

The reactivity of N-heterocyclic diphospholenes towards iron triad carbonyls

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EPR spectrum of 6	1
Molecular structure of 5	2
NMR spectra.....	2
Crystallographic data.....	8
Quantum chemical calculations.....	10
Cartesian coordinates of the calculated structures.....	11

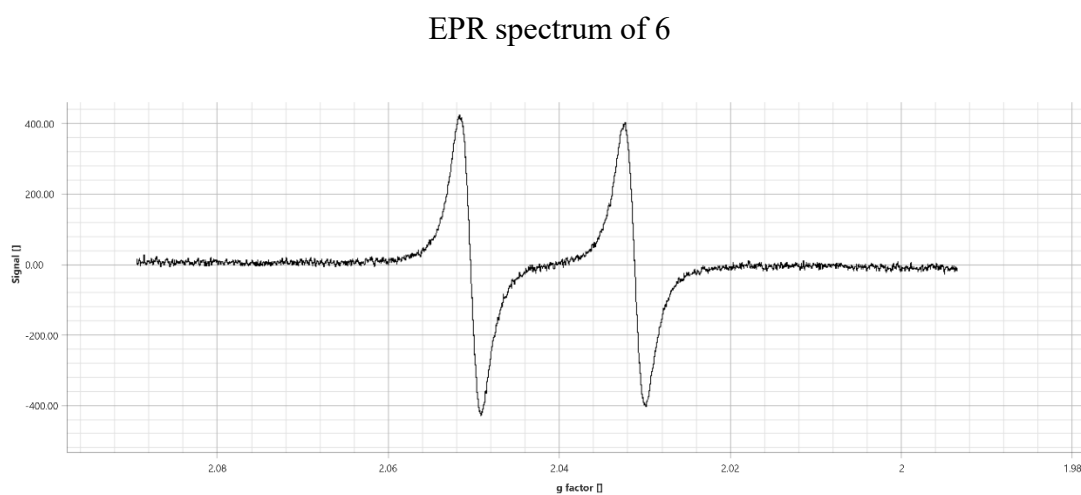


Figure S1. EPR spectrum of **6** in toluene at 293 K. $g=2.042$, $a(^{31}\text{P}) = 3.31$ mT.

Molecular structure of **5**

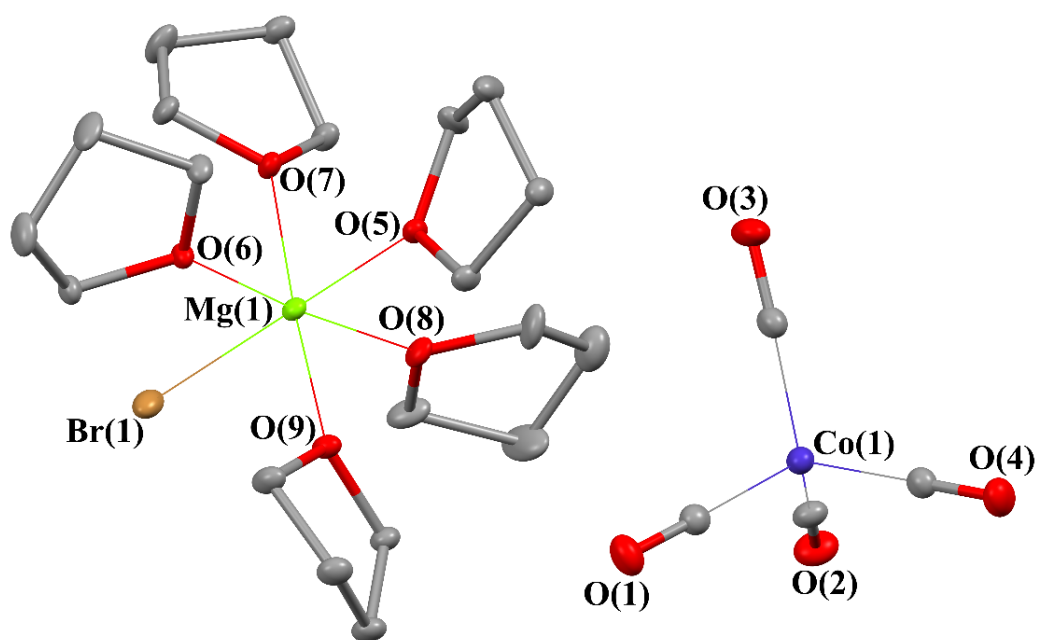
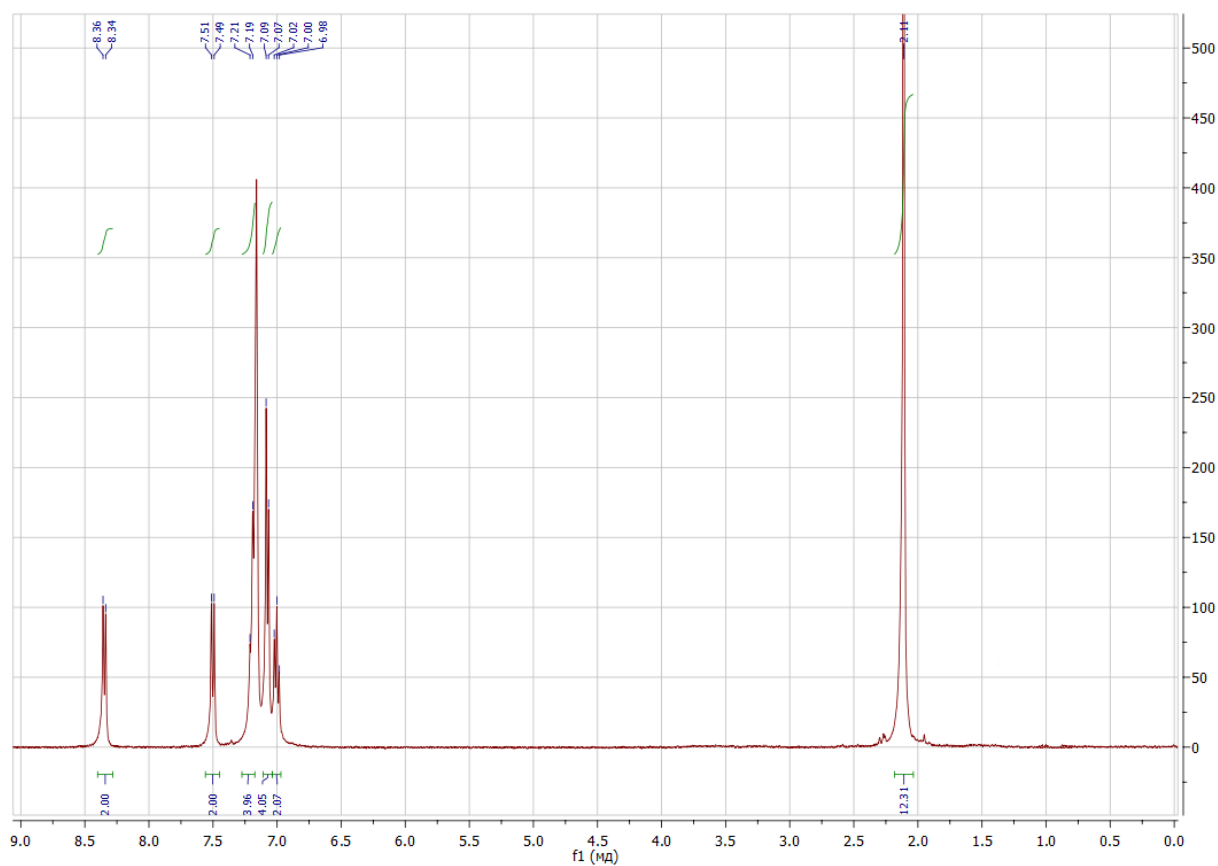
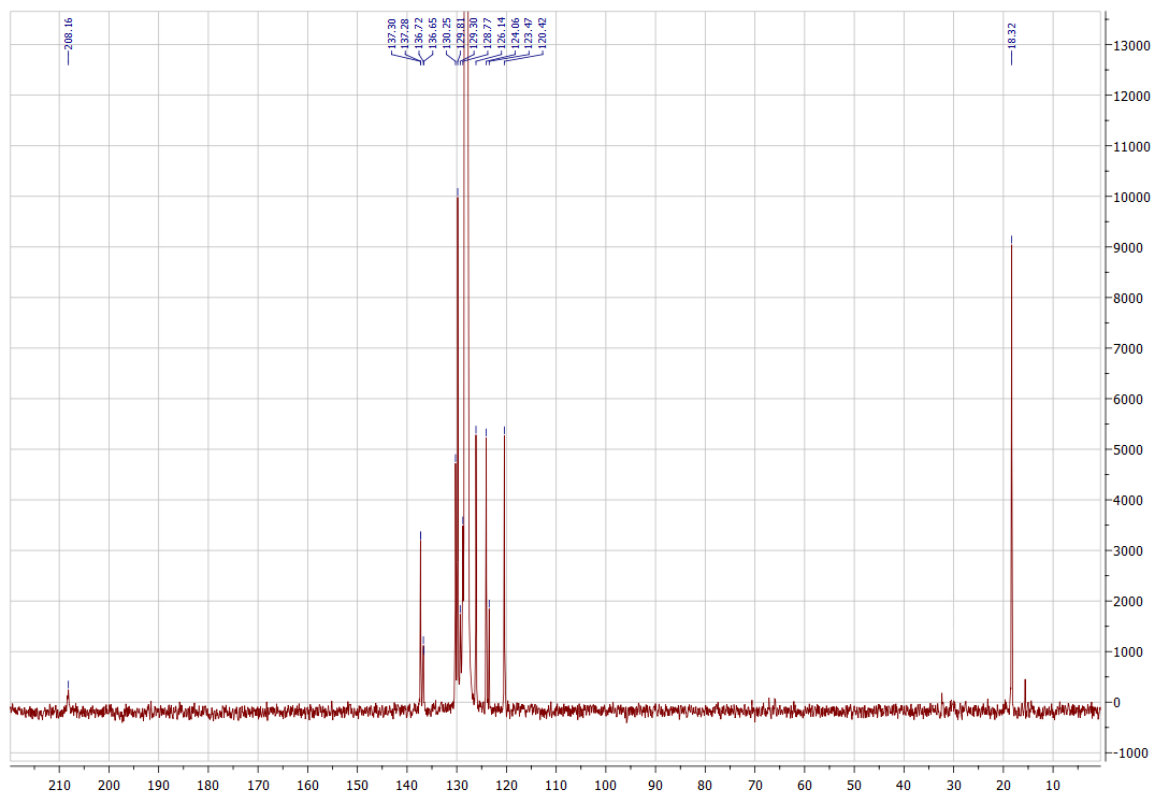


Figure S2. Molecular structure of $\text{Mg}(\text{THF})_5\text{Br}[\text{Co}(\text{CO})_4]$

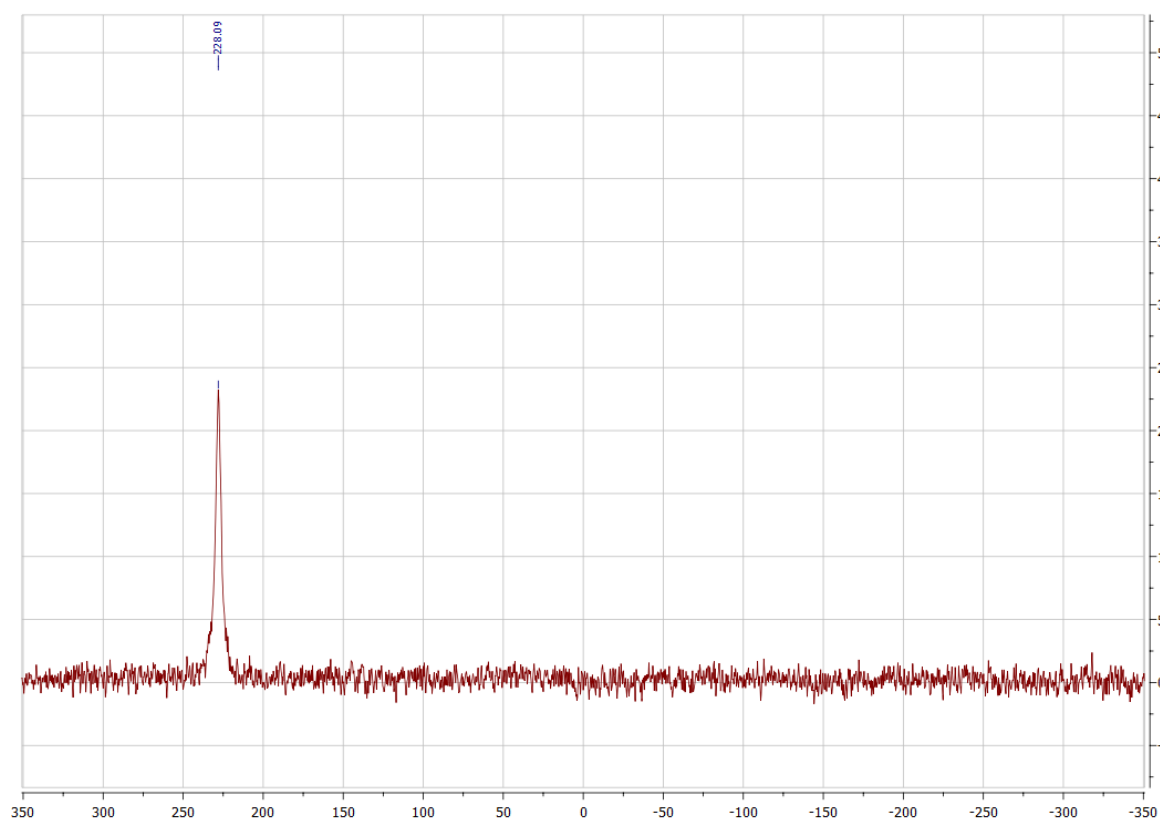
NMR spectra



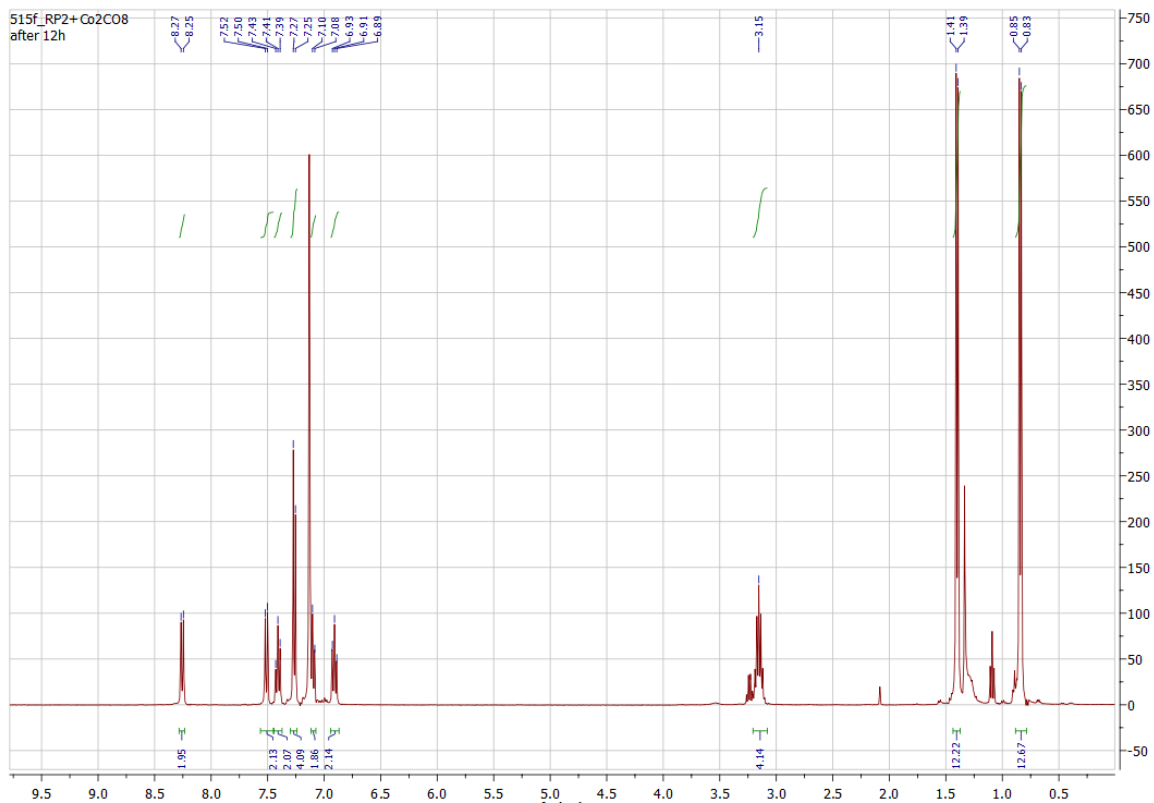
^1H NMR of **3**



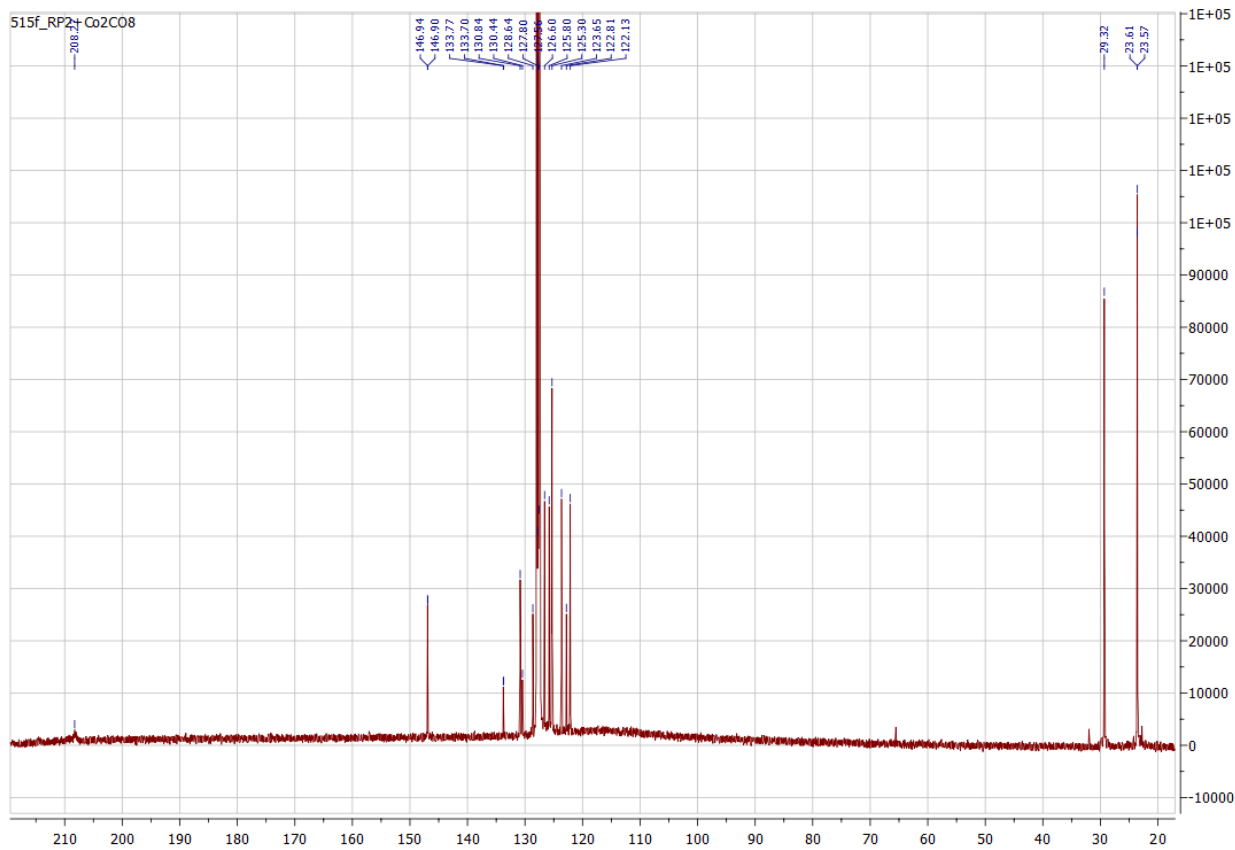
^{13}C NMR of **3**



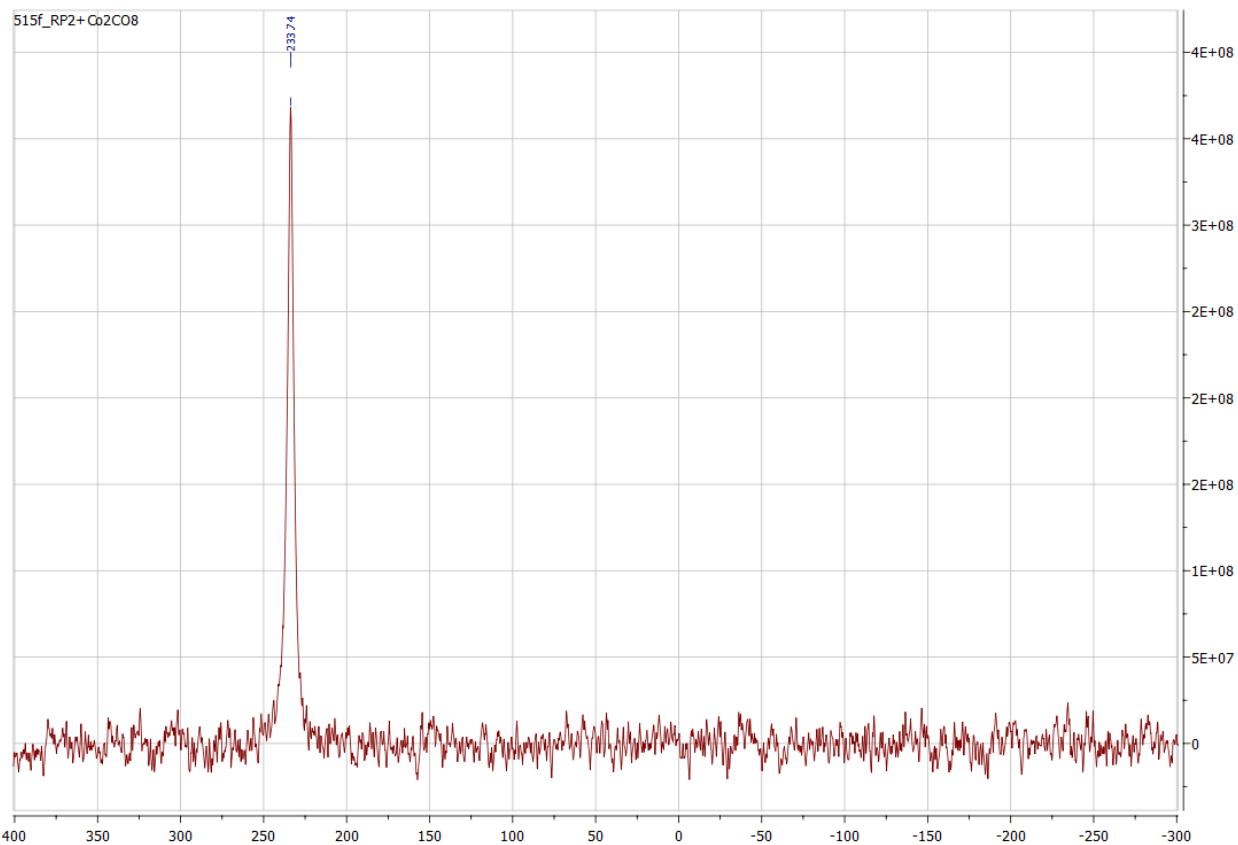
^{31}P NMR of **3**



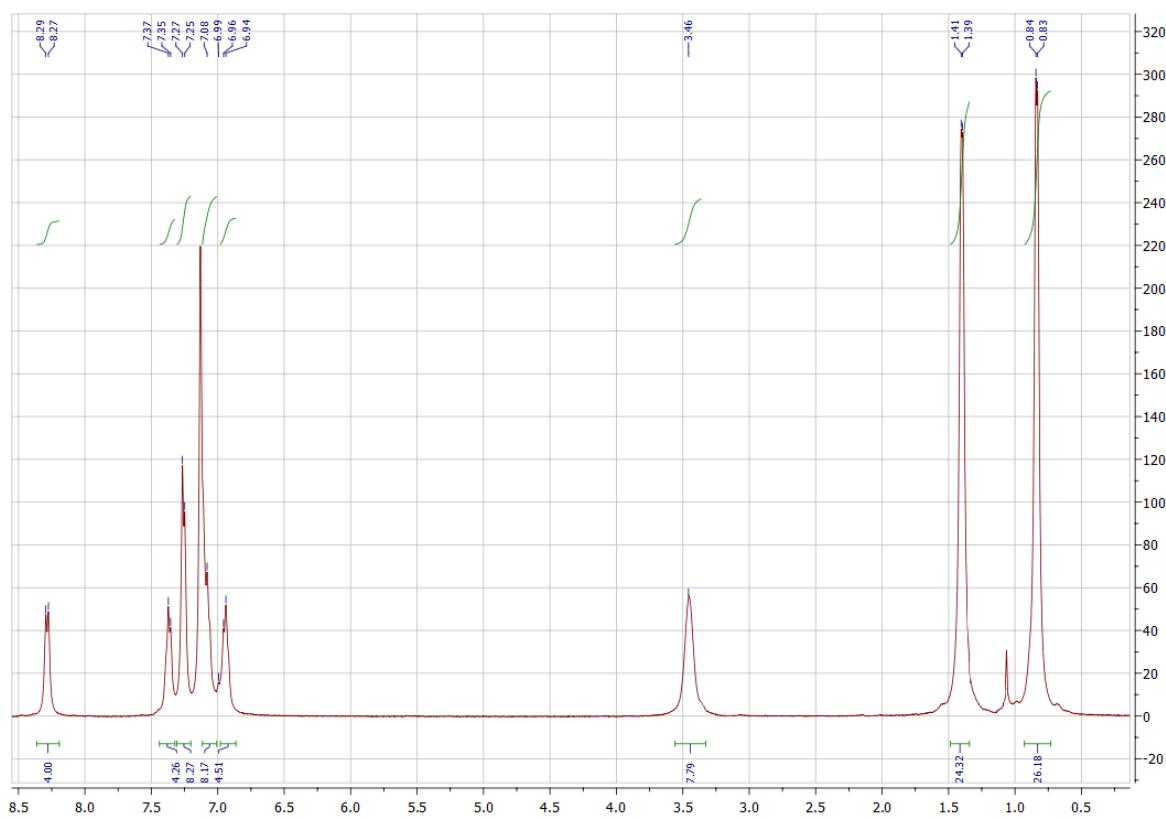
^1H NMR of **4**



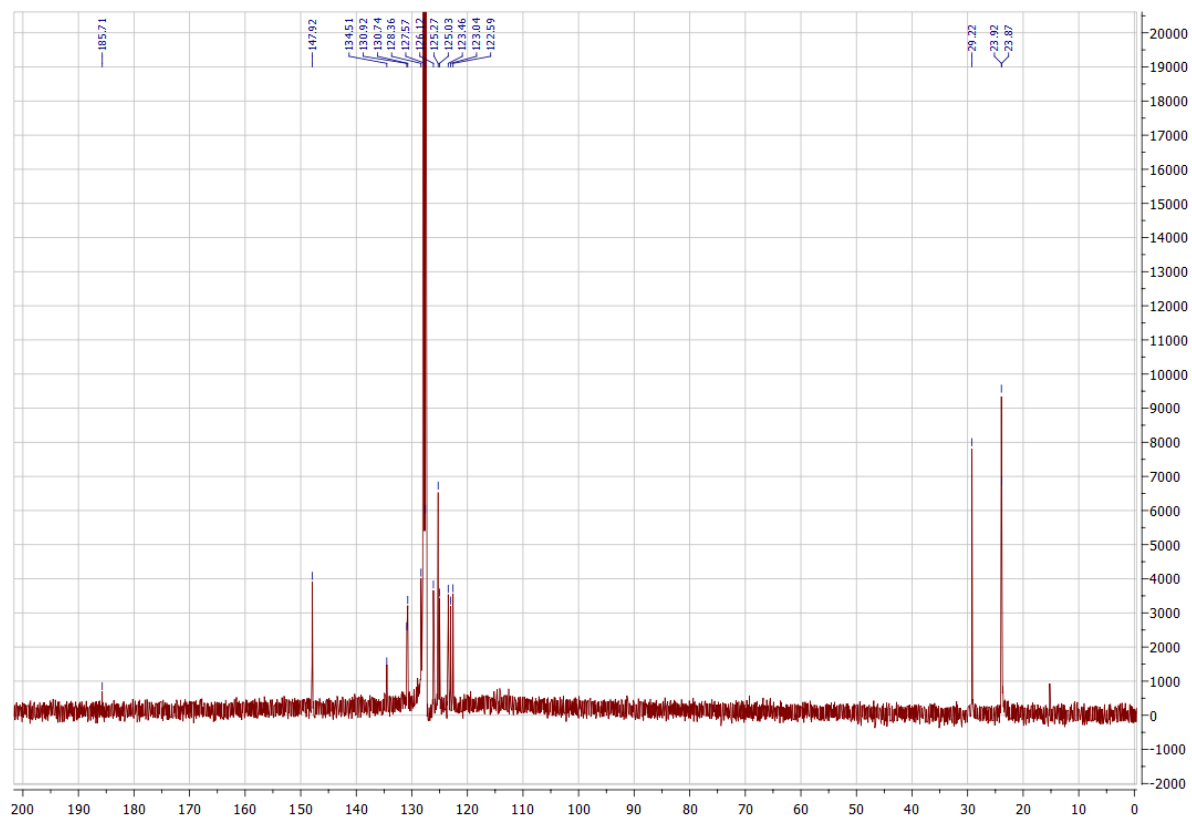
^{13}C NMR of **4**



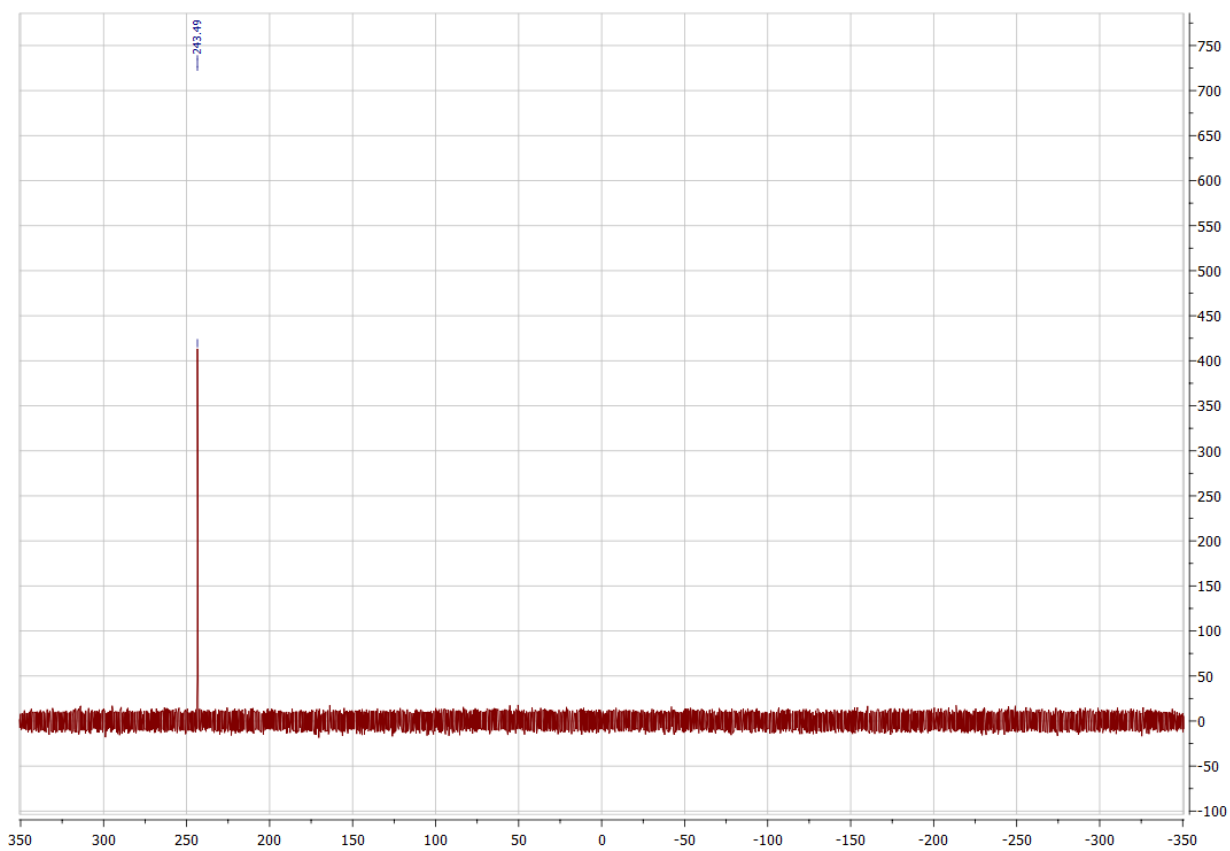
^{31}P NMR of 4



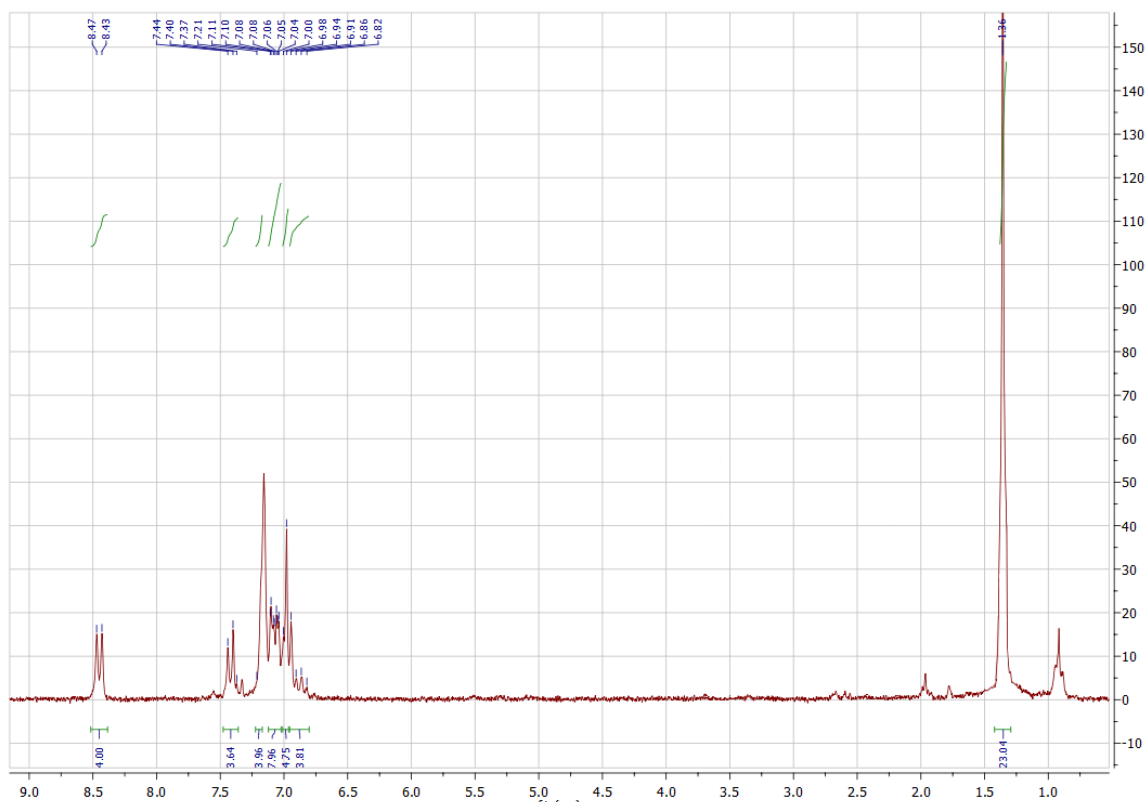
^1H NMR of 6



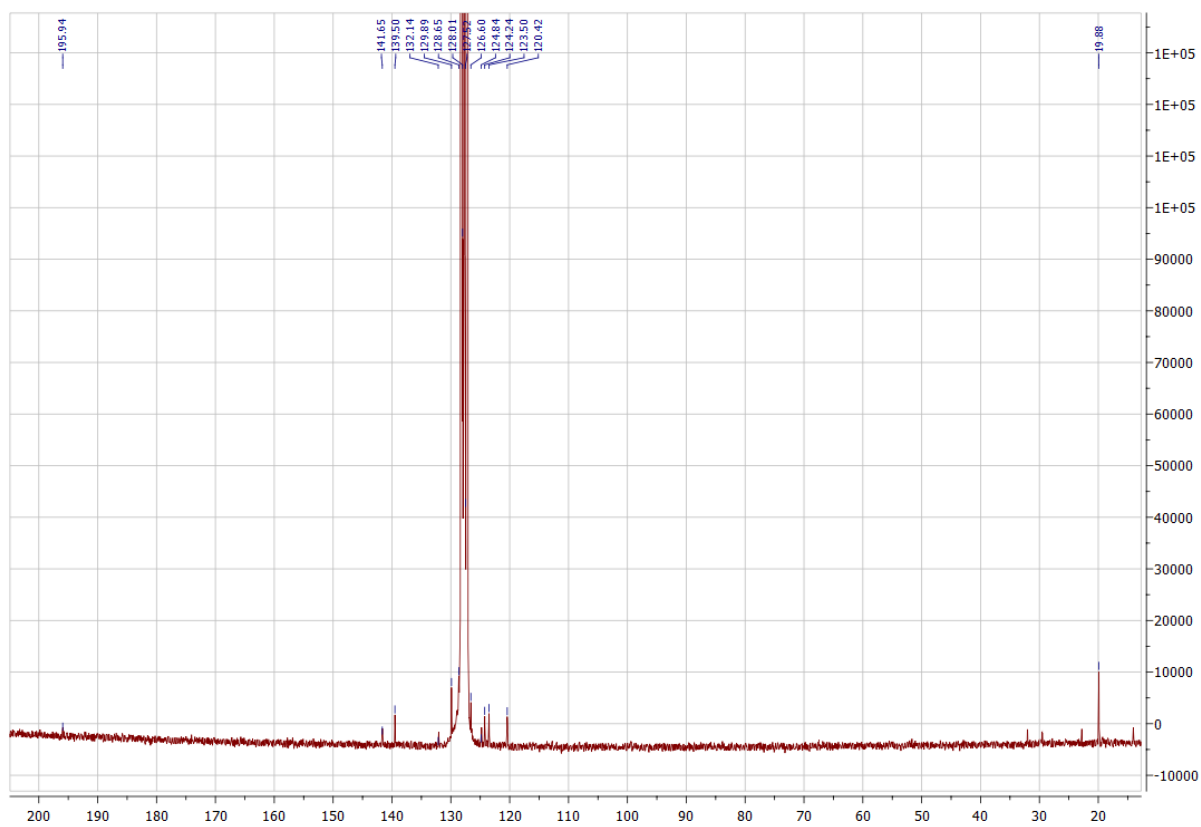
^{13}C NMR of **6**



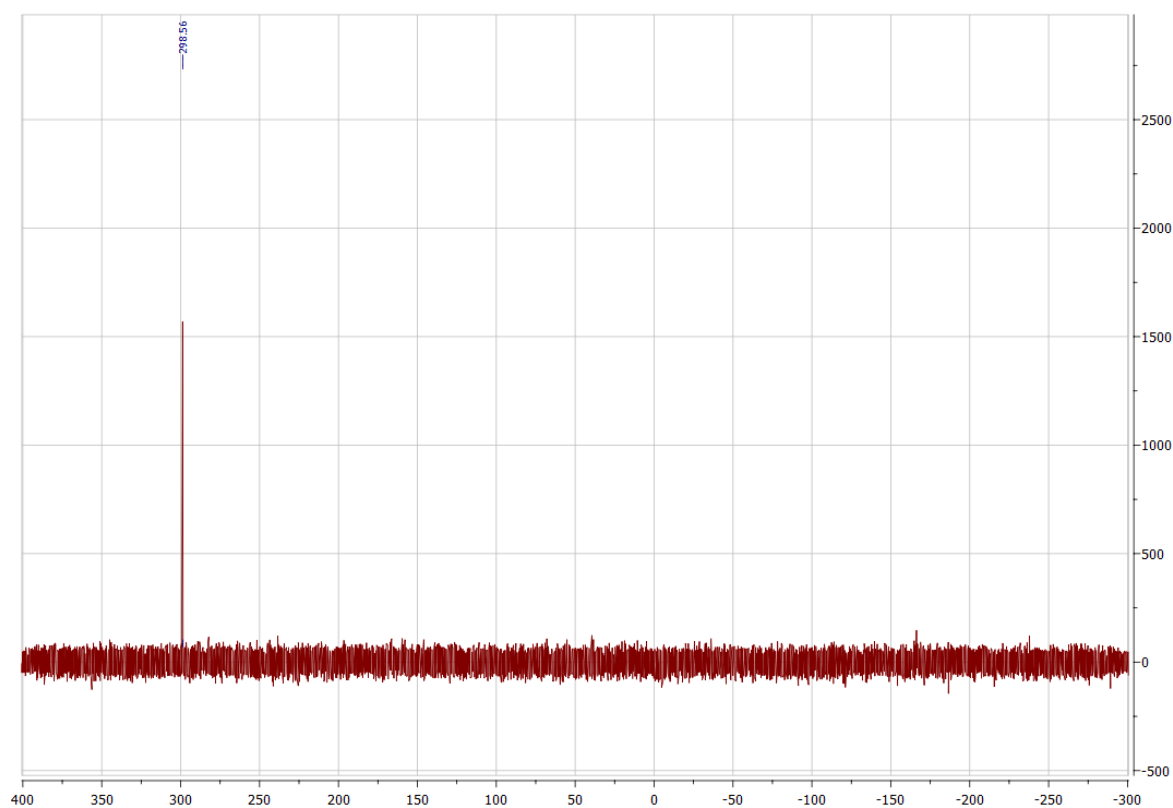
^{31}P NMR of **6**



^1H NMR of 7



^{13}C NMR of 7



^{31}P NMR of **7**

Crystallographic data

Table S1. The selected bond lengths (Å) and angles (°) in the compounds **4**, **6** and **7**.

Bonds, Å	4 (M = Co)	6 (M = Fe)	7 (M = Ni)
M(1)-P(1)	1.9962(4)	2.0370(8)	2.1477(3)
P(1)-N(1)	1.6729(12)	1.693(2)	1.7182(9)
P(1)-N(2)	1.6686(12)	1.689(2)	1.7164(9)
N(1)-C(1)	1.4034(17)	1.415(3)	1.4089(13)
N(2)-C(2)	1.4035(18)	1.408(3)	1.4155(13)
C(1)-C(2)	1.3818(19)	1.376(4)	1.3760(14)
M(1)-C _{CO}	1.7767(16) ÷ 1.7823(18)	1.768(3) ÷ 1.810(3)	1.7866(12) ÷ 1.8068(12)
M(1)-P(1A)			2.2171(3)
M···M		2.7166(5)	2.5263(3)
M(2)-P(2)		2.0298(8)	
P(2)-N(3)		1.693(2)	
P(2)-N(4)		1.693(2)	
N(3)-C(39)		1.405(3)	
N(4)-C(40)		1.412(3)	
C(39)-C(40)		1.383(3)	
M(2)-C _{CO}		1.779(3) ÷ 1.808(3)	
C≡O	1.142(2) ÷ 1.146(2)	1.148(3) ÷ 1.156(3)	1.1407(15), 1.1408(15)
Angles, °	4 (M = Co)	6 (M = Fe)	7 (M = Ni)
C _{CO} -M-C _{CO}	104.55(8) ÷ 117.16(7)	92.15(13) ÷ 153.34(12)	104.98(6)
N(1)-P(1)-N(2)	89.89(6)	89.26(11)	90.44(4)
N(1)-P(1)-M(1)	134.27(5)	135.68(8)	133.22(3)
N(2)-P(1)-M(1)	135.74(4)	131.58(8)	122.28(3)
M(1)-P(1)-M(1A)			70.711(10)

N(1)-P(1)-M(1A)			119.87(3)
N(2)-P(1)-M(1A)			124.65(3)
N(3)-P(2)-N(4)		89.00(10)	
N(3)-P(2)-M(2)		134.57(8)	
N(4)-P(2)-M(2)		134.50(8)	
M-C≡O	177.12(15) ÷ 177.88(18)	174.0(3) ÷ 179.2(3)	168.50(11), 171.67(12)

Table S2. Crystallographic data and structure refinement details for compounds 4-7.

Compound	4	5	6	7
Empirical formula	C ₄₁ H ₄₂ CoN ₂ O ₃ P	C ₂₈ H ₄₈ BrCoMgO ₁₀	C ₈₆ H ₉₄ Fe ₂ N ₄ O ₇ P ₂	C ₈₀ H ₈₄ N ₄ Ni ₂ O ₈ P ₂
Formula weight	700.66	707.81	1469.29	1408.87
Temperature [K]	100(2)	100(2)	100(2)	100(2)
Crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>Cc</i>	<i>P</i> -1	<i>P</i> -1
Unit cell dimensions				
<i>a</i> [Å]	14.1235(2)	12.9480(2)	14.9695(3)	11.8356(3)
<i>b</i> [Å]	12.3282(2)	23.6942(3)	16.1526(3)	12.3643(4)
<i>c</i> [Å]	21.0680(3)	10.69920(10)	17.9588(3)	13.0056(4)
α [°]	90	90	78.315(2)	104.9470(10)
β [°]	91.3690(10)	93.5980(10)	73.465(2)	96.6470(10)
γ [°]	90	90	68.266(2)	108.7910(10)
<i>V</i> [Å ³]	3667.26(9)	3275.96(7)	3843.80(14)	1699.19(9)
<i>Z</i>	4	4	2	1
<i>d</i> _{calc} [g cm ⁻³]	1.269	1.435	1.269	1.377
μ [mm ⁻¹]	0.551	1.813	0.476	0.663
<i>F</i> ₀₀₀	1472	1480	1552	742
Crystal dimensions [mm ³]	0.38 × 0.33 × 0.11	0.78 × 0.53 × 0.32	0.35 × 0.25 × 0.24	0.34 × 0.28 × 0.14
θ range for data collection [°]	2.902–28.698	3.023–30.033	2.858–26.022	2.552–35.631
Reflections collected	52679	46071	58766	35302
Independent reflections (<i>R</i> _{int})	9476 (<i>R</i> _{int} = 0.0426)	9565 (<i>R</i> _{int} = 0.0339)	15135 (<i>R</i> _{int} = 0.0621)	15580 (<i>R</i> _{int} = 0.0271)
Completeness to θ [%]	99.8	99.8	99.8	99.9
Data/restraints/parameters	9476 / 0 / 441	9565 / 2 / 371	15135 / 1 / 933	15580 / 12 / 456
Final <i>R</i> indices [<i>I</i> > 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0347 <i>wR</i> ₂ = 0.0801	<i>R</i> ₁ = 0.0378 <i>wR</i> ₂ = 0.0960	<i>R</i> ₁ = 0.0484 <i>wR</i> ₂ = 0.1052	<i>R</i> ₁ = 0.0396 <i>wR</i> ₂ = 0.0904
Final <i>R</i> indices (all data)	<i>R</i> ₁ = 0.0500 <i>wR</i> ₂ = 0.0855	<i>R</i> ₁ = 0.0394 <i>wR</i> ₂ = 0.0974	<i>R</i> ₁ = 0.0805 <i>wR</i> ₂ = 0.1170	<i>R</i> ₁ = 0.0568 <i>wR</i> ₂ = 0.0970
<i>S</i> (<i>F</i> ²)	1.020	1.028	1.021	1.039
Absolute structure parameter	-	0.496(8)	-	-
Largest diff. peak and hole [e Å ⁻³]	0.388 / -0.329	1.159 / -0.505	0.690 / -0.490	0.733 / -0.399

Quantum chemical calculations

Table S3. Total energies (E_{total} , a.u.) of the structures calculated by the DFT wB97XD/6-311++G(d,p) method.

Structure	E_{total}
4	-3332.458696
a-Fe	-3213.371779
a-Ni	-3457.993501
b-Co	-6664.932829
6	-6426.807099
b-Ni	-3457.993501
c-Co	-6438.284555
c-Fe	-6200.142512
7	-6689.391159

Table S4. Fuzzy bond order calculated by the DFT wB97XD/6-311++G(d,p) method

Compound	M–P	N–P	M–M
4m	1.77	1.32	–
6m	1.74	1.30	0.71
7m	1.04	1.23	0.56

Table S5. Calculated bond lengths (Å) and angles (°) in the compounds **4m**, **6m** and **7m**.

Bonds, Å	4m (M = Co)	6m (M = Fe)	7m (M = Ni)
M(1)-P(1)	1.9835	2.0090	2.2214
P(1)-N(1)	1.6820	1.6890	1.7247
P(1)-N(2)	1.6826	1.6894	1.7209
N(1)-C(1)	1.3995	1.4036	1.4029
N(2)-C(2)	1.3999	1.4013	1.4150
C(1)-C(2)	1.3757	1.3746	1.3669
M(1)-C _{CO}	1.7786 ÷ 1.7929	1.7591 ÷ 1.8029	1.7992 ÷ 1.8159
M(1)-P(1A)			2.1602
M···M		2.6820	2.5588
M(2)-P(2)		2.0092	
P(2)-N(3)		1.6892	
P(2)-N(4)		1.6895	
N(3)-C(39)		1.4037	
N(4)-C(40)		1.4012	
C(39)-C(40)		1.3745	

M(2)-C _{CO}		1.7588 ÷ 1.8030	
C≡O	1.141 ÷ 1.145	1.1455 ÷ 1.1508	1.1381, 1.1404
Angles, °	4m (M = Co)	6m (M = Fe)	7m (M = Ni)
C _{CO} -M-C _{CO}	106.15 ÷ 112.61	93.19 ÷ 152.36	105.54, 105.57
N(1)-P(1)-N(2)	89.12	89.05	90.37
N(1)-P(1)-M(1)	134.28	134.89	120.72
N(2)-P(1)-M(1)	135.57	133.21	124.11
M(1)-P(1)-M(1A)			71.45
N(1)-P(1)-M(1A)			131.09
N(2)-P(1)-M(1A)			123.45
N(3)-P(2)-N(4)		89.05	
N(3)-P(2)-M(2)		134.90	
N(4)-P(2)-M(2)		133.26	
M-C≡O	178.74 ÷ 179.77	174.25 ÷ 177.03	167.49(1), 171.65(1)

Cartesian coordinates of the calculated structures

66

a-Fe

26	-3.149116000	0.042399000	-0.059250000
15	-1.121900000	0.015079000	-0.009453000
7	0.061218000	-1.189371000	0.070463000
7	0.093216000	1.187386000	0.072759000
6	1.376071000	-0.705612000	0.133293000
6	1.394518000	0.668086000	0.134663000
6	2.626624000	1.412069000	0.200787000
6	2.685109000	2.821463000	0.292495000
1	1.776868000	3.399785000	0.347171000
6	3.886891000	3.486298000	0.319832000
1	3.899183000	4.567693000	0.393227000
6	5.085026000	2.768306000	0.257429000
1	6.036821000	3.286666000	0.270947000
6	5.051953000	1.396084000	0.193573000
1	5.994158000	0.866671000	0.163706000
6	3.839173000	0.676952000	0.176125000
6	3.819665000	-0.780706000	0.171885000
6	5.012735000	-1.532377000	0.182607000
1	5.968656000	-1.028164000	0.153636000
6	5.008776000	-2.905387000	0.237863000
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6	3.791890000	-3.591027000	0.298292000
1	3.774417000	-4.672802000	0.364677000
6	2.608412000	-2.893816000	0.277248000
1	1.685357000	-3.448158000	0.330098000
6	2.587756000	-1.482870000	0.194372000
6	-0.360991000	-2.547512000	-0.106855000
6	-0.817131000	-3.260141000	1.004953000
6	-1.246736000	-4.569511000	0.804329000
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6	-1.221623000	-5.138015000	-0.461226000
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6	-0.735303000	3.282704000	0.998353000
6	-1.124476000	4.603842000	0.793057000

1	-1.472389000	5.191109000	1.635977000
6	-1.070770000	5.170750000	-0.472374000
1	-1.378952000	6.200256000	-0.615783000
6	-0.631919000	4.424744000	-1.557796000
1	-0.600385000	4.872251000	-2.545220000
6	-0.240145000	3.099784000	-1.396386000
6	-3.481489000	1.756804000	-0.648806000
8	-3.741565000	2.802721000	-1.026099000
6	-3.853959000	0.053925000	1.580040000
8	-4.229703000	0.059622000	2.664248000
6	-3.530340000	-1.665102000	-0.639161000
8	-3.820601000	-2.705826000	-1.008688000
6	-0.822027000	-2.633806000	2.371832000
1	-1.064955000	-3.374318000	3.134869000
1	0.152238000	-2.197986000	2.608870000
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6	0.150408000	-2.280052000	-2.560202000
1	1.193961000	-1.981645000	-2.422797000
1	0.076274000	-2.849004000	-3.487741000
1	-0.439699000	-1.365461000	-2.672652000
6	-0.770607000	2.658639000	2.365809000
1	-1.535194000	1.878130000	2.417524000
1	0.188423000	2.194567000	2.611412000
1	-0.997498000	3.407090000	3.126078000
6	0.240082000	2.273760000	-2.556650000
1	0.152651000	2.829361000	-3.491041000
1	1.287340000	1.984885000	-2.425373000
1	-0.343654000	1.353268000	-2.650211000

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4

27	-3.062057000	-0.085072000	0.026203000
15	-1.079646000	-0.034253000	0.068988000
7	0.084983000	1.179348000	0.078251000
7	0.152158000	-1.180422000	0.056065000
6	1.408325000	0.724218000	0.066616000
6	1.448023000	-0.650807000	0.050221000
6	2.693908000	-1.377061000	0.019613000
6	2.777652000	-2.787349000	0.007556000
1	1.881035000	-3.385023000	0.034227000
6	3.991072000	-3.430520000	-0.038972000
1	4.022713000	-4.513943000	-0.048119000
6	5.174661000	-2.688324000	-0.074968000
1	6.135272000	-3.188649000	-0.115008000
6	5.116509000	-1.315379000	-0.057939000
1	6.048483000	-0.768184000	-0.083931000
6	3.891925000	-0.619065000	-0.007812000
6	3.849522000	0.839228000	0.024745000
6	5.030924000	1.608677000	0.019272000
1	5.993979000	1.119648000	-0.024111000
6	5.006833000	2.981829000	0.071447000
1	5.936465000	3.539126000	0.066457000
6	3.781136000	3.649709000	0.137471000
1	3.747661000	4.731841000	0.189307000
6	2.608117000	2.934181000	0.139285000
1	1.677431000	3.475179000	0.193766000
6	2.608910000	1.522855000	0.075786000

6	-0.381738000	2.534805000	-0.008204000
6	-0.541157000	3.102926000	-1.274299000
6	-1.025145000	4.405806000	-1.343522000
1	-1.156369000	4.873015000	-2.313431000
6	-1.346618000	5.103726000	-0.187096000
1	-1.730282000	6.115335000	-0.257705000
6	-1.187193000	4.511396000	1.057765000
1	-1.446940000	5.059329000	1.956849000
6	-0.702627000	3.211194000	1.170122000
6	-0.234878000	-2.562639000	0.020911000
6	-0.432417000	-3.168205000	-1.222022000
6	-0.831432000	-4.501429000	-1.236151000
1	-0.988370000	-4.998148000	-2.187410000
6	-1.034237000	-5.192736000	-0.049469000
1	-1.350002000	-6.229535000	-0.077224000
6	-0.842996000	-4.562478000	1.171889000
1	-1.013475000	-5.104646000	2.095449000
6	-0.443677000	-3.230371000	1.229098000
6	-3.624404000	-1.691572000	0.589554000
8	-3.982169000	-2.717924000	0.944761000
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6	-3.724581000	1.256763000	1.004236000
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1	-0.341378000	2.929950000	-3.406296000
1	0.868876000	2.018378000	-2.489629000
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6	-0.511519000	2.556729000	2.509819000
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1	-0.694348000	3.268700000	3.315407000
1	-1.203297000	1.718539000	2.636505000
6	-0.205414000	-2.400558000	-2.494328000
1	-0.940234000	-1.595745000	-2.595327000
1	0.788566000	-1.944812000	-2.511876000
1	-0.298652000	-3.054272000	-3.362305000
6	-0.236392000	-2.527123000	2.541213000
1	-0.334058000	-3.225984000	3.372719000
1	0.753420000	-2.065090000	2.593070000
1	-0.978463000	-1.733558000	2.675188000

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a-Ni

28	-2.989273000	-0.458535000	-0.219813000
15	-1.036660000	-0.222813000	0.880181000
7	-0.088466000	1.189389000	0.597827000
7	0.329855000	-1.192439000	0.475505000
6	1.262681000	0.897814000	0.400317000
6	1.501983000	-0.455317000	0.313035000
6	2.831158000	-0.966074000	0.077589000
6	3.134617000	-2.344895000	0.025934000
1	2.364502000	-3.076938000	0.210918000
6	4.404311000	-2.787814000	-0.258756000
1	4.604967000	-3.852432000	-0.294348000
6	5.427140000	-1.866498000	-0.501941000
1	6.428809000	-2.208398000	-0.736018000

6	5.161177000	-0.519788000	-0.428798000
1	5.973606000	0.171422000	-0.606977000
6	3.875720000	-0.027046000	-0.127533000
6	3.624804000	1.401974000	0.017279000
6	4.655264000	2.357068000	-0.097708000
1	5.660311000	2.042663000	-0.344536000
6	4.429235000	3.696870000	0.113326000
1	5.244815000	4.404539000	0.018319000
6	3.151175000	4.139384000	0.473191000
1	2.971562000	5.190039000	0.669923000
6	2.120406000	3.238120000	0.583145000
1	1.141401000	3.593979000	0.868939000
6	2.324424000	1.863731000	0.332423000
6	-0.753640000	2.388032000	0.184910000
6	-0.722804000	2.764644000	-1.164138000
6	-1.420684000	3.910228000	-1.537665000
1	-1.411068000	4.215085000	-2.578820000
6	-2.137451000	4.647621000	-0.607021000
1	-2.682016000	5.531578000	-0.919251000
6	-2.160039000	4.252083000	0.722542000
1	-2.719841000	4.829785000	1.450349000
6	-1.466684000	3.119933000	1.141893000
6	0.131200000	-2.594486000	0.273552000
6	-0.012686000	-3.074978000	-1.033106000
6	-0.236438000	-4.436887000	-1.207802000
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6	-0.179436000	-4.789729000	1.171893000
1	-0.240514000	-5.460739000	2.022074000
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6	-3.330047000	-2.243662000	-0.194760000
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6	-4.154356000	0.522136000	0.781750000
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1	0.284284000	-3.702820000	3.508377000
1	1.223251000	-2.356845000	2.838696000
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132

6

26	1.155350000	-1.516627000	-0.679731000
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7	4.305488000	-0.789623000	0.364467000
7	-3.461516000	0.990009000	0.953028000
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6	5.308067000	0.154504000	0.105604000
6	6.675939000	0.123952000	0.562153000
6	7.212896000	-0.907275000	1.366863000
1	6.597197000	-1.737333000	1.670790000
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6	9.354106000	0.177205000	1.414845000
1	10.387392000	0.204031000	1.741249000
6	8.854382000	1.190727000	0.633622000
1	9.520438000	1.998731000	0.365341000
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6	7.836068000	3.351347000	-1.049108000
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6	7.376640000	4.374656000	-1.842158000
1	8.044409000	5.178074000	-2.131159000
6	6.047817000	4.366830000	-2.275125000
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6	5.208829000	3.344775000	-1.902671000
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6	2.382680000	1.763369000	-2.992846000
6	1.537701000	2.671253000	-3.623660000
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6	1.142971000	3.806472000	-1.537285000
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6	4.436899000	-2.018025000	1.091531000
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6	4.933568000	-4.352553000	1.117711000
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6	4.655563000	-4.383063000	2.477331000
1	4.736285000	-5.316594000	3.022728000
6	4.268556000	-3.227765000	3.141664000
1	4.050249000	-3.260305000	4.203519000
6	4.149151000	-2.021202000	2.458408000
6	-4.821465000	1.183530000	0.664193000
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6	-7.211233000	-0.909291000	-1.367186000
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1	-8.897552000	-1.690970000	-2.404089000
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6	1.366587000	-2.868875000	0.493855000
8	1.508659000	-3.766323000	1.191561000
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6	-1.366819000	-2.870699000	-0.489914000
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132

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7	-4.759756000	0.810933000	0.053883000
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6	5.549400000	-0.352350000	-0.067009000
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1	7.339646000	-6.101604000	1.120349000
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6	4.385355000	2.898237000	-3.069487000
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1	-9.977365000	-1.319687000	2.869678000
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8	-1.614958000	3.855055000	0.779167000
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1	4.121116000	-0.712136000	5.303976000
1	5.099943000	-0.849447000	3.833294000
1	3.932704000	0.463711000	3.996245000
6	1.886508000	-2.443988000	0.093945000
1	2.855458000	-2.682060000	-0.352809000
1	1.176110000	-3.213687000	-0.208217000
1	1.549784000	-1.492802000	-0.330494000
6	5.926033000	3.239302000	0.935658000
1	5.113534000	3.203366000	1.667553000
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1	3.327347000	0.579785000	-3.686089000
1	4.536874000	-0.293092000	-2.731970000
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132

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15	3.917554000	-1.012336000	-1.527103000
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7	-4.998862000	-0.890081000	0.192038000
7	4.019716000	0.698518000	-1.738066000
7	5.001146000	-0.888186000	-0.190469000
6	-5.023435000	1.274341000	0.947956000
6	-5.568094000	0.376626000	0.058945000
6	-6.604311000	0.772715000	-0.864261000
6	-7.253938000	-0.129135000	-1.736621000
1	-7.027425000	-1.182658000	-1.693833000
6	-8.183906000	0.304874000	-2.650693000

1	-8.663696000	-0.410954000	-3.308230000
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1	-9.225520000	2.014662000	-3.459535000
6	-7.915901000	2.552752000	-1.862942000
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6	-6.973103000	2.142414000	-0.899165000
6	-6.429261000	3.077714000	0.078192000
6	-6.851728000	4.421363000	0.137209000
1	-7.557516000	4.798091000	-0.590565000
6	-6.407367000	5.279648000	1.115147000
1	-6.755231000	6.306199000	1.132446000
6	-5.529628000	4.814385000	2.100646000
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6	-5.087460000	3.514147000	2.067093000
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6	-5.497978000	2.628963000	1.045612000
6	-2.945313000	1.427401000	2.338913000
6	-2.751978000	1.320809000	3.722217000
6	-1.709233000	2.040484000	4.299394000
1	-1.546175000	1.967755000	5.369493000
6	-0.894095000	2.855828000	3.527400000
1	-0.092689000	3.418728000	3.992499000
6	-1.097332000	2.938550000	2.158982000
1	-0.450191000	3.564634000	1.553735000
6	-2.106548000	2.210443000	1.535265000
6	-5.109082000	-1.984026000	-0.722853000
6	-5.882048000	-3.094176000	-0.365419000
6	-5.969866000	-4.148740000	-1.271581000
1	-6.567230000	-5.017719000	-1.016422000
6	-5.315210000	-4.091923000	-2.493781000
1	-5.396539000	-4.918647000	-3.190589000
6	-4.553512000	-2.980792000	-2.826119000
1	-4.034026000	-2.944227000	-3.777405000
6	-4.428261000	-1.912823000	-1.943405000
6	5.020791000	1.274747000	-0.950924000
6	5.567067000	0.380228000	-0.059679000
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6	7.254170000	-0.118116000	1.736828000
1	7.030895000	-1.172380000	1.695366000
6	8.182667000	0.319936000	2.650464000
1	8.664637000	-0.393557000	3.308941000
6	8.499382000	1.679511000	2.728181000
1	9.218974000	2.033897000	3.457282000
6	7.908095000	2.565950000	1.859674000
1	8.185920000	3.608927000	1.927113000
6	6.966776000	2.151402000	0.896230000
6	6.420808000	3.083556000	-0.082948000
6	6.839297000	4.428361000	-0.143540000
1	7.543103000	4.808282000	0.584493000
6	6.393565000	5.283807000	-1.123346000
1	6.738300000	6.311389000	-1.141865000
6	5.518387000	4.814330000	-2.109114000
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6	5.079934000	3.512855000	-2.073952000
1	4.413166000	3.166606000	-2.849456000
6	5.491771000	2.630513000	-1.050550000
6	2.944266000	1.419506000	-2.344988000

6	2.102008000	2.201692000	-1.544164000
6	1.091847000	2.925770000	-2.170903000
1	0.441600000	3.550289000	-1.567506000
6	0.891055000	2.840030000	-3.539495000
1	0.088717000	3.399647000	-4.006943000
6	1.709684000	2.025491000	-4.308607000
1	1.548507000	1.950199000	-5.378813000
6	2.753426000	1.309681000	-3.728356000
6	5.112766000	-1.979272000	0.727630000
6	4.432230000	-1.905352000	1.948128000
6	4.559341000	-2.970480000	2.834067000
1	4.040253000	-2.931628000	3.785481000
6	5.322507000	-4.081520000	2.504886000
1	5.405395000	-4.905900000	3.204278000
6	5.976747000	-4.141167000	1.282574000
1	6.575224000	-5.010083000	1.029832000
6	5.887127000	-3.089505000	0.373270000
6	-1.775055000	-2.913086000	-0.193039000
8	-1.645785000	-3.509198000	-1.153473000
6	-1.889683000	-3.183179000	2.782631000
8	-1.846127000	-3.914898000	3.652690000
6	-0.602871000	-0.772536000	1.595472000
8	0.261030000	-0.047681000	1.753585000
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8	-0.260601000	-0.060084000	-1.757937000
6	1.779464000	-2.912818000	0.201742000
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6	1.898337000	-3.195593000	-2.772629000
8	1.858442000	-3.931154000	-3.639615000
6	2.260258000	2.261423000	-0.050943000
1	3.037233000	2.974863000	0.240687000
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1	2.537166000	1.288804000	0.357409000
6	3.664357000	0.462039000	-4.574432000
1	3.502276000	0.664286000	-5.634327000
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6	3.591702000	-0.708771000	2.288592000
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1	7.188569000	-2.197182000	-1.091075000
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128

c-Fe

26	-0.080471000	-0.160083000	-1.382352000
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7	2.916735000	-1.262449000	-0.009191000
6	4.316870000	0.579171000	-0.108333000
6	4.236452000	-0.770716000	0.075915000
6	5.384925000	-1.568808000	0.379426000
6	5.282306000	-2.926278000	0.756614000
1	4.310295000	-3.395299000	0.813245000
6	6.401386000	-3.657730000	1.069312000
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6	7.666467000	-3.057282000	1.019770000
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6	7.783408000	-1.732519000	0.672261000
1	8.770012000	-1.288660000	0.666213000
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6	6.763431000	0.457957000	-0.009042000
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1	8.924178000	0.522462000	0.003620000
6	8.128269000	2.408261000	-0.521150000
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6	6.973286000	3.159072000	-0.768080000
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6	5.593216000	1.232046000	-0.232228000
6	2.777999000	2.558549000	-0.003716000
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6	2.711958000	4.441291000	1.477608000
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6	2.229989000	5.234880000	0.447798000
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6	2.603842000	-2.493101000	-0.671834000
6	1.797149000	-3.429197000	-0.006689000
6	1.486113000	-4.620963000	-0.657894000
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6	1.956835000	-4.883646000	-1.933798000
1	1.706470000	-5.816130000	-2.427468000
6	2.768235000	-3.956478000	-2.569471000
1	3.150216000	-4.163572000	-3.563678000
6	3.114010000	-2.754883000	-1.955963000
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6	0.991076000	-0.316942000	-2.798052000
8	-2.447294000	-0.286468000	-3.108034000
6	-1.550952000	-0.247482000	-2.398125000
26	0.064701000	0.224287000	1.229973000

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6	-4.234588000	0.588843000	-0.280626000
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6	-6.533673000	3.235931000	-1.619076000
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1	-8.641271000	3.003277000	-2.032437000
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1	-3.817123000	1.120522000	2.539773000
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6	2.207561000	2.801180000	-2.459513000
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1	4.548603000	2.003044000	2.278604000
6	4.048880000	-1.817437000	-2.674438000
1	5.080630000	-1.985234000	-2.350522000
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1	3.819563000	-0.769196000	-2.488726000
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1	1.145960000	-4.148383000	1.906826000
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1	-2.606599000	-2.778014000	-1.816697000
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1	-1.678514000	-4.290565000	-1.814903000

128

c-Co

27	-0.045014000	-0.385678000	-1.194541000
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6	6.762756000	3.494453000	-0.648159000
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6	2.580895000	2.582331000	-0.256412000
6	2.575173000	3.308078000	0.939521000
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1	2.116786000	5.205871000	1.816621000
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6	-7.956545000	-1.427500000	-0.044551000
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1	-8.975916000	-3.235059000	0.453328000
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6	-2.805410000	2.500669000	0.403865000
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128

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