095997000  |
|   | 6  | 0.983622000  | -1.610755000 | 1.303614000  |
|   | 7  | 0.220379000  | -0.693918000 | 0.712562000  |
|   | 1  | -1.354280000 | -3.444801000 | 2.896344000  |
|   | 1  | -2.777174000 | -1.711205000 | 1.801439000  |
|   | 1  | 1.113402000  | -3.340865000 | 2.553950000  |
|   | 15 | 2.762736000  | -1.458033000 | 1.024902000  |
|   | 15 | -2.042716000 | 0.553555000  | 0.087111000  |
|   | 8  | -1.156396000 | 1.409733000  | -0.737238000 |
|   | 8  | 3.248643000  | -2.818530000 | 0.431183000  |
|   | 8  | 3.026863000  | -0.228491000 | 0.252166000  |
|   | 6  | 3.780859000  | -2.470079000 | -1.949767000 |
|   | 6  | 3.674547000  | -3.137405000 | -3.314523000 |
|   | 6  | 2.222943000  | -3.364347000 | -3.703426000 |
|   | 6  | 1.498203000  | -4.172095000 | -2.640472000 |
|   | 6  | 1.607888000  | -3.506497000 | -1.275439000 |
|   | 6  | 3.065053000  | -3.319623000 | -0.929354000 |
|   | 1  | 3.317975000  | -1.485289000 | -1.985415000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 1  | 4.820445000  | -2.338886000 | -1.653123000 |
| 1  | 4.201613000  | -4.096204000 | -3.290934000 |
| 1  | 4.178076000  | -2.525446000 | -4.060197000 |
| 1  | 2.166905000  | -3.875754000 | -4.663791000 |
| 1  | 1.728278000  | -2.400973000 | -3.827331000 |
| 1  | 1.926733000  | -5.177423000 | -2.584404000 |
| 1  | 0.448476000  | -4.300819000 | -2.901455000 |
| 1  | 1.116009000  | -4.105899000 | -0.508278000 |
| 1  | 1.119203000  | -2.531434000 | -1.314213000 |
| 1  | 3.546231000  | -4.296446000 | -0.873227000 |
| 82 | 1.274363000  | 1.500188000  | -0.518663000 |
| 7  | 0.669897000  | 3.035844000  | 2.078620000  |
| 8  | 0.542564000  | 3.502386000  | 3.195038000  |
| 8  | 0.576320000  | 1.767991000  | 1.902660000  |
| 8  | 0.884782000  | 3.743937000  | 1.073045000  |
| 7  | 0.942139000  | 0.421080000  | -3.325366000 |
| 8  | 0.911796000  | -0.121401000 | -4.414609000 |
| 8  | 0.865826000  | 1.658930000  | -3.188489000 |
| 8  | 1.051595000  | -0.290308000 | -2.262276000 |
| 8  | 3.445369000  | -1.601066000 | 2.422518000  |
| 6  | 2.251775000  | -0.237723000 | 4.086792000  |
| 6  | 2.471092000  | 0.708645000  | 5.260077000  |
| 6  | 3.236612000  | 1.948127000  | 4.830709000  |
| 6  | 4.549143000  | 1.575005000  | 4.164093000  |
| 6  | 4.313712000  | 0.642754000  | 2.984611000  |
| 6  | 3.581281000  | -0.585782000 | 3.465643000  |
| 1  | 1.619364000  | 0.257285000  | 3.347012000  |
| 1  | 1.743139000  | -1.146381000 | 4.410847000  |
| 1  | 3.029110000  | 0.187463000  | 6.043826000  |
| 1  | 1.510212000  | 0.983552000  | 5.689840000  |
| 1  | 3.416482000  | 2.593619000  | 5.689151000  |
| 1  | 2.619334000  | 2.520788000  | 4.137312000  |
| 1  | 5.202342000  | 1.082495000  | 4.890373000  |
| 1  | 5.077489000  | 2.464952000  | 3.827568000  |
| 1  | 5.249603000  | 0.356038000  | 2.507667000  |
| 1  | 3.709901000  | 1.150660000  | 2.233197000  |
| 1  | 4.199984000  | -1.103824000 | 4.198852000  |
| 8  | -3.211383000 | -0.148449000 | -0.685722000 |
| 6  | -2.055508000 | -1.713030000 | -2.213079000 |
| 6  | -2.188760000 | -2.363887000 | -3.584623000 |
| 6  | -2.222963000 | -1.326378000 | -4.695030000 |
| 6  | -3.306494000 | -0.290039000 | -4.452645000 |
| 6  | -3.149224000 | 0.357206000  | -3.084148000 |
| 6  | -3.175957000 | -0.720482000 | -2.028469000 |
| 1  | -1.095099000 | -1.195713000 | -2.148569000 |
| 1  | -2.084247000 | -2.465132000 | -1.422866000 |
| 1  | -3.107275000 | -2.957803000 | -3.609256000 |
| 1  | -1.364800000 | -3.057811000 | -3.741044000 |
| 1  | -2.378584000 | -1.816128000 | -5.655501000 |
| 1  | -1.253959000 | -0.831439000 | -4.750754000 |
| 1  | -4.290248000 | -0.765358000 | -4.511575000 |
| 1  | -3.285090000 | 0.473913000  | -5.227099000 |

|  |    |              |              |              |
|--|----|--------------|--------------|--------------|
|  | 1  | -3.945648000 | 1.076096000  | -2.894132000 |
|  | 1  | -2.201405000 | 0.893951000  | -3.024584000 |
|  | 1  | -4.131534000 | -1.244113000 | -2.076453000 |
|  | 8  | -2.786234000 | 1.206031000  | 1.287107000  |
|  | 6  | -4.169730000 | 2.796529000  | -0.021590000 |
|  | 6  | -4.862241000 | 4.149621000  | 0.068898000  |
|  | 6  | -3.874163000 | 5.251714000  | 0.411042000  |
|  | 6  | -3.139026000 | 4.935259000  | 1.701523000  |
|  | 6  | -2.449692000 | 3.582795000  | 1.618986000  |
|  | 6  | -3.452171000 | 2.512494000  | 1.276720000  |
|  | 1  | -3.439334000 | 2.820166000  | -0.834052000 |
|  | 1  | -4.880975000 | 2.003133000  | -0.244311000 |
|  | 1  | -5.636296000 | 4.107125000  | 0.839960000  |
|  | 1  | -5.372945000 | 4.361712000  | -0.868741000 |
|  | 1  | -4.388377000 | 6.208490000  | 0.488447000  |
|  | 1  | -3.150135000 | 5.349820000  | -0.401431000 |
|  | 1  | -3.853634000 | 4.929779000  | 2.529614000  |
|  | 1  | -2.404020000 | 5.702755000  | 1.932260000  |
|  | 1  | -1.953123000 | 3.337528000  | 2.554759000  |
|  | 1  | -1.686315000 | 3.608398000  | 0.840064000  |
|  | 1  | -4.181739000 | 2.415040000  | 2.080755000  |
| Py-PO-cHex *Pb(NO <sub>3</sub> ) <sub>2</sub><br>(non-classical structure) | 6  | -1.160616000 | -0.362708000 | -0.228925000 |
|  | 6  | -1.730152000 | -1.619395000 | -0.357583000 |
|  | 6  | -1.004838000 | -2.720238000 | 0.065302000  |
|  | 6  | 0.268907000  | -2.530678000 | 0.565338000  |
|  | 6  | 0.770607000  | -1.236759000 | 0.627453000  |
|  | 7  | 0.062995000  | -0.171276000 | 0.262835000  |
|  | 1  | -1.416135000 | -3.713067000 | -0.022826000 |
|  | 1  | -2.706307000 | -1.727172000 | -0.799636000 |
|  | 1  | 0.884953000  | -3.361179000 | 0.869297000  |
|  | 15 | 2.469533000  | -0.869394000 | 1.118125000  |
|  | 15 | -1.898881000 | 1.170318000  | -0.826050000 |
|  | 8  | -0.926034000 | 1.993662000  | -1.559502000 |
|  | 8  | 3.327526000  | -2.129862000 | 0.799434000  |
|  | 8  | 2.889919000  | 0.408121000  | 0.501764000  |
|  | 6  | 3.139067000  | -2.989464000 | -1.480392000 |
|  | 6  | 3.877084000  | -3.142818000 | -2.802756000 |
|  | 6  | 5.219886000  | -3.824799000 | -2.607322000 |
|  | 6  | 6.062958000  | -3.075067000 | -1.589836000 |
|  | 6  | 5.322679000  | -2.932479000 | -0.267135000 |
|  | 6  | 4.010174000  | -2.239710000 | -0.506760000 |
|  | 1  | 2.906832000  | -3.972357000 | -1.058596000 |
|  | 1  | 2.201816000  | -2.460323000 | -1.642100000 |
|  | 1  | 4.030210000  | -2.150350000 | -3.228002000 |
|  | 1  | 3.257643000  | -3.693440000 | -3.508134000 |
|  | 1  | 5.749176000  | -3.898132000 | -3.555828000 |
|  | 1  | 5.060618000  | -4.849271000 | -2.257763000 |
|  | 1  | 6.293422000  | -2.081128000 | -1.978719000 |
|  | 1  | 7.014792000  | -3.577343000 | -1.426512000 |
|  | 1  | 5.911213000  | -2.370870000 | 0.456090000  |
|  | 1  | 5.127612000  | -3.917384000 | 0.164263000  |
|  | 1  | 4.178696000  | -1.228400000 | -0.868358000 |

|   |              |              |              |
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| 8 | 2.494569000  | -0.907219000 | 2.689628000  |
| 6 | 2.877311000  | 1.169371000  | 3.858590000  |
| 6 | 2.229550000  | 2.260519000  | 4.696415000  |
| 6 | 1.478550000  | 1.665120000  | 5.874388000  |
| 6 | 0.440841000  | 0.662965000  | 5.399232000  |
| 6 | 1.077202000  | -0.429755000 | 4.553702000  |
| 6 | 1.836846000  | 0.177349000  | 3.402496000  |
| 1 | 3.619079000  | 0.634132000  | 4.455131000  |
| 1 | 3.392663000  | 1.578599000  | 2.992548000  |
| 1 | 1.532468000  | 2.828045000  | 4.073853000  |
| 1 | 2.984793000  | 2.967478000  | 5.033121000  |
| 1 | 1.007250000  | 2.448585000  | 6.465365000  |
| 1 | 2.188815000  | 1.160088000  | 6.533739000  |
| 1 | -0.308044000 | 1.186555000  | 4.799984000  |
| 1 | -0.090329000 | 0.222571000  | 6.241276000  |
| 1 | 0.327832000  | -1.125249000 | 4.175307000  |
| 1 | 1.777341000  | -1.011113000 | 5.156809000  |
| 1 | 1.134916000  | 0.673790000  | 2.723523000  |
| 8 | -3.136815000 | 0.641264000  | -1.631249000 |
| 6 | -2.609728000 | 0.763632000  | -4.015928000 |
| 6 | -3.137959000 | 1.218109000  | -5.366512000 |
| 6 | -3.422361000 | 2.709964000  | -5.362274000 |
| 6 | -4.393108000 | 3.072626000  | -4.250853000 |
| 6 | -3.868432000 | 2.620499000  | -2.895389000 |
| 6 | -3.588198000 | 1.138062000  | -2.930899000 |
| 1 | -1.656712000 | 1.252149000  | -3.814949000 |
| 1 | -2.431548000 | -0.309908000 | -4.003982000 |
| 1 | -4.059749000 | 0.677854000  | -5.602014000 |
| 1 | -2.420425000 | 0.959177000  | -6.141305000 |
| 1 | -3.817607000 | 3.025182000  | -6.326589000 |
| 1 | -2.486447000 | 3.252754000  | -5.213171000 |
| 1 | -5.356332000 | 2.592397000  | -4.445143000 |
| 1 | -4.582058000 | 4.144270000  | -4.233049000 |
| 1 | -4.581576000 | 2.847490000  | -2.102676000 |
| 1 | -2.941430000 | 3.146932000  | -2.664603000 |
| 1 | -4.523424000 | 0.596584000  | -3.077586000 |
| 8 | -2.429662000 | 1.983502000  | 0.410624000  |
| 6 | -2.406990000 | 1.033727000  | 2.638913000  |
| 6 | -3.264961000 | 0.741637000  | 3.859604000  |
| 6 | -4.395505000 | -0.211368000 | 3.511310000  |
| 6 | -5.233587000 | 0.341615000  | 2.371824000  |
| 6 | -4.378092000 | 0.629579000  | 1.147444000  |
| 6 | -3.263883000 | 1.581007000  | 1.519353000  |
| 1 | -1.922778000 | 0.113865000  | 2.302845000  |
| 1 | -1.616755000 | 1.747527000  | 2.866893000  |
| 1 | -3.688253000 | 1.677342000  | 4.233633000  |
| 1 | -2.650365000 | 0.338548000  | 4.662395000  |
| 1 | -5.016747000 | -0.400362000 | 4.384856000  |
| 1 | -3.972623000 | -1.174881000 | 3.213854000  |
| 1 | -5.717032000 | 1.265881000  | 2.697944000  |
| 1 | -6.033451000 | -0.347323000 | 2.108082000  |
| 1 | -4.973328000 | 1.045253000  | 0.337448000  |

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|  | 1  | -3.947900000 | -0.304205000 | 0.781329000  |
|  | 1  | -3.707781000 | 2.522223000  | 1.846560000  |
|  | 82 | 1.812190000  | 1.578502000  | -1.562970000 |
|  | 7  | 4.466500000  | 1.340407000  | -2.775697000 |
|  | 8  | 5.578236000  | 1.128187000  | -3.192945000 |
|  | 8  | 3.996294000  | 2.497443000  | -2.637523000 |
|  | 8  | 3.700885000  | 0.363554000  | -2.442642000 |
|  | 7  | 0.712804000  | -0.196585000 | -3.575447000 |
|  | 8  | 0.216445000  | -0.951541000 | -4.376997000 |
|  | 8  | 1.053392000  | 0.978652000  | -3.871908000 |
|  | 8  | 0.899849000  | -0.560087000 | -2.362882000 |
| Py-PO- cHex *Cd(NO <sub>3</sub> ) <sub>2</sub> | 6  | -1.287212000 | -0.853176000 | 0.926037000  |
|  | 6  | -1.857340000 | -1.868018000 | 1.679468000  |
|  | 6  | -1.025992000 | -2.823696000 | 2.237867000  |
|  | 6  | 0.339550000  | -2.732786000 | 2.033552000  |
|  | 6  | 0.829958000  | -1.681038000 | 1.273047000  |
|  | 7  | 0.026174000  | -0.770303000 | 0.729307000  |
|  | 1  | -1.437123000 | -3.626916000 | 2.828372000  |
|  | 1  | -2.925679000 | -1.900682000 | 1.819729000  |
|  | 1  | 1.019300000  | -3.454458000 | 2.457848000  |
|  | 15 | 2.595294000  | -1.421541000 | 0.958808000  |
|  | 15 | -2.236795000 | 0.466543000  | 0.135342000  |
|  | 8  | -1.346812000 | 1.355982000  | -0.638021000 |
|  | 8  | 3.151985000  | -2.749336000 | 0.357308000  |
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|  | 6  | 3.711932000  | -2.296614000 | -2.002217000 |
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|  | 6  | 2.239983000  | -3.229572000 | -3.810244000 |
|  | 6  | 1.558573000  | -4.121823000 | -2.787149000 |
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|  | 1  | 3.199167000  | -1.336401000 | -2.009013000 |
|  | 1  | 4.736982000  | -2.113868000 | -1.683733000 |
|  | 1  | 4.256265000  | -3.840607000 | -3.393698000 |
|  | 1  | 4.137545000  | -2.246883000 | -4.105855000 |
|  | 1  | 2.231313000  | -3.705618000 | -4.789905000 |
|  | 1  | 1.681244000  | -2.297888000 | -3.906678000 |
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|  | 1  | 0.527489000  | -4.321376000 | -3.074541000 |
|  | 1  | 1.125094000  | -4.134969000 | -0.660914000 |
|  | 1  | 1.047970000  | -2.543988000 | -1.431407000 |
|  | 1  | 3.571537000  | -4.165272000 | -0.981612000 |
|  | 48 | 0.982626000  | 1.148521000  | -0.497645000 |
|  | 7  | 0.991864000  | 3.139692000  | 1.420790000  |
|  | 8  | 0.953979000  | 4.055096000  | 2.214423000  |
|  | 8  | 0.794793000  | 1.938391000  | 1.778138000  |
|  | 8  | 1.224070000  | 3.336166000  | 0.188483000  |
|  | 7  | 1.277387000  | 0.455674000  | -3.155773000 |
|  | 8  | 1.420318000  | 0.200259000  | -4.332097000 |
|  | 8  | 1.709363000  | 1.533784000  | -2.649331000 |
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| 6 | 4.210425000  | 1.766816000  | 4.031124000  |
| 6 | 4.049552000  | 0.793662000  | 2.871895000  |
| 6 | 3.390145000  | -0.467859000 | 3.373365000  |
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| 1 | 1.587213000  | -1.128061000 | 4.324267000  |
| 1 | 2.781133000  | 0.327431000  | 5.932265000  |
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| 1 | 4.885555000  | 1.335131000  | 4.776264000  |
| 1 | 4.683681000  | 2.680699000  | 3.678073000  |
| 1 | 5.009244000  | 0.553215000  | 2.417229000  |
| 1 | 3.426192000  | 1.242700000  | 2.100581000  |
| 1 | 4.034768000  | -0.941577000 | 4.113875000  |
| 8 | -3.392840000 | -0.209715000 | -0.681500000 |
| 6 | -2.249110000 | -1.932518000 | -2.018312000 |
| 6 | -2.220661000 | -2.589459000 | -3.390990000 |
| 6 | -1.925167000 | -1.571036000 | -4.478098000 |
| 6 | -2.935603000 | -0.437094000 | -4.438896000 |
| 6 | -2.956816000 | 0.226974000  | -3.069135000 |
| 6 | -3.256747000 | -0.808374000 | -2.012031000 |
| 1 | -1.258172000 | -1.527972000 | -1.802977000 |
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| 1 | -1.933009000 | -2.050950000 | -5.455686000 |
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| 6 | -2.741851000 | 4.809206000  | 1.922051000  |
| 6 | -2.257534000 | 3.382027000  | 1.724856000  |
| 6 | -3.431613000 | 2.477821000  | 1.448549000  |
| 1 | -3.564928000 | 2.857823000  | -0.644958000 |
| 1 | -5.049389000 | 2.232760000  | 0.063661000  |
| 1 | -5.402737000 | 4.373845000  | 1.257158000  |
| 1 | -5.243940000 | 4.666337000  | -0.458103000 |
| 1 | -3.900836000 | 6.294408000  | 0.871055000  |
| 1 | -2.874156000 | 5.316470000  | -0.153658000 |
| 1 | -3.371500000 | 4.866526000  | 2.814752000  |
| 1 | -1.885770000 | 5.455217000  | 2.101813000  |
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| 1 | -1.581728000 | 3.348086000  | 0.870254000  |

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|  | 1  | -4.092665000 | 2.453603000  | 2.314699000  |
| Py-PO- cHex *Cu(NO <sub>3</sub> ) <sub>2</sub> | 6  | -1.110819000 | -0.827408000 | 0.712251000  |
|  | 6  | -1.700457000 | -1.932534000 | 1.303825000  |
|  | 6  | -0.888735000 | -2.938938000 | 1.797143000  |
|  | 6  | 0.482872000  | -2.799822000 | 1.697275000  |
|  | 6  | 1.000633000  | -1.659650000 | 1.100536000  |
|  | 7  | 0.213163000  | -0.702102000 | 0.611057000  |
|  | 1  | -1.319170000 | -3.814186000 | 2.257050000  |
|  | 1  | -2.774666000 | -1.993058000 | 1.366994000  |
|  | 1  | 1.153249000  | -3.553848000 | 2.077778000  |
|  | 15 | 2.778166000  | -1.329085000 | 0.984257000  |
|  | 15 | -2.051635000 | 0.567384000  | 0.052369000  |
|  | 8  | -1.184285000 | 1.427246000  | -0.768897000 |
|  | 8  | 3.452775000  | -2.614022000 | 0.409986000  |
|  | 8  | 2.964794000  | -0.050107000 | 0.280912000  |
|  | 6  | 3.828019000  | -2.016429000 | -1.967921000 |
|  | 6  | 3.923875000  | -2.636367000 | -3.355497000 |
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|  | 1  | 3.070520000  | -1.234746000 | -1.963276000 |
|  | 1  | 4.765891000  | -1.545419000 | -1.679209000 |
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|  | 1  | 2.991041000  | -5.173943000 | -2.696885000 |
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|  | 1  | 4.251548000  | -3.839609000 | -0.948226000 |
|  | 29 | 1.054412000  | 1.025526000  | -0.343962000 |
|  | 7  | 1.356022000  | 3.096261000  | 0.906527000  |
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|  | 8  | 1.628065000  | 3.029574000  | -0.320881000 |
|  | 7  | 0.812451000  | -0.220246000 | -2.839315000 |
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|  | 8  | 0.297708000  | -1.124873000 | -2.171446000 |
|  | 8  | 3.337251000  | -1.449164000 | 2.443422000  |
|  | 6  | 1.810899000  | -0.156820000 | 3.876913000  |
|  | 6  | 1.771445000  | 0.823590000  | 5.040158000  |
|  | 6  | 2.513583000  | 2.103489000  | 4.697689000  |
|  | 6  | 3.945814000  | 1.803208000  | 4.289696000  |
|  | 6  | 3.987529000  | 0.829322000  | 3.121141000  |
|  | 6  | 3.243786000  | -0.432489000 | 3.487480000  |
|  | 1  | 1.283539000  | 0.283756000  | 3.030289000  |
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|  | 1 | 2.003725000  | 2.606411000  | 3.873975000  |
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|  | 1 | 4.467012000  | 2.719241000  | 4.018997000  |
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|  | 1 | 3.519612000  | 1.280451000  | 2.248164000  |
|  | 1 | 3.751058000  | -0.918169000 | 4.321762000  |
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|  | 1 | -4.267401000 | -0.355204000 | -4.590359000 |
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|  | 1 | -3.396194000 | 1.322775000  | -2.967441000 |
|  | 1 | -1.865022000 | 0.478719000  | -2.908467000 |
|  | 1 | -4.558338000 | -0.646223000 | -2.080214000 |
|  | 8 | -2.618358000 | 1.174519000  | 1.379722000  |
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|  | 6 | -4.652974000 | 4.303680000  | 0.715909000  |
|  | 6 | -3.526475000 | 5.320055000  | 0.790316000  |
|  | 6 | -2.506826000 | 4.923551000  | 1.844476000  |
|  | 6 | -1.968477000 | 3.525805000  | 1.582483000  |
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|  | 1 | -3.925151000 | 6.311816000  | 0.998342000  |
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|  | 1 | -1.681724000 | 5.631878000  | 1.873376000  |
|  | 1 | -1.256032000 | 3.223423000  | 2.346854000  |
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|  | 1 | -3.614411000 | 2.510196000  | 2.492328000  |
| Py-PO- cHex *Zn(NO <sub>3</sub> ) <sub>2</sub> | 6 | -1.239056000 | -0.806743000 | 0.975007000  |
|  | 6 | -1.801611000 | -1.810888000 | 1.744562000  |
|  | 6 | -0.969040000 | -2.781654000 | 2.276881000  |
|  | 6 | 0.391448000  | -2.715066000 | 2.032324000  |
|  | 6 | 0.877244000  | -1.670606000 | 1.260938000  |
|  | 7 | 0.069766000  | -0.748948000 | 0.742265000  |
|  | 1 | -1.376292000 | -3.577981000 | 2.879114000  |
|  | 1 | -2.865472000 | -1.826922000 | 1.916932000  |
|  | 1 | 1.070655000  | -3.448393000 | 2.436705000  |



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| 15 | -2.144294000 | 0.530452000  | 0.169330000  |
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| 8  | 3.208745000  | -2.670158000 | 0.250345000  |
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| 6  | 3.553114000  | -2.783211000 | -3.522345000 |
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| 1  | 2.116947000  | -5.060568000 | -2.837364000 |
| 1  | 0.523665000  | -4.378297000 | -3.061992000 |
| 1  | 1.250303000  | -4.199748000 | -0.680769000 |
| 1  | 1.016903000  | -2.607896000 | -1.410854000 |
| 1  | 3.665919000  | -4.051476000 | -1.111734000 |
| 30 | 0.902512000  | 0.937386000  | -0.381643000 |
| 7  | 0.890162000  | 2.695570000  | 1.729722000  |
| 8  | 0.994351000  | 3.718830000  | 2.376506000  |
| 8  | 0.361910000  | 1.660649000  | 2.178834000  |
| 8  | 1.344821000  | 2.663571000  | 0.527170000  |
| 7  | 1.099074000  | 0.489751000  | -2.913012000 |
| 8  | 1.216630000  | 0.389705000  | -4.113917000 |
| 8  | 1.452682000  | 1.536163000  | -2.286706000 |
| 8  | 0.617611000  | -0.441497000 | -2.202308000 |
| 8  | 3.412709000  | -1.426743000 | 2.224422000  |
| 6  | 2.180326000  | -0.403627000 | 4.081700000  |
| 6  | 2.334246000  | 0.528514000  | 5.275747000  |
| 6  | 2.745053000  | 1.920861000  | 4.828843000  |
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| 1  | 1.376688000  | -0.030400000 | 3.445219000  |
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| 1  | 3.089947000  | 0.121859000  | 5.954530000  |
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| 1  | 1.942586000  | 2.362929000  | 4.238117000  |
| 1  | 4.847691000  | 1.532211000  | 4.620679000  |
| 1  | 4.278316000  | 2.868643000  | 3.644639000  |
| 1  | 4.787239000  | 0.874398000  | 2.231647000  |
| 1  | 3.099787000  | 1.322881000  | 2.130269000  |
| 1  | 4.264243000  | -0.829888000 | 3.925109000  |
| 8  | -3.310662000 | -0.111684000 | -0.659309000 |
| 6  | -2.292666000 | -1.955890000 | -1.928204000 |
| 6  | -2.289111000 | -2.647457000 | -3.284410000 |

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|   | 6  | -2.802273000 | -0.471409000 | -4.398984000 |
|   | 6  | -2.798470000 | 0.229019000  | -3.047301000 |
|   | 6  | -3.200468000 | -0.751302000 | -1.971740000 |
|   | 1  | -1.277589000 | -1.629035000 | -1.699397000 |
|   | 1  | -2.617506000 | -2.637423000 | -1.140883000 |
|   | 1  | -3.287896000 | -3.043574000 | -3.490698000 |
|   | 1  | -1.617281000 | -3.503989000 | -3.254117000 |
|   | 1  | -1.913307000 | -2.185594000 | -5.353730000 |
|   | 1  | -0.858933000 | -1.355320000 | -4.226246000 |
|   | 1  | -3.821072000 | -0.787074000 | -4.643711000 |
|   | 1  | -2.499480000 | 0.230551000  | -5.172949000 |
|   | 1  | -3.481776000 | 1.077848000  | -3.042719000 |
|   | 1  | -1.802172000 | 0.609581000  | -2.832820000 |
|   | 1  | -4.224913000 | -1.080417000 | -2.148882000 |
|   | 8  | -2.901108000 | 1.200607000  | 1.350153000  |
|   | 6  | -4.111070000 | 2.948449000  | 0.091248000  |
|   | 6  | -4.632120000 | 4.375862000  | 0.193242000  |
|   | 6  | -3.505914000 | 5.352334000  | 0.487070000  |
|   | 6  | -2.759920000 | 4.955721000  | 1.749255000  |
|   | 6  | -2.235018000 | 3.532469000  | 1.645722000  |
|   | 6  | -3.376230000 | 2.590283000  | 1.360898000  |
|   | 1  | -3.420901000 | 2.874779000  | -0.752759000 |
|   | 1  | -4.922059000 | 2.243714000  | -0.085629000 |
|   | 1  | -5.375211000 | 4.429468000  | 0.993559000  |
|   | 1  | -5.149314000 | 4.642912000  | -0.726565000 |
|   | 1  | -3.896977000 | 6.364813000  | 0.574980000  |
|   | 1  | -2.807390000 | 5.357204000  | -0.352899000 |
|   | 1  | -3.431885000 | 5.039053000  | 2.608465000  |
|   | 1  | -1.928902000 | 5.631078000  | 1.938841000  |
|   | 1  | -1.716503000 | 3.229761000  | 2.551508000  |
|   | 1  | -1.518077000 | 3.471707000  | 0.825870000  |
|   | 1  | -4.075624000 | 2.591101000  | 2.196573000  |
| Py-PO-C5*Pb(NO <sub>3</sub> ) <sub>2</sub><br>(classical structure) | 6  | -3.086650000 | -1.620276000 | 1.944559000  |
|   | 6  | -3.968746000 | -1.100766000 | 1.040245000  |
|   | 6  | -3.490830000 | -0.317559000 | -0.018147000 |
|   | 6  | -2.096517000 | -0.106658000 | -0.107239000 |
|   | 7  | -1.239393000 | -0.639763000 | 0.778821000  |
|   | 6  | -1.720111000 | -1.362657000 | 1.773776000  |
|   | 6  | -4.365057000 | 0.259844000  | -0.975918000 |
|   | 6  | -1.584926000 | 0.713690000  | -1.170941000 |
|   | 6  | -2.491486000 | 1.278782000  | -2.096387000 |
|   | 6  | -3.883556000 | 1.028943000  | -1.978186000 |
|   | 6  | -1.968946000 | 2.086993000  | -3.113920000 |
|   | 1  | -2.640139000 | 2.534260000  | -3.831648000 |
|   | 6  | -0.620214000 | 2.293760000  | -3.183176000 |
|   | 6  | 0.202118000  | 1.681063000  | -2.228174000 |
|   | 7  | -0.262955000 | 0.925253000  | -1.251781000 |
|   | 1  | -5.423682000 | 0.071790000  | -0.881311000 |
|   | 1  | -3.415341000 | -2.219531000 | 2.777964000  |
|   | 1  | -5.030010000 | -1.278684000 | 1.128331000  |
|   | 15 | -0.532242000 | -2.036200000 | 2.959013000  |

|  |    |              |              |              |
|--|----|--------------|--------------|--------------|
|  | 1  | -4.546833000 | 1.472088000  | -2.705272000 |
|  | 1  | -0.178050000 | 2.902042000  | -3.955396000 |
|  | 15 | 1.994135000  | 1.894241000  | -2.330090000 |
|  | 8  | 2.675011000  | 1.033423000  | -1.347513000 |
|  | 8  | 0.829615000  | -1.574577000 | 2.642453000  |
|  | 8  | -0.791145000 | -3.578226000 | 2.995608000  |
|  | 6  | -0.249642000 | -4.454515000 | 1.963545000  |
|  | 1  | -0.241379000 | -5.434874000 | 2.429080000  |
|  | 1  | 0.771032000  | -4.153563000 | 1.746127000  |
|  | 6  | -1.094164000 | -4.444012000 | 0.719288000  |
|  | 6  | -0.642622000 | -5.497694000 | -0.273280000 |
|  | 1  | -1.027592000 | -3.463974000 | 0.242230000  |
|  | 1  | -2.141686000 | -4.597704000 | 0.990502000  |
|  | 1  | 0.423056000  | -5.373588000 | -0.468160000 |
|  | 6  | -1.395189000 | -5.415521000 | -1.587610000 |
|  | 1  | -0.769598000 | -6.492686000 | 0.162628000  |
|  | 1  | -2.460607000 | -5.584942000 | -1.409273000 |
|  | 6  | -0.872179000 | -6.396240000 | -2.614831000 |
|  | 1  | -1.305156000 | -4.400814000 | -1.980348000 |
|  | 82 | 1.443781000  | -0.389104000 | 0.426172000  |
|  | 7  | 1.477623000  | 1.941136000  | 2.385510000  |
|  | 8  | 2.553299000  | 1.320993000  | 2.272813000  |
|  | 8  | 1.274053000  | 2.738068000  | 3.286700000  |
|  | 8  | 0.564208000  | 1.719768000  | 1.512416000  |
|  | 7  | 1.144391000  | -2.881369000 | -1.416779000 |
|  | 8  | 1.621477000  | -3.071803000 | -0.272652000 |
|  | 8  | 1.252395000  | -3.711604000 | -2.305824000 |
|  | 8  | 0.535916000  | -1.782843000 | -1.628001000 |
|  | 8  | 2.230026000  | 3.439370000  | -2.235540000 |
|  | 6  | 1.876675000  | 4.125922000  | -1.000042000 |
|  | 1  | 0.970566000  | 3.681706000  | -0.583306000 |
|  | 1  | 1.645924000  | 5.140333000  | -1.311841000 |
|  | 6  | 2.991066000  | 4.090122000  | 0.006500000  |
|  | 6  | 2.629562000  | 4.913289000  | 1.229375000  |
|  | 1  | 3.904745000  | 4.467932000  | -0.454350000 |
|  | 1  | 3.183768000  | 3.057357000  | 0.296053000  |
|  | 1  | 2.524788000  | 5.965276000  | 0.946703000  |
|  | 6  | 3.642609000  | 4.785395000  | 2.350061000  |
|  | 1  | 1.652793000  | 4.599544000  | 1.604995000  |
|  | 1  | 3.739485000  | 3.733005000  | 2.616622000  |
|  | 6  | 3.245952000  | 5.584165000  | 3.572917000  |
|  | 1  | 4.622712000  | 5.107503000  | 1.989867000  |
|  | 8  | 2.383307000  | 1.672690000  | -3.830987000 |
|  | 6  | 2.645258000  | 0.320805000  | -4.307998000 |
|  | 1  | 3.256456000  | -0.191296000 | -3.568137000 |
|  | 1  | 3.236104000  | 0.464384000  | -5.206920000 |
|  | 6  | 1.371187000  | -0.427671000 | -4.582207000 |
|  | 6  | 1.632438000  | -1.837220000 | -5.076229000 |
|  | 1  | 0.771900000  | 0.128698000  | -5.306892000 |
|  | 1  | 0.789217000  | -0.504442000 | -3.663700000 |
|  | 1  | 2.197594000  | -1.813376000 | -6.012679000 |
|  | 6  | 0.348534000  | -2.621177000 | -5.265251000 |

|   |    |              |              |              |
|---|----|--------------|--------------|--------------|
|   | 1  | 2.251928000  | -2.362724000 | -4.346912000 |
|   | 1  | -0.196655000 | -2.607977000 | -4.321202000 |
|   | 6  | 0.601462000  | -4.053580000 | -5.682722000 |
|   | 1  | -0.279547000 | -2.116569000 | -6.004533000 |
|   | 8  | -1.090113000 | -1.663166000 | 4.374205000  |
|   | 6  | -0.741416000 | -0.388304000 | 4.982768000  |
|   | 1  | 0.339413000  | -0.273694000 | 4.944650000  |
|   | 1  | -1.044323000 | -0.501508000 | 6.018875000  |
|   | 6  | -1.439598000 | 0.769660000  | 4.324829000  |
|   | 6  | -1.225337000 | 2.059363000  | 5.092701000  |
|   | 1  | -2.507107000 | 0.548448000  | 4.245770000  |
|   | 1  | -1.060246000 | 0.903264000  | 3.309124000  |
|   | 1  | -1.674729000 | 1.980022000  | 6.086850000  |
|   | 6  | -1.791627000 | 3.261203000  | 4.362854000  |
|   | 1  | -0.156104000 | 2.214004000  | 5.241364000  |
|   | 1  | -1.366172000 | 3.281076000  | 3.359420000  |
|   | 6  | -1.487558000 | 4.563922000  | 5.071294000  |
|   | 1  | -2.872059000 | 3.139635000  | 4.246581000  |
|   | 1  | 3.141280000  | 6.643287000  | 3.337838000  |
|   | 1  | 3.980908000  | 5.494578000  | 4.369083000  |
|   | 1  | 2.292370000  | 5.232746000  | 3.962552000  |
|   | 1  | -1.890731000 | 4.569650000  | 6.083439000  |
|   | 1  | -1.906641000 | 5.417959000  | 4.544504000  |
|   | 1  | -0.412193000 | 4.716314000  | 5.143875000  |
|   | 1  | 1.188123000  | -4.569242000 | -4.925602000 |
|   | 1  | 1.150444000  | -4.102638000 | -6.622836000 |
|   | 1  | -0.326463000 | -4.605610000 | -5.814441000 |
|   | 1  | -1.415755000 | -6.324579000 | -3.554134000 |
|   | 1  | -0.956865000 | -7.423147000 | -2.260772000 |
|   | 1  | 0.177177000  | -6.199090000 | -2.822352000 |
| Py-PO-C5*Pb(NO <sub>3</sub> ) <sub>2</sub><br>(non-classical structure) | 6  | -3.849601000 | -2.061116000 | 0.664455000  |
|   | 6  | -4.494421000 | -1.560833000 | -0.435415000 |
|   | 6  | -3.835832000 | -0.651619000 | -1.272882000 |
|   | 6  | -2.505487000 | -0.310180000 | -0.947038000 |
|   | 7  | -1.874561000 | -0.825843000 | 0.114810000  |
|   | 6  | -2.530912000 | -1.658618000 | 0.900180000  |
|   | 6  | -4.450469000 | -0.080063000 | -2.419541000 |
|   | 6  | -1.790366000 | 0.615474000  | -1.782581000 |
|   | 6  | -2.436292000 | 1.156324000  | -2.915341000 |
|   | 6  | -3.777757000 | 0.790363000  | -3.208209000 |
|   | 6  | -1.700782000 | 2.035406000  | -3.719860000 |
|   | 1  | -2.166081000 | 2.472264000  | -4.590914000 |
|   | 6  | -0.394820000 | 2.302136000  | -3.407678000 |
|   | 6  | 0.161770000  | 1.691073000  | -2.275466000 |
|   | 7  | -0.521297000 | 0.901856000  | -1.468948000 |
|   | 1  | -5.466437000 | -0.362581000 | -2.650697000 |
|   | 1  | -4.325965000 | -2.758115000 | 1.333332000  |
|   | 1  | -5.506530000 | -1.856933000 | -0.667432000 |
|   | 15 | -1.620050000 | -2.153907000 | 2.371813000  |
|   | 1  | -4.246871000 | 1.215962000  | -4.082505000 |
|   | 1  | 0.212938000  | 2.945495000  | -4.022616000 |
|   | 15 | 1.911229000  | 1.887488000  | -1.870186000 |

|  |   |              |              |              |
|--|---|--------------|--------------|--------------|
|  | 8 | 2.387750000  | 0.798830000  | -1.006153000 |
|  | 8 | -0.188461000 | -1.820095000 | 2.303987000  |
|  | 8 | -2.054994000 | -3.644423000 | 2.538276000  |
|  | 6 | -1.520386000 | -4.442100000 | 3.633673000  |
|  | 1 | -2.288236000 | -5.183650000 | 3.833877000  |
|  | 1 | -1.423134000 | -3.807996000 | 4.515088000  |
|  | 6 | -0.215822000 | -5.073307000 | 3.243507000  |
|  | 6 | 0.317816000  | -5.988472000 | 4.329388000  |
|  | 1 | 0.510980000  | -4.291272000 | 3.023492000  |
|  | 1 | -0.362475000 | -5.627528000 | 2.319806000  |
|  | 1 | 0.337020000  | -5.457044000 | 5.284375000  |
|  | 6 | 1.711714000  | -6.510937000 | 4.018752000  |
|  | 1 | -0.364059000 | -6.833271000 | 4.462905000  |
|  | 6 | 1.789034000  | -7.302833000 | 2.727437000  |
|  | 1 | 2.049638000  | -7.128718000 | 4.851678000  |
|  | 1 | 2.400784000  | -5.665577000 | 3.967402000  |
|  | 8 | 2.060310000  | 3.349295000  | -1.293128000 |
|  | 6 | 1.448847000  | 3.646655000  | -0.023028000 |
|  | 1 | 1.587576000  | 2.801167000  | 0.651307000  |
|  | 1 | 0.377133000  | 3.789093000  | -0.177616000 |
|  | 6 | 2.088796000  | 4.889799000  | 0.524028000  |
|  | 6 | 1.447116000  | 5.332213000  | 1.823315000  |
|  | 1 | 2.013554000  | 5.683157000  | -0.220647000 |
|  | 1 | 3.152530000  | 4.701970000  | 0.672207000  |
|  | 1 | 0.386500000  | 5.537866000  | 1.656461000  |
|  | 6 | 2.109826000  | 6.558846000  | 2.418871000  |
|  | 1 | 1.481376000  | 4.514698000  | 2.549791000  |
|  | 1 | 3.166297000  | 6.344641000  | 2.589913000  |
|  | 6 | 1.461713000  | 7.013000000  | 3.710095000  |
|  | 1 | 2.084005000  | 7.368440000  | 1.686886000  |
|  | 8 | 2.658049000  | 2.102292000  | -3.229504000 |
|  | 6 | 3.193562000  | 0.972600000  | -3.972548000 |
|  | 1 | 3.427647000  | 0.169767000  | -3.276251000 |
|  | 1 | 4.123242000  | 1.339314000  | -4.397947000 |
|  | 6 | 2.238284000  | 0.526745000  | -5.043759000 |
|  | 6 | 2.869446000  | -0.509474000 | -5.952947000 |
|  | 1 | 1.929438000  | 1.397929000  | -5.626485000 |
|  | 1 | 1.339498000  | 0.109060000  | -4.587045000 |
|  | 1 | 3.753046000  | -0.084039000 | -6.438209000 |
|  | 6 | 1.906669000  | -1.020558000 | -7.005662000 |
|  | 1 | 3.217443000  | -1.352841000 | -5.354505000 |
|  | 1 | 1.028464000  | -1.423746000 | -6.502032000 |
|  | 6 | 2.525744000  | -2.083368000 | -7.888669000 |
|  | 1 | 1.560987000  | -0.182032000 | -7.616029000 |
|  | 8 | -2.355601000 | -1.451834000 | 3.591758000  |
|  | 6 | -1.877359000 | -0.190661000 | 4.099604000  |
|  | 1 | -0.817920000 | -0.284331000 | 4.328456000  |
|  | 1 | -2.423713000 | -0.044840000 | 5.027436000  |
|  | 6 | -2.124053000 | 0.948740000  | 3.144149000  |
|  | 6 | -1.816320000 | 2.287684000  | 3.784283000  |
|  | 1 | -3.167132000 | 0.923059000  | 2.820759000  |
|  | 1 | -1.512541000 | 0.814049000  | 2.249771000  |

|  |    |              |              |              |
|--|----|--------------|--------------|--------------|
|  | 1  | -2.452864000 | 2.424514000  | 4.662533000  |
|  | 6  | -2.011743000 | 3.459553000  | 2.841861000  |
|  | 1  | -0.787896000 | 2.291549000  | 4.155378000  |
|  | 1  | -1.327718000 | 3.356240000  | 1.995415000  |
|  | 6  | -1.799864000 | 4.793694000  | 3.525927000  |
|  | 1  | -3.018248000 | 3.416054000  | 2.420216000  |
|  | 82 | 0.935928000  | -1.426756000 | -0.171254000 |
|  | 7  | 1.218320000  | -2.197718000 | -2.999059000 |
|  | 8  | 1.287456000  | -2.552317000 | -4.155714000 |
|  | 8  | 0.313422000  | -1.386718000 | -2.614229000 |
|  | 8  | 2.036618000  | -2.594089000 | -2.126412000 |
|  | 7  | 0.267961000  | -4.285376000 | -0.012507000 |
|  | 8  | -0.095580000 | -5.439347000 | -0.051605000 |
|  | 8  | -0.494125000 | -3.355088000 | -0.467984000 |
|  | 8  | 1.367844000  | -3.934295000 | 0.472090000  |
|  | 1  | 1.958743000  | 7.886537000  | 4.123587000  |
|  | 1  | 1.495826000  | 6.227707000  | 4.464056000  |
|  | 1  | 0.414961000  | 7.270334000  | 3.556677000  |
|  | 1  | -2.502264000 | 4.925569000  | 4.347334000  |
|  | 1  | -1.933449000 | 5.628349000  | 2.841595000  |
|  | 1  | -0.796146000 | 4.867471000  | 3.940993000  |
|  | 1  | 1.828406000  | -2.437761000 | -8.643777000 |
|  | 1  | 2.836006000  | -2.942074000 | -7.296713000 |
|  | 1  | 3.406817000  | -1.704223000 | -8.405401000 |
|  | 1  | 1.073006000  | -8.124868000 | 2.730587000  |
|  | 1  | 2.779093000  | -7.731124000 | 2.590989000  |
|  | 1  | 1.578454000  | -6.685814000 | 1.857569000  |
| Py-PO-C5*Cd(NO <sub>3</sub> ) <sub>2</sub> | 6  | -3.452790000 | -1.607911000 | 1.933294000  |
|  | 6  | -4.335699000 | -1.030501000 | 1.060203000  |
|  | 6  | -3.853672000 | -0.237011000 | 0.009710000  |
|  | 6  | -2.457357000 | -0.064962000 | -0.085562000 |
|  | 7  | -1.604665000 | -0.632773000 | 0.775028000  |
|  | 6  | -2.082398000 | -1.384128000 | 1.748098000  |
|  | 6  | -4.704986000 | 0.383863000  | -0.944094000 |
|  | 6  | -1.918931000 | 0.739733000  | -1.144730000 |
|  | 6  | -2.794729000 | 1.338897000  | -2.073129000 |
|  | 6  | -4.196117000 | 1.139855000  | -1.946346000 |
|  | 6  | -2.222106000 | 2.116806000  | -3.089436000 |
|  | 1  | -2.862166000 | 2.589531000  | -3.819343000 |
|  | 6  | -0.862074000 | 2.268838000  | -3.141452000 |
|  | 6  | -0.076828000 | 1.631101000  | -2.171203000 |
|  | 7  | -0.592501000 | 0.892523000  | -1.209118000 |
|  | 1  | -5.770523000 | 0.236982000  | -0.852882000 |
|  | 1  | -3.788981000 | -2.230096000 | 2.746780000  |
|  | 1  | -5.399731000 | -1.181637000 | 1.164426000  |
|  | 15 | -0.821059000 | -2.136289000 | 2.801457000  |
|  | 1  | -4.848313000 | 1.607508000  | -2.668298000 |
|  | 1  | -0.389327000 | 2.862473000  | -3.907085000 |
|  | 15 | 1.724535000  | 1.777513000  | -2.134113000 |
|  | 8  | 2.271658000  | 0.911963000  | -1.076553000 |
|  | 8  | 0.516154000  | -1.778956000 | 2.301069000  |
|  | 8  | -1.166106000 | -3.663349000 | 2.867975000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 6  | -0.617830000 | -4.563187000 | 1.863642000  |
| 1  | -0.781891000 | -5.553453000 | 2.276064000  |
| 1  | 0.452499000  | -4.383486000 | 1.793536000  |
| 6  | -1.289117000 | -4.395604000 | 0.528982000  |
| 6  | -0.761714000 | -5.382180000 | -0.494321000 |
| 1  | -1.109834000 | -3.386361000 | 0.155260000  |
| 1  | -2.369312000 | -4.509460000 | 0.649696000  |
| 1  | 0.324639000  | -5.295510000 | -0.554825000 |
| 6  | -1.342619000 | -5.145063000 | -1.873978000 |
| 1  | -0.975094000 | -6.405164000 | -0.171024000 |
| 1  | -2.429670000 | -5.256099000 | -1.833678000 |
| 6  | -0.759328000 | -6.078617000 | -2.912299000 |
| 1  | -1.142365000 | -4.110789000 | -2.157948000 |
| 48 | 0.901075000  | -0.351288000 | 0.415315000  |
| 7  | 1.537268000  | 1.664749000  | 2.235585000  |
| 8  | 2.262525000  | 0.653856000  | 2.054876000  |
| 8  | 1.810902000  | 2.509354000  | 3.071196000  |
| 8  | 0.494774000  | 1.769839000  | 1.511694000  |
| 7  | 1.404100000  | -2.587132000 | -1.186002000 |
| 8  | 2.220047000  | -2.164863000 | -0.326070000 |
| 8  | 1.651809000  | -3.550367000 | -1.890699000 |
| 8  | 0.299957000  | -1.962479000 | -1.291707000 |
| 8  | 2.008345000  | 3.314628000  | -2.052664000 |
| 6  | 1.635226000  | 4.035609000  | -0.844089000 |
| 1  | 0.789191000  | 3.542184000  | -0.363632000 |
| 1  | 1.314081000  | 5.012941000  | -1.193969000 |
| 6  | 2.793202000  | 4.141749000  | 0.105798000  |
| 6  | 2.445353000  | 5.038741000  | 1.278034000  |
| 1  | 3.658604000  | 4.534108000  | -0.430637000 |
| 1  | 3.063919000  | 3.145348000  | 0.457702000  |
| 1  | 2.201621000  | 6.040983000  | 0.911418000  |
| 6  | 3.561332000  | 5.129822000  | 2.299358000  |
| 1  | 1.549416000  | 4.656789000  | 1.770818000  |
| 1  | 3.797638000  | 4.124423000  | 2.646774000  |
| 6  | 3.190539000  | 6.000972000  | 3.480518000  |
| 1  | 4.463130000  | 5.514725000  | 1.817328000  |
| 8  | 2.244398000  | 1.509198000  | -3.586094000 |
| 6  | 2.639024000  | 0.162691000  | -3.968801000 |
| 1  | 3.226795000  | -0.267422000 | -3.161415000 |
| 1  | 3.281339000  | 0.307367000  | -4.831771000 |
| 6  | 1.448773000  | -0.694049000 | -4.300395000 |
| 6  | 1.874902000  | -2.053900000 | -4.818887000 |
| 1  | 0.833828000  | -0.182150000 | -5.044482000 |
| 1  | 0.832123000  | -0.829739000 | -3.409114000 |
| 1  | 2.460330000  | -1.929494000 | -5.734746000 |
| 6  | 0.699782000  | -2.973142000 | -5.085706000 |
| 1  | 2.532344000  | -2.531159000 | -4.090235000 |
| 1  | 0.144635000  | -3.103271000 | -4.155419000 |
| 6  | 1.137169000  | -4.321991000 | -5.615518000 |
| 1  | 0.019217000  | -2.494172000 | -5.794665000 |
| 8  | -1.163202000 | -1.729200000 | 4.273897000  |
| 6  | -0.602822000 | -0.509045000 | 4.836620000  |

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|  | 1  | 0.466689000  | -0.502109000 | 4.639481000  |
|  | 1  | -0.762555000 | -0.613719000 | 5.904996000  |
|  | 6  | -1.265450000 | 0.726202000  | 4.293137000  |
|  | 6  | -0.769198000 | 1.974530000  | 4.999039000  |
|  | 1  | -2.349109000 | 0.633211000  | 4.397325000  |
|  | 1  | -1.050260000 | 0.818942000  | 3.226961000  |
|  | 1  | -1.095033000 | 1.962449000  | 6.043001000  |
|  | 6  | -1.237486000 | 3.248480000  | 4.323816000  |
|  | 1  | 0.321872000  | 1.972810000  | 5.011577000  |
|  | 1  | -0.894848000 | 3.230430000  | 3.288916000  |
|  | 6  | -0.714437000 | 4.489784000  | 5.014304000  |
|  | 1  | -2.330507000 | 3.265622000  | 4.295620000  |
|  | 1  | 2.955943000  | 7.017551000  | 3.165801000  |
|  | 1  | 3.996158000  | 6.058020000  | 4.208410000  |
|  | 1  | 2.313710000  | 5.603489000  | 3.988922000  |
|  | 1  | -1.052798000 | 4.543265000  | 6.048645000  |
|  | 1  | -1.039300000 | 5.398914000  | 4.513584000  |
|  | 1  | 0.374079000  | 4.488582000  | 5.023708000  |
|  | 1  | 1.778215000  | -4.826234000 | -4.894729000 |
|  | 1  | 1.700250000  | -4.217658000 | -6.542412000 |
|  | 1  | 0.289743000  | -4.973326000 | -5.814239000 |
|  | 1  | -1.185597000 | -5.902713000 | -3.897312000 |
|  | 1  | -0.939031000 | -7.122077000 | -2.654868000 |
|  | 1  | 0.316607000  | -5.934656000 | -2.987702000 |
| Py-PO-C5*Cu(NO <sub>3</sub> ) <sub>2</sub> | 6  | -3.375706000 | -1.646675000 | 1.910011000  |
|  | 6  | -4.270514000 | -1.149739000 | 1.000364000  |
|  | 6  | -3.811576000 | -0.347417000 | -0.053905000 |
|  | 6  | -2.427870000 | -0.096609000 | -0.117204000 |
|  | 7  | -1.561332000 | -0.591880000 | 0.773696000  |
|  | 6  | -2.016089000 | -1.340760000 | 1.759247000  |
|  | 6  | -4.667648000 | 0.208244000  | -1.043512000 |
|  | 6  | -1.905975000 | 0.713908000  | -1.173562000 |
|  | 6  | -2.780036000 | 1.244798000  | -2.140440000 |
|  | 6  | -4.172012000 | 0.972580000  | -2.046823000 |
|  | 6  | -2.212546000 | 2.021309000  | -3.160957000 |
|  | 1  | -2.849003000 | 2.444299000  | -3.923812000 |
|  | 6  | -0.858736000 | 2.226548000  | -3.179727000 |
|  | 6  | -0.072813000 | 1.649142000  | -2.172706000 |
|  | 7  | -0.585847000 | 0.920591000  | -1.201322000 |
|  | 1  | -5.725771000 | 0.004234000  | -0.979844000 |
|  | 1  | -3.693525000 | -2.266319000 | 2.732772000  |
|  | 1  | -5.324964000 | -1.367660000 | 1.081691000  |
|  | 15 | -0.746359000 | -1.945925000 | 2.894172000  |
|  | 1  | -4.827607000 | 1.387882000  | -2.797139000 |
|  | 1  | -0.387480000 | 2.811821000  | -3.952620000 |
|  | 15 | 1.724389000  | 1.812650000  | -2.110481000 |
|  | 8  | 2.245414000  | 0.922078000  | -1.066988000 |
|  | 8  | 0.564159000  | -1.426244000 | 2.491222000  |
|  | 8  | -0.927067000 | -3.504116000 | 2.946787000  |
|  | 6  | -0.275491000 | -4.326565000 | 1.939143000  |
|  | 1  | -0.165110000 | -5.296978000 | 2.413035000  |
|  | 1  | 0.712140000  | -3.916036000 | 1.740893000  |



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| 6  | -1.087217000 | -4.418042000 | 0.676273000  |
| 6  | -0.451898000 | -5.371656000 | -0.318157000 |
| 1  | -1.167095000 | -3.429124000 | 0.221096000  |
| 1  | -2.103349000 | -4.738731000 | 0.916989000  |
| 1  | 0.586917000  | -5.080088000 | -0.482447000 |
| 6  | -1.169336000 | -5.392233000 | -1.653998000 |
| 1  | -0.428018000 | -6.380418000 | 0.103922000  |
| 1  | -2.200156000 | -5.725169000 | -1.506388000 |
| 6  | -0.474032000 | -6.278393000 | -2.665468000 |
| 1  | -1.223750000 | -4.373329000 | -2.039633000 |
| 29 | 0.643347000  | -0.142763000 | 0.405877000  |
| 7  | 1.651426000  | 1.373730000  | 2.148549000  |
| 8  | 2.415880000  | 0.487187000  | 1.769373000  |
| 8  | 1.870914000  | 2.141424000  | 3.060650000  |
| 8  | 0.524877000  | 1.465483000  | 1.500015000  |
| 7  | 0.635155000  | -2.288774000 | -1.434055000 |
| 8  | 1.193491000  | -1.797873000 | -0.377208000 |
| 8  | 1.232756000  | -3.175085000 | -2.019972000 |
| 8  | -0.465635000 | -1.859084000 | -1.787896000 |
| 8  | 1.996948000  | 3.354839000  | -1.986264000 |
| 6  | 1.678423000  | 4.005531000  | -0.727041000 |
| 1  | 0.826672000  | 3.508463000  | -0.258447000 |
| 1  | 1.376220000  | 5.012463000  | -1.001887000 |
| 6  | 2.863303000  | 4.011616000  | 0.196051000  |
| 6  | 2.575766000  | 4.805435000  | 1.456026000  |
| 1  | 3.720271000  | 4.433844000  | -0.331169000 |
| 1  | 3.125401000  | 2.982803000  | 0.445056000  |
| 1  | 2.353556000  | 5.844337000  | 1.193365000  |
| 6  | 3.724552000  | 4.766306000  | 2.444023000  |
| 1  | 1.680631000  | 4.408389000  | 1.940092000  |
| 1  | 3.945119000  | 3.725527000  | 2.680503000  |
| 6  | 3.419008000  | 5.523772000  | 3.718275000  |
| 1  | 4.620676000  | 5.174250000  | 1.970868000  |
| 8  | 2.250879000  | 1.596739000  | -3.572103000 |
| 6  | 2.598029000  | 0.255080000  | -4.010598000 |
| 1  | 3.130610000  | -0.245103000 | -3.204923000 |
| 1  | 3.282262000  | 0.409618000  | -4.839180000 |
| 6  | 1.382341000  | -0.523107000 | -4.432849000 |
| 6  | 1.750265000  | -1.895913000 | -4.961327000 |
| 1  | 0.836231000  | 0.043400000  | -5.191034000 |
| 1  | 0.707740000  | -0.640649000 | -3.583040000 |
| 1  | 2.378599000  | -1.793594000 | -5.850955000 |
| 6  | 0.532398000  | -2.739094000 | -5.284329000 |
| 1  | 2.349068000  | -2.418310000 | -4.213472000 |
| 1  | -0.088395000 | -2.806354000 | -4.390499000 |
| 6  | 0.901138000  | -4.130187000 | -5.754157000 |
| 1  | -0.067658000 | -2.233043000 | -6.045222000 |
| 8  | -1.257625000 | -1.576811000 | 4.333641000  |
| 6  | -0.801695000 | -0.336654000 | 4.939516000  |
| 1  | 0.284076000  | -0.309246000 | 4.884872000  |
| 1  | -1.098420000 | -0.422305000 | 5.980131000  |
| 6  | -1.400919000 | 0.875920000  | 4.281002000  |

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|  | 6  | -0.925902000 | 2.160694000  | 4.932609000  |
|  | 1  | -2.491049000 | 0.808918000  | 4.309931000  |
|  | 1  | -1.104643000 | 0.897633000  | 3.231443000  |
|  | 1  | -1.301032000 | 2.224843000  | 5.957797000  |
|  | 6  | -1.344514000 | 3.390521000  | 4.151028000  |
|  | 1  | 0.163366000  | 2.145577000  | 4.997306000  |
|  | 1  | -0.967446000 | 3.292486000  | 3.131439000  |
|  | 6  | -0.829056000 | 4.673946000  | 4.766270000  |
|  | 1  | -2.434715000 | 3.421499000  | 4.077278000  |
|  | 1  | 3.195534000  | 6.570488000  | 3.514066000  |
|  | 1  | 4.252047000  | 5.494574000  | 4.416281000  |
|  | 1  | 2.553326000  | 5.096051000  | 4.221492000  |
|  | 1  | -1.191580000 | 4.799846000  | 5.785804000  |
|  | 1  | -1.136579000 | 5.548037000  | 4.197074000  |
|  | 1  | 0.258998000  | 4.671028000  | 4.803732000  |
|  | 1  | 1.471040000  | -4.653492000 | -4.988395000 |
|  | 1  | 1.512186000  | -4.097240000 | -6.655649000 |
|  | 1  | 0.019863000  | -4.728529000 | -5.973337000 |
|  | 1  | -0.997878000 | -6.292120000 | -3.618508000 |
|  | 1  | -0.403693000 | -7.306542000 | -2.311568000 |
|  | 1  | 0.536956000  | -5.920402000 | -2.850528000 |
| Py-PO-C5*Zn(NO <sub>3</sub> ) <sub>2</sub> | 6  | -3.433926000 | -1.533245000 | 2.004265000  |
|  | 6  | -4.360452000 | -0.982501000 | 1.155964000  |
|  | 6  | -3.931797000 | -0.192620000 | 0.078245000  |
|  | 6  | -2.544225000 | -0.001504000 | -0.060836000 |
|  | 7  | -1.648579000 | -0.539573000 | 0.768481000  |
|  | 6  | -2.074738000 | -1.285775000 | 1.765557000  |
|  | 6  | -4.809103000 | 0.406341000  | -0.868316000 |
|  | 6  | -2.039881000 | 0.786773000  | -1.142248000 |
|  | 6  | -2.933098000 | 1.355241000  | -2.069920000 |
|  | 6  | -4.330103000 | 1.145954000  | -1.900276000 |
|  | 6  | -2.372894000 | 2.100957000  | -3.118091000 |
|  | 1  | -3.019809000 | 2.554552000  | -3.854196000 |
|  | 6  | -1.010896000 | 2.243268000  | -3.196853000 |
|  | 6  | -0.213970000 | 1.636135000  | -2.215644000 |
|  | 7  | -0.716560000 | 0.936548000  | -1.220199000 |
|  | 1  | -5.871824000 | 0.255006000  | -0.752511000 |
|  | 1  | -3.731025000 | -2.151196000 | 2.836251000  |
|  | 1  | -5.416489000 | -1.153951000 | 1.302503000  |
|  | 15 | -0.712131000 | -1.958371000 | 2.737802000  |
|  | 1  | -5.006931000 | 1.590234000  | -2.614529000 |
|  | 1  | -0.550241000 | 2.807951000  | -3.991441000 |
|  | 15 | 1.585752000  | 1.726500000  | -2.149744000 |
|  | 8  | 2.061756000  | 0.844012000  | -1.069734000 |
|  | 8  | 0.557509000  | -1.497132000 | 2.148100000  |
|  | 8  | -0.923412000 | -3.509297000 | 2.811087000  |
|  | 6  | -0.362710000 | -4.354874000 | 1.768431000  |
|  | 1  | -0.356700000 | -5.348783000 | 2.204615000  |
|  | 1  | 0.664719000  | -4.043733000 | 1.591383000  |
|  | 6  | -1.173440000 | -4.302262000 | 0.503697000  |
|  | 6  | -0.630912000 | -5.253715000 | -0.545274000 |
|  | 1  | -1.142628000 | -3.289892000 | 0.098460000  |

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| 1  | -2.217232000 | -4.531873000 | 0.729685000  |
| 1  | 0.444202000  | -5.099782000 | -0.651748000 |
| 6  | -1.279713000 | -5.048192000 | -1.899196000 |
| 1  | -0.768188000 | -6.288266000 | -0.218812000 |
| 1  | -2.359125000 | -5.199213000 | -1.813793000 |
| 6  | -0.707222000 | -5.964421000 | -2.958976000 |
| 1  | -1.132566000 | -4.007416000 | -2.193711000 |
| 30 | 0.843618000  | -0.244272000 | 0.373323000  |
| 7  | 1.588210000  | 1.451793000  | 2.171441000  |
| 8  | 2.429457000  | 0.601809000  | 1.841194000  |
| 8  | 1.743554000  | 2.237909000  | 3.088830000  |
| 8  | 0.495349000  | 1.469912000  | 1.484190000  |
| 7  | 1.518271000  | -2.325569000 | -1.003441000 |
| 8  | 2.345682000  | -1.905758000 | -0.176599000 |
| 8  | 1.729156000  | -3.252143000 | -1.764931000 |
| 8  | 0.384172000  | -1.713214000 | -1.027744000 |
| 8  | 1.935539000  | 3.250549000  | -2.050342000 |
| 6  | 1.611180000  | 3.952090000  | -0.816300000 |
| 1  | 0.740712000  | 3.490509000  | -0.346608000 |
| 1  | 1.340139000  | 4.956002000  | -1.131181000 |
| 6  | 2.781732000  | 3.957868000  | 0.123644000  |
| 6  | 2.488933000  | 4.795266000  | 1.354053000  |
| 1  | 3.656074000  | 4.346182000  | -0.401187000 |
| 1  | 3.015474000  | 2.931640000  | 0.408879000  |
| 1  | 2.283327000  | 5.828045000  | 1.055368000  |
| 6  | 3.623341000  | 4.774147000  | 2.358959000  |
| 1  | 1.583777000  | 4.422819000  | 1.838265000  |
| 1  | 3.829805000  | 3.738918000  | 2.628942000  |
| 6  | 3.302055000  | 5.569282000  | 3.606175000  |
| 1  | 4.529845000  | 5.162183000  | 1.888594000  |
| 8  | 2.141320000  | 1.430134000  | -3.581071000 |
| 6  | 2.566267000  | 0.083499000  | -3.930852000 |
| 1  | 3.141343000  | -0.323549000 | -3.102751000 |
| 1  | 3.226036000  | 0.225988000  | -4.780992000 |
| 6  | 1.401548000  | -0.802157000 | -4.277823000 |
| 6  | 1.876501000  | -2.134405000 | -4.825050000 |
| 1  | 0.773319000  | -0.296274000 | -5.014767000 |
| 1  | 0.789562000  | -0.970323000 | -3.388770000 |
| 1  | 2.439021000  | -1.967595000 | -5.748538000 |
| 6  | 0.740216000  | -3.101169000 | -5.090330000 |
| 1  | 2.567709000  | -2.592068000 | -4.115486000 |
| 1  | 0.228277000  | -3.300525000 | -4.147646000 |
| 6  | 1.221495000  | -4.400132000 | -5.701710000 |
| 1  | 0.007799000  | -2.628291000 | -5.749870000 |
| 8  | -0.979565000 | -1.590098000 | 4.235088000  |
| 6  | -0.497258000 | -0.328887000 | 4.778799000  |
| 1  | 0.555715000  | -0.227612000 | 4.525048000  |
| 1  | -0.587441000 | -0.453933000 | 5.853246000  |
| 6  | -1.289818000 | 0.848641000  | 4.282391000  |
| 6  | -0.873793000 | 2.128713000  | 4.984710000  |
| 1  | -2.355906000 | 0.658958000  | 4.427172000  |
| 1  | -1.120662000 | 0.968461000  | 3.211426000  |

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|  | 1  | -1.226110000 | 2.117749000  | 6.019705000  |
|  | 6  | -1.383735000 | 3.366423000  | 4.273791000  |
|  | 1  | 0.214915000  | 2.178819000  | 5.021876000  |
|  | 1  | -1.006691000 | 3.347439000  | 3.250080000  |
|  | 6  | -0.953405000 | 4.647052000  | 4.956801000  |
|  | 1  | -2.474234000 | 3.326190000  | 4.205497000  |
|  | 1  | 3.090945000  | 6.611754000  | 3.369022000  |
|  | 1  | 4.122584000  | 5.552976000  | 4.319296000  |
|  | 1  | 2.424269000  | 5.160793000  | 4.104245000  |
|  | 1  | -1.323635000 | 4.694808000  | 5.980219000  |
|  | 1  | -1.317312000 | 5.527821000  | 4.432907000  |
|  | 1  | 0.132603000  | 4.713471000  | 4.998264000  |
|  | 1  | 1.925175000  | -4.901869000 | -5.039673000 |
|  | 1  | 1.731175000  | -4.223366000 | -6.648166000 |
|  | 1  | 0.400632000  | -5.087388000 | -5.890659000 |
|  | 1  | -1.178488000 | -5.807532000 | -3.926647000 |
|  | 1  | -0.841371000 | -7.011968000 | -2.691418000 |
|  | 1  | 0.360174000  | -5.788396000 | -3.079360000 |
| Pb(NO <sub>3</sub> ) <sub>2</sub> *2Py-PO-cHex | 82 | 0.103313000  | 0.708466000  | 2.246166000  |
|  | 15 | 0.703190000  | -1.145152000 | -1.400741000 |
|  | 15 | -1.896949000 | 3.622191000  | 1.293261000  |
|  | 8  | 0.288812000  | -0.364192000 | -0.167067000 |
|  | 8  | 2.282320000  | -1.483198000 | -1.530581000 |
|  | 7  | 0.031196000  | -3.406319000 | -2.698818000 |
|  | 8  | 0.406870000  | -0.406012000 | -2.819135000 |
|  | 7  | -0.916621000 | 2.838434000  | 3.701965000  |
|  | 8  | 1.789178000  | 2.767957000  | 2.097380000  |
|  | 8  | -1.344296000 | 2.283075000  | 0.820823000  |
|  | 8  | 2.914022000  | 0.889983000  | 2.138712000  |
|  | 8  | -1.308470000 | 4.928228000  | 0.545052000  |
|  | 6  | -0.496734000 | -4.634779000 | -2.829045000 |
|  | 6  | -1.970240000 | 5.010405000  | 3.768047000  |
|  | 1  | -2.490340000 | 5.816789000  | 3.230052000  |
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|  | 1  | 0.019034000  | 4.897838000  | 0.568157000  |
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| 8  | 0.076635000  | 0.831724000  | 5.964874000   |
| 6  | 3.113591000  | 1.750999000  | 4.913711000   |
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|  | 6  | -0.433378000 | -1.574320000 | 5.863547000  |
|  | 1  | 0.397630000  | -1.743401000 | 6.584098000  |
|  | 1  | -0.007474000 | -1.639852000 | 4.841607000  |
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|  | 1  | 5.061922000  | 0.177667000  | 7.330415000  |
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|  | 1  | -5.529001000 | -0.111706000 | 1.962472000  |
|  | 6  | -6.156070000 | 0.891755000  | 0.135986000  |
|  | 1  | -6.030914000 | -0.020219000 | -0.483847000 |
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|  | 6  | -6.472411000 | 1.774408000  | 2.493157000  |
|  | 1  | -6.560443000 | 1.493652000  | 3.563219000  |
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|  | 8  | 0.610882000  | 0.895287000  | -0.300601000 |
|  | 8  | 2.468946000  | -0.189234000 | -1.816090000 |
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|  | 8  | 1.439566000  | 2.424929000  | 1.924914000  |
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|  | 8  | -0.516357000 | 5.804765000  | 1.280113000  |
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