# **Can heterometallic 1-dimensional chains support current rectification?**

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#### Supporting information.

### **Computational methods**

All calculations of gas-phase electronic structure were performed using the Amsterdam Density Functional package ADF2012<sup>1</sup> package and the BP86 functional.<sup>2</sup> A double- $\zeta$  Slatertype basis set, extended with a single polarization function, was used to describe the main group atoms, while cobalt was modeled with a triple- $\zeta$  basis set. Electrons in orbitals up to and including 1s {C, N}, 2p{Cl}, 3p {Cr, Mn, Co} and 4p {Mo} were considered part of the core and treated in accordance with the frozen core approximation. The local density approximation was employed for the optimizations,<sup>3</sup> along with the local exchange-correlation potential of Vosko, Wilk and Nusair<sup>4</sup> and gradient corrections to exchange and correlation proposed by Becke and Perdew (BP86).<sup>5</sup> Different configurations were defined using the 'occupations' key. All structures were optimized using the gradient algorithm of Versluis and Ziegler.<sup>6</sup> Transport calculations were performed with ATK11.2.3<sup>7,8</sup> package using the gradient corrected PBE functional.<sup>9</sup> The methodology combines a density functional theory treatment of the electronic structure with the Keldysh non-equilibrium Green's function approach to simulating coherent transport.<sup>10</sup> All atoms were treated with double- $\zeta$  basis set, extended with single polarization function. Core electrons were described by norm-conserving pseudopotentials.<sup>11</sup> The electronic structure of the two-probe systems at equilibrium was converged using a 100 Ry mesh cut-off, finite temperature of 300K at the electrodes, and the real space density constraint at the electrodes. Sampling of the Brillouin zone was performed using a Monkhorst-Pack grid<sup>12</sup> with 300 k-points along the transport direction. In the calculation of the transmission spectra and currents, a 5 x 5 grid was used to sample the Brillouin zone, and the bias window was sampled

at 0.01 eV intervals. The initial spin density for the two-probe calculations was polarized to be consistent with the net spin densities of the isolated molecules in their gas phase ground states. The scattering region contained the EMAC sandwiched between 4 x 4 layer of the Au (111) surface of the source and the drain, respectively. The sulphur atoms of the two NCS<sup>-</sup> ligands are located in a hollow site on the Au (111) surface with Au-S distance 2.52 Å. The precise details of the contact geometry remain a significant issue in all transport calculations – the 'hollow-site' geometry with a gold-sulfur distance of 2.52 Å (corresponding to a distance of ~1.9 Å between the sulfur and the surface) adopted here has been established as the global minimum for many examples of sulfur coordination to Au (111)<sup>13</sup> and is used in the majority of comparative studies.<sup>14</sup> The transmission spectra are not influenced strongly by alternative choices of contact geometry.

Figure S1 Comparison of optimised and X-ray crystallographic structural parameters.



Note X-ray data corresponds to MoWCr while computation relates to Mo<sub>2</sub>Cr.



**Figure S2** Bias-dependence of the transmission spectra for Mo<sub>2</sub>Cr.

O	otimis	ed	Cartesian	coordinates	and tota	l energies	of Mo <sub>2</sub>	Cr.	Mo <sub>2</sub> Mn	and Mo	Co.
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$Mo_2Cr$	$(dpa)_4 (NCS)_2$	${}^{5}B_{1}$ E=-644.90	eV
S	0.00000000	0.00000000	-7.404126000
S	0.00000000	0.00000000	7.447030000
С	0.00000000	0.00000000	-5.791980000
С	0.00000000	0.00000000	5.836557000
N	0.00000000	0.00000000	-4.591682000
N	0.00000000	0.00000000	4.637168000
Мо	0.00000000	0.00000000	-2.272369000
Мо	0.00000000	0.00000000	-0.111881000
Cr	0.00000000	0.00000000	2.542077000
N	-1.147116000	-1.908201000	-2.243923000
N	-1.907213000	1.147086000	-2.245245000
N	1.907213000	-1.147086000	-2.245245000
N	1.147116000	1.908201000	-2.243923000
N	-1.626318000	1.406242000	0.048946000
N	-1.405348000	-1.626771000	0.050303000
N	1.626318000	-1.406242000	0.048946000
N	1.405348000	1.626771000	0.050303000
N	-1.828197000	-1.088703000	2.286798000
N	1.092319000	-1.828076000	2.286609000
N	-1.092319000	1.828076000	2.286609000
N	1.828197000	1.088703000	2.286798000
С	-1.290019000	-2.647036000	-3.371103000
С	-1.806328000	-3.928233000	-3.377444000
С	-2.158539000	-4.509147000	-2.153443000
С	-2.034719000	-3.766904000	-0.994064000
С	-1.569606000	-2.439097000	-1.051046000
С	-2.258435000	-1.674238000	1.125348000
С	-3.575407000	-2.181727000	1.051316000
С	-4.401951000	-2.148570000	2.156085000
С	-3.931896000	-1.594795000	3.350130000
С	-2.656061000	-1.063952000	3.355870000

Н	-0.947804000	-2.163162000	-4.285253000
Н	-1.894455000	-4.470701000	-4.318262000
Н	-2.262823000	-4.205041000	-0.022620000
Н	-3.944307000	-2.560039000	0.099397000
Н	-4.543596000	-1.551416000	4.250547000
н	-2 244525000	-0.590417000	4 247065000
C	2 645722000	-1 289036000	-3 372828000
C	3 926379000	-1 806663000	-3 380129000
C	4 506572000	-2 162190000	-2 156754000
C	3 764483000	-2 039416000	-0 997125000
C	2 437709000	-1 571396000	-1 052897000
C	1 673987000	-2 259540000	1 123782000
C	2 176863000	-3 578103000	1 047577000
C	2 143994000	-4 404832000	2 152093000
C	1 596426000	-3 932879000	3 348272000
C	1 069382000	-2 655554000	3 355909000
ц	0 599613000	-2 242810000	4 248579000
н Ц	1 554157000	-4 544518000	4.248379000
ц	2 550879000	-3 947997000	9.240701000
п u	4 202408000	-3.947097000	-0.026221000
п	4.202408000	1 902020000	-0.020221000
п	4.408841000	-1.893930000	-4.321109000
п	2.101//0000	-0.945252000	-4.286303000
C	2.030001000	1 604706000	2 250120000
C	3.931896000	1.594795000	3.330130000
C	4.401951000	2.1485/0000	2.156085000
C	3.373407000	2.101/2/000	1 125240000
C	2.258435000	1.6/4238000	1.125348000
C	1.569606000	2.439097000	-1.051046000
C	2.034/19000	3.766904000	-0.994064000
C	2.158539000	4.509147000	-2.153443000
C	1.806328000	3.928233000	-3.3//444000
C	1.290019000	2.64/036000	-3.3/1103000
H	0.94/804000	2.163162000	-4.285253000
Н	1.894455000	4.4/0/01000	-4.318262000
Н	2.262823000	4.205041000	-0.022620000
H	3.944307000	2.560039000	0.099397000
Н	4.543596000	1.551416000	4.25054/000
H	2.244525000	0.59041/000	4.24/065000
С	-2.645/22000	1.289036000	-3.3/2828000
C	-3.926379000	1.806663000	-3.380129000
C	-4.5065/2000	2.162190000	-2.156/54000
С	-3.764483000	2.039416000	-0.997125000
С	-2.437709000	1.571396000	-1.052897000
С	-1.673987000	2.259540000	1.123782000
С	-2.176863000	3.578103000	1.047577000
С	-2.143994000	4.404832000	2.152093000
С	-1.596426000	3.932879000	3.348272000
С	-1.069382000	2.655554000	3.355909000
Η	-0.599613000	2.242810000	4.248579000
Η	-1.554157000	4.544518000	4.248701000
Η	-2.550879000	3.947897000	0.094272000
Η	-4.202408000	2.270147000	-0.026221000
Η	-4.468841000	1.893930000	-4.321109000
Η	-2.161770000	0.945232000	-4.286305000
Η	5.539037000	-2.512569000	-2.109438000
Η	2.525181000	-5.424961000	2.076221000
Η	-2.525181000	5.424961000	2.076221000
Η	-5.539037000	2.512569000	-2.109438000

H       -5.420627000       -2.534154000       2.081920000         Mo₂Mn(dpa)₄(NCS)₂ <sup>6</sup> A₁       E=-644.99 eV         S       0.00000000       0.00000000       -7.307665000         S       0.00000000       0.00000000       -7.550773000         C       0.00000000       0.00000000       -5.696951000         N       0.00000000       0.00000000       -4.496895000         N       0.00000000       0.00000000       -2.208579000         Mo       0.00000000       0.00000000       -2.005793000         Mo       0.00000000       0.00000000       -2.01952000         N       1.12746600       -1.910041000       -2.210962000         N       1.909425000       -1.128854000       -2.210962000         N       -1.633896000       -1.414820000       0.082662000         N       -1.633896000       -1.824773000       2.320326000         N       -1.835767000       -1.82173000       2.320326000         N       -1.82620000       -1.896342000       2.321332000         N       -1.82620000       -1.896342000       2.321326000         C       -2.20333900       -2.44355300       -2.14378000         C       -2.20333900	Н	2.507127000	5.542179000	-2.105307000
H       -2.507127000       -5.542179000       -2.105307000         H       5.420627000       2.534154000       2.081920000         Mo <sub>2</sub> Mn (dpa) (NCS) 2 <sup>6</sup> A1       E=-644.99       eV         S       0.00000000       0.00000000       -7.307665000         C       0.00000000       0.00000000       -5.696951000         C       0.00000000       0.00000000       -5.946073000         N       0.00000000       0.00000000       -4.496895000         Mo       0.00000000       0.00000000       -2.208579000         Mo       0.00000000       0.000000000       -2.210193000         N       -1.27466000       -1.91041000       -2.210962000         N       1.99425000       -1.128854000       -2.210193000         N       1.99425000       -1.414820000       0.082662000         N       1.43450000       -1.634773000       0.082061000         N       1.633896000       -1.414820000       2.321332000         N       1.855767000       -1.182173000       2.32326000         N       1.855767000       -1.89632000       2.32332000         N       1.855767000       -1.89043200       2.32332000        C       -2.3333900 <td>Н</td> <td>-5.420627000</td> <td>-2.534154000</td> <td>2.081920000</td>	Н	-5.420627000	-2.534154000	2.081920000
H       5.420627000       2.534154000       2.081920000         Mo₂Mn (dpa) 4 (NCS) 2 <sup>6</sup> A1       E=-644.99 eV         S       0.00000000       0.00000000       -7.307665000         S       0.00000000       0.00000000       -5.696951000         C       0.00000000       0.00000000       -4.496895000         N       0.00000000       0.00000000       -2.208579000         Mo       0.00000000       0.00000000       -2.208579000         Mo       0.00000000       0.00000000       -2.208579000         Mo       0.00000000       0.00000000       -2.208579000         Mo       0.00000000       0.00000000       -2.21092000         N       -1.909425000       -1.128854000       -2.21092000         N       -1.909425000       -1.414820000       0.082662000         N       -1.63389600       -1.414820000       0.082662000         N       -1.43450000       -1.634773000       0.82261000         N       -1.895767000       -1.896342000       2.321332000         N       -1.895767000       -1.896342000       2.321332000         N       -1.895767000       -1.896342000       2.32332000         N       -1.895779000<	Н	-2.507127000	-5.542179000	-2.105307000
Ho2Mn (dpa) (NCS) 2 <sup>6</sup> A1         E=-644.99 eV           S         0.00000000         0.00000000         -7.307665000           S         0.00000000         0.00000000         -5.696951000           C         0.00000000         0.00000000         -4.9685000           N         0.00000000         0.00000000         -4.9685000           N         0.00000000         0.00000000         -2.20857900           Mo         0.00000000         0.00000000         -2.210952000           N         -1.127466000         -1.910041000         -2.210952000           N         -1.909425000         -1.128854000         -2.210952000           N         -1.909425000         -1.128854000         -2.210952000           N         -1.633896000         -1.414820000         0.082662000           N         -1.633896000         -1.414820000         0.082662000           N         -1.863773000         0.082061000         0.82032000           N         -1.853767000         -1.82173000         2.32332000           N         -1.855767000         -1.82173000         2.32326000           N         -1.855767000         -2.82798000         -3.3207000           C         -2.07415000	Н	5.420627000	2.534154000	2.081920000
Mo2Mn (dpa) (NCS) 2         TA1         E=-644.99 eV           S         0.00000000         0.00000000         -7.307665000           S         0.00000000         0.00000000         -5.69650100           C         0.00000000         0.00000000         -5.696591000           N         0.00000000         0.00000000         -4.496895000           N         0.00000000         0.00000000         -4.496895000           Mo         0.00000000         0.00000000         -2.208579000           Mo         0.00000000         0.00000000         -2.210962000           N         -1.127466000         -1.910041000         -2.210962000           N         -1.909425000         -1.128854000         -2.210193000           N         -1.633896000         -1.414820000         0.082662000           N         -1.413450000         -1.634773000         0.082661000           N         1.413450000         -1.82173000         2.32132000           N         1.4182620000         -1.896342000         2.321332000           N         1.4182620000         -1.825300         -2.201332000           N         -1.41345000         -2.42739800         -3.342977000           C         -2.20333900			6	
S         0.00000000         0.00000000         -7.307665000           S         0.00000000         0.00000000         -5.696951000           C         0.00000000         0.00000000         -4.496895000           N         0.00000000         0.00000000         -4.495895000           N         0.00000000         0.00000000         -2.20879000           Mo         0.00000000         0.00000000         -2.20879000           Mn         0.00000000         0.00000000         -2.20879000           Mn         0.00000000         0.00000000         -2.201952000           N         -1.127466000         1.128854000         -2.210193000           N         -1.633896000         -1.414820000         0.082662000           N         -1.63389600         -1.414820000         0.082662000           N         -1.895767000         -1.182173000         2.32132000           N         -1.895767000         -1.82173000         2.321322000           N         -1.82620000         -1.896342000         2.321322000           N         -1.8262000         -1.896342000         2.321322000           N         -1.826000         -3.72399000         -3.34297000           C         -2.741	Mo <sub>2</sub> Mn	$(dpa)_4$ (NCS) <sub>2</sub>	<sup>°</sup> A <sub>1</sub> E=-644.99 eV	
S         0.00000000         0.00000000         7.550773000           C         0.00000000         0.00000000         -5.696951000           N         0.00000000         0.00000000         -4.496895000           N         0.00000000         0.00000000         -2.208579000           Mo         0.00000000         0.00000000         -2.208579000           N         -1.909425000         -1.128854000         -2.210193000           N         1.909425000         -1.418854000         -2.210962000           N         -1.633896000         -1.414820000         0.082662000           N         -1.633896000         -1.414820000         0.082662000           N         -1.82620000         -1.824773000         0.82061000           N         -1.82620000         -1.8634773000         -2.32326000           N         -1.82620000         -1.86342000         -3.360670000           C         <	S	0.00000000	0.00000000	-7.307665000
C         0.00000000         0.00000000         -5.696951000           C         0.00000000         0.00000000         -4.496895000           N         0.00000000         0.00000000         -2.208579000           Mo         0.00000000         0.00000000         -2.208579000           Mo         0.00000000         0.00000000         -2.210952000           Mn         0.00000000         1.128854000         -2.210952000           N         -1.909425000         1.128854000         -2.210962000           N         1.909425000         1.418854000         -2.210962000           N         1.909425000         1.418854000         -2.210962000           N         1.4335000         1.634773000         0.082662000           N         1.413450000         1.634773000         0.082661000           N         1.413450000         1.82173000         2.320326000           N         1.413450000         1.82173000         2.32132000           N         1.895767000         1.82173000         2.322326000           N         1.895767000         1.82173000         2.322326000           C         -2.20339000         -4.486571000         -2.34607000          C         -2.32423000	S	0.00000000	0.00000000	7.550773000
C         0.00000000         0.0000000         -446073000           N         0.0000000         0.0000000         -4.49685000           N         0.0000000         0.0000000         -2.208579000           Mo         0.0000000         0.0000000         -2.208579000           Mn         0.0000000         0.0000000         -2.210962000           N         -1.127466000         -1.910041000         -2.210193000           N         -1.909425000         -1.128854000         -2.210193000           N         -1.633896000         1.41482000         0.082662000           N         -1.633896000         -1.41482000         0.082061000           N         -1.43450000         -1.634773000         0.082061000           N         -1.4895767000         -1.896342000         2.32132000           N         -1.182620000         -1.896342000         2.321322000           N         -1.895767000         -1.896342000         2.321322000           N         -1.826279800         -3.342907000         C           C         -2.20339000         -2.44279800         -3.342907000           C         -2.210339000         -2.435355000         -1.026121000          C         -2.57439900	С	0.00000000	0.00000000	-5.696951000
N         0.00000000         0.00000000         -4.496895000           N         0.00000000         0.00000000         4.746522000           Mo         0.00000000         0.00000000         -2.2857900           Mn         0.00000000         0.00000000         2.210962000           N         -1.127466000         -1.91041000         -2.210962000           N         1.909425000         -1.128854000         -2.210193000           N         1.909425000         -1.128854000         -2.210962000           N         1.909425000         -1.128854000         -2.210962000           N         1.413450000         -1.634773000         0.082662000           N         -1.633896000         -1.414820000         0.082662000           N         1.43450000         -1.634773000         0.082061000           N         1.895767000         -1.896342000         2.321322000           N         1.182620000         -1.896342000         2.321322000           N         1.895767000         -1.896342000         2.321322000           N         1.895767000         -2.14373000         -2.31232000           C         -2.203339000         -4.46571000         -2.1437478000           C	С	0.00000000	0.00000000	5.946073000
N         0.00000000         0.00000000         4.746522000           Mo         0.00000000         0.00000000         -2.208579000           Mo         0.00000000         0.00000000         -2.2108579000           Mn         0.1127466000         -1.910041000         -2.210962000           N         -1.127466000         -1.128854000         -2.210193000           N         1.127466000         1.128854000         -2.210962000           N         1.127466000         1.414820000         0.082662000           N         -1.413450000         -1.634773000         0.082662000           N         -1.413450000         -1.634773000         0.082662000           N         -1.485767000         -1.82173000         2.320326000           N         -1.82620000         -1.895342000         2.321322000           N         -1.82620000         -3.89842000         2.321322000           N         -1.82620000         -3.9988400         -3.342907000           C         -2.20333900         -4.486571000         -2.143478000           C         -2.20333900         -2.43535500         -1.026121000           C         -2.312242000         -1.685314000         -1.26352000           C <td>Ν</td> <td>0.00000000</td> <td>0.00000000</td> <td>-4.496895000</td>	Ν	0.00000000	0.00000000	-4.496895000
Mo         0.00000000         0.00000000         -2.208579000           Mn         0.0000000         0.0000000         -0.47122000           Mn         0.0000000         0.0000000         2.745753000           N         -1.127466000         -1.910041000         -2.210962000           N         -1.909425000         1.128854000         -2.210193000           N         1.127466000         1.910041000         -2.210962000           N         -1.633896000         1.414820000         0.082662000           N         -1.633896000         -1.414820000         0.082662000           N         -1.43450000         -1.634773000         0.082061000           N         -1.432620000         -1.896342000         2.321322000           N         -1.182620000         -1.896342000         2.321322000           N         -1.182620000         -3.342907000         2.321322000           N         -1.82620000         -2.642798000         -3.342907000           C         -2.07415000         -3.75239900         -2.143478000           C         -2.07415000         -3.75239900         -0.98822000           C         -3.64805000         -2.121299000         0.975951000           C	Ν	0.00000000	0.00000000	4.746522000
Mo0.000000000.00000000-0.047122000Mn0.000000000.000000002.745753000N-1.127466000-1.910041000-2.210193000N1.909425000-1.128854000-2.210193000N1.909425000-1.128854000-2.210193000N1.1274660001.910041000-2.210962000N-1.633896000-1.4148200000.082662000N-1.633896000-1.4148200000.082662000N1.6339567000-1.842730002.320326000N1.182620000-1.8963420002.32132000N1.8957670001.1821730002.320326000N1.895767000-2.64279800-3.342907000C-2.203339000-4.486571000-3.36067000C-2.074150000-3.75239900-0.980832000C-1.574893000-2.121990000.975951000C-3.648050000-2.121290000.975951000C-4.507812000-2.164660000-4.251420000C-4.51433000-1.6410900003.293599000C-2.751225000-1.1723920003.61541000H-0.90927000-2.164660000-4.251420000H-4.691120000-2.12458000-3.46824000H-2.351759000-0.7610990004.289975000C2.641393000-1.274580000-3.34237000C2.641393000-2.12452000-3.34237000C2.641393000-2.1446562000-0.015724000C3.97978000 </td <td>Мо</td> <td>0.00000000</td> <td>0.00000000</td> <td>-2.208579000</td>	Мо	0.00000000	0.00000000	-2.208579000
Mn0.000000000.000000002.745753000N-1.127466000-1.910041000-2.210962000N1.9094250001.128854000-2.210193000N1.1274660001.910041000-2.210962000N-1.6338960001.4148200000.082662000N-1.633896000-1.4148200000.082662000N-1.633896000-1.4148200000.082662000N1.41345000-1.6347730002.320326000N1.41345000-1.8963420002.32132000N-1.182620000-1.8963420002.32132000N1.8957670001.1821730002.320326000C-1.272165000-2.642798000-3.34290700C-1.820179000-3.99884000-3.360670000C-2.074150000-3.752399000-0.980832000C-2.074150000-2.1212990000.975951000C-2.31242000-1.6653140001.126352000C-3.64805000-2.1049260002.056723000C-4.507812000-2.164660000-4.251420000H-0.909297000-2.164660000-4.251420000H-2.32768000-4.48554000-0.013724000H-2.351759000-1.6710820004.289975000C2.64133000-1.27458000-3.342372000C2.43407000-1.5776000004.289975000C2.641393000-2.210427000-2.144054000C2.434047000-1.577600000-3.942372000C2.4353540000	Мо	0.00000000	0.00000000	-0.047122000
N         -1.127466000         -1.910041000         -2.210962000           N         -1.909425000         -1.128854000         -2.210193000           N         1.909425000         -1.128854000         -2.210193000           N         -1.633896000         1.414820000         -2.210962000           N         -1.633896000         -1.634773000         0.082662000           N         -1.633896000         -1.634773000         0.082662000           N         -1.413450000         -1.634773000         0.082661000           N         -1.895767000         -1.182173000         2.320326000           N         -1.182620000         -1.896342000         2.32132000           N         -1.82620000         -2.642798000         -3.342907000           C         -1.272165000         -2.642798000         -3.342907000           C         -2.03399000         -4.485571000         -2.143478000           C         -2.074150000         -3.752399000         -0.980832000           C         -3.648050000         -2.12129900         0.975951000           C         -3.64805000         -2.104926000         2.956723000           C         -4.507812000         -2.164660000         -4.251420000	Mn	0.00000000	0.00000000	2.745753000
N         -1.909425000         1.128854000         -2.210193000           N         1.909425000         -1.128854000         -2.210193000           N         1.127466000         1.910041000         -2.210962000           N         -1.633896000         1.414820000         0.082662000           N         -1.633896000         -1.414820000         0.082662000           N         1.633896000         -1.414820000         0.082662000           N         1.633896000         -1.414820000         0.082662000           N         1.43450000         -1.634773000         2.320326000           N         1.895767000         -1.820173000         2.321332000           N         -1.820179000         -3.909884000         -3.360670000           C         -1.272165000         -2.642798000         -3.342907000           C         -2.074150000         -2.752399000         -0.980832000           C         -2.074150000         -2.143478000         C.26121000           C         -2.312242000         -1.685314000         1.126352000           C         -3.648050000         -2.114299000         3.93599000           C         -4.057812000         -2.164660000         -4.251420000	Ν	-1.127466000	-1.910041000	-2.210962000
N         1.909425000         -1.128854000         -2.210193000           N         1.127466000         1.910041000         -2.210962000           N         -1.633896000         1.414820000         0.082662000           N         -1.413450000         -1.634773000         0.082662000           N         1.413450000         1.634773000         0.082662000           N         1.413450000         1.634773000         0.082662000           N         1.413450000         1.634773000         2.320326000           N         -1.182620000         1.896342000         2.321332000           N         -1.182620000         1.896342000         2.321332000           N         1.895767000         1.182173000         2.320326000           C         -1.272165000         -2.642798000         -3.342907000           C         -2.074150000         -3.75239900         -0.980832000           C         -2.07415000         -3.75239900         -0.980832000           C         -2.312242000         -1.685314000         1.12652000           C         -3.648050000         -2.104926000         2.056723000           C         -2.751225000         -1.172392000         3.361541000           H <td>Ν</td> <td>-1.909425000</td> <td>1.128854000</td> <td>-2.210193000</td>	Ν	-1.909425000	1.128854000	-2.210193000
N         1.127466000         1.910041000         -2.210962000           N         -1.633896000         1.414820000         0.082662000           N         -1.413450000         -1.634773000         0.082662000           N         1.633896000         -1.414820000         0.082662000           N         1.633896000         -1.414820000         0.082662000           N         1.413450000         1.634773000         2.320326000           N         -1.182620000         -1.896342000         2.321332000           N         -1.182620000         -1.896342000         2.320326000           C         -1.272165000         -2.642798000         -3.342907000           C         -2.20339000         -4.48571000         -2.143478000           C         -2.074150000         -3.752399000         -0.980832000           C         -2.312242000         -1.685314000         1.126352000           C         -3.648050000         -2.121299000         0.975951000           C         -2.751225000         -1.172392000         3.361541000           H         -0.909297000         -2.164660000         -4.251420000           H         -4.051433000         -1.617082000         4.251420000	Ν	1.909425000	-1.128854000	-2.210193000
N         -1.633896000         1.414820000         0.082662000           N         -1.413450000         -1.634773000         0.082061000           N         1.633896000         -1.414820000         0.082662000           N         1.413450000         -1.634773000         0.082061000           N         1.413450000         -1.414820000         2.320326000           N         -1.895767000         -1.896342000         2.321332000           N         -1.895767000         1.182173000         2.320326000           C         -1.27165000         -2.642798000         -3.342907000           C         -1.820179000         -3.999884000         -3.360670000           C         -2.074150000         -3.752399000         -0.980832000           C         -2.074150000         -3.752399000         -0.980832000           C         -3.648050000         -2.121299000         0.975951000           C         -3.648050000         -2.104926000         2.056723000           C         -2.751225000         -1.172392000         3.361541000           H         -0.909297000         -2.164660000         -4.251420000           H         -1.909865000         -4.446562000         -4.304824000	Ν	1.127466000	1.910041000	-2.210962000
N         -1.413450000         -1.634773000         0.082061000           N         1.633896000         -1.414820000         0.082662000           N         1.413450000         1.634773000         0.082662000           N         -1.4395767000         -1.182173000         2.320326000           N         -1.895767000         -1.896342000         2.321332000           N         -1.82620000         1.896342000         2.32132000           N         1.895767000         1.182173000         2.320326000           C         -1.272165000         -2.642798000         -3.342907000           C         -2.03339000         -4.486571000         -2.143478000           C         -2.074150000         -3.752399000         -0.980832000           C         -2.312242000         -1.685314000         1.126352000           C         -3.648050000         -2.104926000         2.056723000           C         -4.051433000         -1.64109000         3.2959000           C         -2.751225000         -1.172392000         3.361541000           H         -0.909297000         -2.164660000         -4.251420000           H         -1.909865000         -4.48510000         -0.013724000 <t< td=""><td>Ν</td><td>-1.633896000</td><td>1.414820000</td><td>0.082662000</td></t<>	Ν	-1.633896000	1.414820000	0.082662000
N         1.633896000         -1.414820000         0.082662000           N         1.413450000         1.634773000         0.082061000           N         -1.895767000         -1.182173000         2.320326000           N         1.182620000         -1.896342000         2.321332000           N         -1.182620000         1.896342000         2.321332000           N         1.895767000         1.182173000         2.320326000           C         -1.272165000         -2.642798000         -3.342907000           C         -1.820179000         -3.909884000         -3.360670000           C         -2.03339000         -4.48571000         -2.143478000           C         -2.074150000         -3.752399000         -0.980832000           C         -2.312242000         -1.685314000         1.126352000           C         -3.64805000         -2.104926000         2.0575951000           C         -4.507812000         -2.164660000         -4.304824000           H         -0.909297000         -2.164660000         -4.304824000           H         -0.909297000         -2.16436000         -0.013724000           H         -2.327680000         -2.43554000         -3.342372000	Ν	-1,413450000	-1.634773000	0.082061000
N         1.413450000         1.634773000         0.082061000           N         -1.895767000         -1.182173000         2.320326000           N         1.182620000         -1.896342000         2.321332000           N         -1.182620000         1.896342000         2.320326000           N         -1.18262000         1.896342000         2.320326000           N         -1.895767000         1.182173000         2.320326000           C         -1.272165000         -2.642798000         -3.342907000           C         -1.820179000         -3.909884000         -3.360670000           C         -2.074150000         -3.752399000         -0.980832000           C         -2.312242000         -1.685314000         1.126352000           C         -3.648050000         -2.121299000         0.975951000           C         -4.507812000         -2.164660000         -4.25142000           H         -0.909297000         -2.164660000         -4.25142000           H         -0.909297000         -2.164660000         -4.25142000           H         -2.327680000         -4.186100000         -0.01372400           H         -2.351759000         -2.616099000         -3.342372000	N	1.633896000	-1.414820000	0.082662000
N         -1.895767000         -1.182173000         2.320326000           N         1.182620000         -1.896342000         2.321332000           N         -1.182620000         1.896342000         2.321332000           N         1.895767000         1.182173000         2.320326000           C         -1.272165000         -2.642798000         -3.342907000           C         -1.820179000         -3.909884000         -3.360670000           C         -2.203339000         -4.486571000         -2.143478000           C         -2.074150000         -3.752399000         -0.980832000           C         -2.312242000         -1.685314000         1.126352000           C         -3.648050000         -2.104926000         2.056723000           C         -4.507812000         -2.104926000         2.056723000           C         -4.51433000         -1.641090000         3.293509000           C         -2.751225000         -1.172392000         3.361541000           H         -0.909297000         -2.164660000         -4.25142000           H         -1.909865000         -4.46562000         -4.304824000           H         -2.327680000         -1.617082000         4.175093000	Ν	1.413450000	1.634773000	0.082061000
N         1.182620000         -1.896342000         2.321332000           N         -1.182620000         1.896342000         2.321332000           N         1.895767000         1.182173000         2.320326000           C         -1.272165000         -2.642798000         -3.342907000           C         -1.820179000         -3.909884000         -3.360670000           C         -2.03339000         -4.486571000         -2.143478000           C         -2.074150000         -3.752399000         -0.980832000           C         -2.312242000         -1.685314000         1.126352000           C         -3.648050000         -2.104926000         2.056723000           C         -4.051433000         -1.641090000         3.293509000           C         -2.751225000         -1.172392000         3.361541000           H         -0.909297000         -2.164660000         -4.251420000           H         -1.909865000         -4.446562000         -4.304824000           H         -2.351759000         -0.761009000         4.289975000           C         2.641393000         -1.274580000         -3.342372000           C         2.641393000         -1.274580000         -3.360842000	N	-1.895767000	-1.182173000	2.320326000
N         -1.182620000         1.896342000         2.321332000           N         1.895767000         1.182173000         2.320326000           C         -1.272165000         -2.642798000         -3.342907000           C         -1.820179000         -3.909884000         -3.360670000           C         -2.203339000         -4.486571000         -2.143478000           C         -2.074150000         -3.752399000         -0.980832000           C         -2.312242000         -1.685314000         1.126352000           C         -3.648050000         -2.104926000         2.056723000           C         -4.507812000         -2.104926000         2.056723000           C         -4.051433000         -1.641090000         3.293509000           C         -2.751225000         -1.172392000         3.361541000           H         -0.909297000         -2.164660000         -4.25142000           H         -1.909865000         -4.48562000         -4.304824000           H         -2.327680000         -4.186100000         -0.013724000           H         -4.691120000         -1.61708200         4.175093000           C         2.641393000         -1.274580000         -3.342372000	N	1.182620000	-1.896342000	2.321332000
N         1.895767000         1.182173000         2.320326000           C         -1.272165000         -2.642798000         -3.342907000           C         -1.820179000         -3.909884000         -3.360670000           C         -2.203339000         -4.486571000         -2.143478000           C         -2.074150000         -3.752399000         -0.980832000           C         -2.312242000         -1.685314000         1.126352000           C         -3.648050000         -2.114926000         2.056723000           C         -4.507812000         -2.104926000         2.056723000           C         -4.507812000         -2.164660000         -4.25142000           H         -0.909297000         -2.164660000         -4.25142000           H         -0.909297000         -2.435354000         -0.013724000           H         -2.327680000         -4.186100000         -0.013724000           H         -2.351759000         -0.761009000         4.289975000           C         2.641393000         -1.27458000         -3.342372000           C         2.641393000         -1.27458000         -3.360842000           C         3.907300000         -2.079902000         -0.981059000	N	-1.182620000	1.896342000	2.321332000
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N	1.895767000	1.182173000	2.320326000
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С	-1.272165000	-2.642798000	-3.342907000
C-2.20339000-4.486571000-2.143478000C-2.074150000-3.752399000-0.980832000C-1.574893000-2.435355000-1.026121000C-2.312242000-1.6853140001.126352000C-3.648050000-2.1212990000.975951000C-4.507812000-2.1049260002.056723000C-4.051433000-1.6410900003.293509000C-2.751225000-1.1723920003.361541000H-0.909297000-2.164660000-4.251420000H-1.909865000-4.48656200-4.304824000H-2.327680000-4.186100000-0.013724000H-4.691120000-1.6170820004.175093000H-2.351759000-0.7610090004.289975000C2.641393000-1.274580000-3.360842000C3.907300000-1.825211000-3.360842000C3.749973000-2.3140630001.1225603000C2.16142000-3.6506380000.975876000C2.162176000-4.5093700002.057351000C1.642778000-4.5093700002.057351000C1.642778000-4.5093700003.363169000H0.765434000-2.3504270004.292125000H1.621146000-4.6901500004.177200000H2.424801000-4.06377000-0.006282000H4.183435000-2.334915000-0.014289000	С	-1.820179000	-3.909884000	-3.360670000
C-2.074150000-3.752399000-0.980832000C-1.574893000-2.435355000-1.026121000C-2.312242000-1.6853140001.126352000C-3.648050000-2.1212990000.975951000C-4.507812000-2.1049260002.056723000C-4.507812000-1.6410900003.293509000C-4.051433000-1.6410900003.293509000C-2.751225000-1.1723920003.361541000H-0.909297000-2.164660000-4.251420000H-1.909865000-4.446562000-4.304824000H-2.327680000-4.186100000-0.013724000H-4.691120000-1.6170820004.175093000H-4.691120000-1.825211000-3.360842000C2.641393000-1.274580000-3.360842000C2.641393000-2.210427000-2.144054000C3.749973000-2.079902000-0.981059000C2.1682945000-2.3140630001.1226633000C2.16142000-3.6506380000.975876000C2.162176000-4.5093700002.057351000C2.1642778000-4.0513220003.295020000C1.1642778000-2.3504270004.292125000H1.621146000-4.6901500004.17720000H2.424801000-4.06377000-0.014289000	C	-2.203339000	-4.486571000	-2.143478000
C-1.574893000-2.435355000-1.026121000C-2.312242000-1.6853140001.126352000C-3.648050000-2.1212990000.975951000C-4.507812000-2.1049260002.056723000C-4.051433000-1.6410900003.293509000C-2.751225000-1.1723920003.361541000H-0.909297000-2.164660000-4.251420000H-1.909865000-4.446562000-4.304824000H-2.327680000-4.186100000-0.013724000H-4.691120000-1.6170820004.175093000H-2.351759000-0.7610090004.289975000C2.641393000-1.274580000-3.360842000C3.907300000-1.577600000-1.025603000C2.434047000-1.57760000-1.025603000C2.102176000-4.509370002.314063000C2.102176000-4.509370002.057351000C2.102176000-4.509370002.057351000C1.642778000-4.051322003.295020000C1.174681000-2.3504270004.292125000H0.765434000-2.3504270004.292125000H1.621146000-4.6901500004.177200000H2.424801000-4.06377000-0.014289000	C	-2 074150000	-3.752399000	-0.980832000
C         -2.312242000         -1.685314000         1.126352000           C         -3.648050000         -2.121299000         0.975951000           C         -4.507812000         -2.104926000         2.056723000           C         -4.051433000         -1.641090000         3.293509000           C         -2.751225000         -1.172392000         3.361541000           H         -0.909297000         -2.164660000         -4.251420000           H         -1.909865000         -4.446562000         -4.304824000           H         -2.327680000         -4.186100000         -0.013724000           H         -4.691120000         -1.617082000         4.175093000           H         -4.691120000         -1.825211000         -3.342372000           C         2.641393000         -1.274580000         -3.342372000           C         3.907300000         -2.210427000         -2.144054000           C         3.90730000         -2.314063000         1.126691000           C         2.434047000         -1.577600000         -1.025603000           C         2.16142000         -3.650638000         0.975876000           C         2.102176000         -4.509370000         2.057351000	C	-1.574893000	-2.435355000	-1.026121000
C       -3.648050000       -2.121299000       0.975951000         C       -4.507812000       -2.104926000       2.056723000         C       -4.051433000       -1.641090000       3.293509000         C       -2.751225000       -1.172392000       3.361541000         H       -0.909297000       -2.164660000       -4.251420000         H       -1.909865000       -4.446562000       -4.304824000         H       -2.327680000       -4.186100000       -0.013724000         H       -4.002639000       -2.433540000       -0.005530000         H       -4.691120000       -1.617082000       4.175093000         C       2.641393000       -1.274580000       -3.342372000         C       3.907300000       -1.825211000       -3.360842000         C       3.749973000       -2.079902000       -0.981059000         C       2.434047000       -1.577600000       -1.025603000         C       2.164278000       -2.314063000       1.126691000         C       2.1642778000       -4.051322000       3.295020000         C       1.642778000       -4.051322000       3.295020000         C       1.174681000       -2.350427000       4.292125000	С	-2.312242000	-1.685314000	1.126352000
C-4.507812000-2.1049260002.056723000C-4.051433000-1.6410900003.293509000C-2.751225000-1.1723920003.361541000H-0.909297000-2.164660000-4.251420000H-1.909865000-4.446562000-4.304824000H-2.327680000-4.186100000-0.013724000H-4.691120000-1.6170820004.175093000H-4.691120000-1.6170820004.289975000C2.641393000-1.274580000-3.342372000C2.641393000-1.274580000-3.360842000C3.907300000-1.825211000-3.360842000C3.749973000-2.079902000-0.981059000C2.116142000-3.6506380000.975876000C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.363169000H0.765434000-2.3504270004.292125000H1.621146000-4.6901500004.177200000H2.424801000-4.06377000-0.006282000H4.183435000-2.334915000-0.014289000	C	-3.648050000	-2.121299000	0.975951000
C-4.051433000-1.6410900003.293509000C-2.751225000-1.1723920003.361541000H-0.909297000-2.164660000-4.251420000H-1.909865000-4.446562000-4.304824000H-2.327680000-4.186100000-0.013724000H-4.002639000-2.433540000-0.005530000H-4.691120000-1.6170820004.175093000C2.641393000-1.274580000-3.342372000C3.907300000-1.825211000-3.360842000C3.749973000-2.079902000-0.981059000C2.434047000-1.5776000001.126691000C2.16142000-3.6506380000.975876000C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.363169000H0.765434000-2.3504270004.292125000H1.621146000-4.6901500004.177200000H2.424801000-4.006377000-0.014289000	C	-4.507812000	-2.104926000	2.056723000
C-2.751225000-1.1723920003.361541000H-0.909297000-2.164660000-4.251420000H-1.909865000-4.446562000-4.304824000H-2.327680000-4.186100000-0.013724000H-4.002639000-2.433540000-0.005530000H-4.691120000-1.6170820004.175093000C2.641393000-1.274580000-3.342372000C3.907300000-1.274580000-3.360842000C3.749973000-2.210427000-2.144054000C3.749973000-2.3140630001.126691000C2.16142000-3.6506380000.975876000C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.295020000C1.174681000-2.3504270004.292125000H0.765434000-2.3504270004.292125000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	C	-4.051433000	-1.641090000	3.293509000
H-0.909297000-2.164660000-4.251420000H-1.909865000-4.446562000-4.304824000H-2.327680000-4.186100000-0.013724000H-4.002639000-2.433540000-0.005530000H-4.691120000-1.6170820004.175093000H-2.351759000-0.7610090004.289975000C2.641393000-1.274580000-3.342372000C3.907300000-1.825211000-3.360842000C4.483372000-2.079902000-0.981059000C2.434047000-1.5776000001.025603000C2.102176000-4.5093700002.057351000C2.102176000-4.0513220003.295020000C1.642778000-4.0513220003.363169000H0.765434000-2.3504270004.292125000H1.621146000-4.6901500004.177200000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	C	-2.751225000	-1.172392000	3.361541000
H-1.909865000-4.446562000-4.304824000H-2.327680000-4.186100000-0.013724000H-4.002639000-2.433540000-0.005530000H-4.691120000-1.6170820004.175093000H-2.351759000-0.7610090004.289975000C2.641393000-1.274580000-3.342372000C3.907300000-1.825211000-3.360842000C4.483372000-2.210427000-2.144054000C3.749973000-2.079902000-0.981059000C2.434047000-1.5776000001.025603000C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.295020000C1.642778000-4.0513220003.363169000H0.765434000-2.3504270004.292125000H1.621146000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	H	-0.909297000	-2.164660000	-4.251420000
H-2.327680000-4.186100000-0.013724000H-4.002639000-2.433540000-0.005530000H-4.691120000-1.6170820004.175093000H-2.351759000-0.7610090004.289975000C2.641393000-1.274580000-3.342372000C3.907300000-1.825211000-3.360842000C4.483372000-2.210427000-2.144054000C3.749973000-2.079902000-0.981059000C2.434047000-1.5776000001.025603000C2.1682945000-2.3140630001.126691000C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.363169000H0.765434000-2.3504270004.292125000H1.621146000-4.6901500004.177200000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	H	-1.909865000	-4.446562000	-4.304824000
H-4.002639000-2.433540000-0.005530000H-4.691120000-1.6170820004.175093000H-2.351759000-0.7610090004.289975000C2.641393000-1.274580000-3.342372000C3.907300000-1.825211000-3.360842000C4.483372000-2.210427000-2.144054000C3.749973000-2.079902000-0.981059000C2.434047000-1.577600000-1.025603000C2.16142000-3.6506380000.975876000C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.295020000C1.174681000-2.3504270004.292125000H0.765434000-2.3504270004.177200000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	Н	-2.327680000	-4.186100000	-0.013724000
H-4.691120000-1.6170820004.175093000H-2.351759000-0.7610090004.289975000C2.641393000-1.274580000-3.342372000C3.907300000-1.825211000-3.360842000C4.483372000-2.210427000-2.144054000C3.749973000-2.079902000-0.981059000C2.434047000-1.577600000-1.025603000C1.682945000-2.3140630001.126691000C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.295020000C1.174681000-2.3504270004.292125000H1.621146000-4.6901500004.177200000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	Н	-4.002639000	-2.433540000	-0.005530000
H-2.351759000-0.7610090004.289975000C2.641393000-1.274580000-3.342372000C3.907300000-1.825211000-3.360842000C4.483372000-2.210427000-2.144054000C3.749973000-2.079902000-0.981059000C2.434047000-1.577600000-1.025603000C1.682945000-2.3140630001.126691000C2.116142000-3.6506380000.975876000C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.295020000C1.174681000-2.7508340003.363169000H0.765434000-2.3504270004.192125000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	Н	-4.691120000	-1.617082000	4.175093000
C2.641393000-1.274580000-3.342372000C3.907300000-1.825211000-3.360842000C4.483372000-2.210427000-2.144054000C3.749973000-2.079902000-0.981059000C2.434047000-1.577600000-1.025603000C1.682945000-2.3140630001.126691000C2.116142000-3.6506380000.975876000C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.295020000C1.174681000-2.7508340003.363169000H1.621146000-4.6901500004.177200000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	Н	-2.351759000	-0.761009000	4.289975000
C3.907300000-1.825211000-3.360842000C4.483372000-2.210427000-2.144054000C3.749973000-2.079902000-0.981059000C2.434047000-1.577600000-1.025603000C1.682945000-2.3140630001.126691000C2.116142000-3.6506380000.975876000C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.295020000C1.174681000-2.7508340003.363169000H0.765434000-4.6901500004.177200000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	С	2.641393000	-1.274580000	-3.342372000
C4.483372000-2.210427000-2.144054000C3.749973000-2.079902000-0.981059000C2.434047000-1.577600000-1.025603000C1.682945000-2.3140630001.126691000C2.116142000-3.6506380000.975876000C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.295020000C1.174681000-2.7508340003.363169000H0.765434000-2.3504270004.177200000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	С	3.907300000	-1.825211000	-3.360842000
C3.749973000-2.079902000-0.981059000C2.434047000-1.577600000-1.025603000C1.682945000-2.3140630001.126691000C2.116142000-3.6506380000.975876000C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.295020000C1.174681000-2.7508340003.363169000H0.765434000-2.3504270004.292125000H1.621146000-4.0901500004.177200000H2.424801000-2.334915000-0.014289000	С	4.483372000	-2.210427000	-2.144054000
C2.434047000-1.577600000-1.025603000C1.682945000-2.3140630001.126691000C2.116142000-3.6506380000.975876000C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.295020000C1.174681000-2.7508340003.363169000H0.765434000-2.3504270004.292125000H1.621146000-4.6901500004.177200000H2.424801000-2.334915000-0.014289000	С	3.749973000	-2.079902000	-0.981059000
C1.682945000-2.3140630001.126691000C2.116142000-3.6506380000.975876000C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.295020000C1.174681000-2.7508340003.363169000H0.765434000-2.3504270004.292125000H1.621146000-4.6901500004.177200000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	С	2.434047000	-1.577600000	-1.025603000
C2.116142000-3.6506380000.975876000C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.295020000C1.174681000-2.7508340003.363169000H0.765434000-2.3504270004.292125000H1.621146000-4.6901500004.177200000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	С	1.682945000	-2.314063000	1.126691000
C2.102176000-4.5093700002.057351000C1.642778000-4.0513220003.295020000C1.174681000-2.7508340003.363169000H0.765434000-2.3504270004.292125000H1.621146000-4.6901500004.177200000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	С	2.116142000	-3.650638000	0.975876000
C1.642778000-4.0513220003.295020000C1.174681000-2.7508340003.363169000H0.765434000-2.3504270004.292125000H1.621146000-4.6901500004.177200000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	С	2.102176000	-4.509370000	2.057351000
C1.174681000-2.7508340003.363169000H0.765434000-2.3504270004.292125000H1.621146000-4.6901500004.177200000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	С	1.642778000	-4.051322000	3.295020000
H0.765434000-2.3504270004.292125000H1.621146000-4.6901500004.177200000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	С	1.174681000	-2.750834000	3.363169000
H1.621146000-4.6901500004.177200000H2.424801000-4.006377000-0.006282000H4.183435000-2.334915000-0.014289000	Н	0.765434000	-2.350427000	4.292125000
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Н	4.443382000	-1.915612000	-4.305105000
Н	2.163716000	-0.910180000	-4.250421000
С	2.751225000	1.172392000	3.361541000
С	4.051433000	1.641090000	3.293509000
С	4.507812000	2.104926000	2.056723000
С	3.648050000	2.121299000	0.975951000
С	2.312242000	1.685314000	1.126352000
С	1.574893000	2.435355000	-1.026121000
С	2.074150000	3.752399000	-0.980832000
С	2.203339000	4.486571000	-2.143478000
С	1.820179000	3.909884000	-3.360670000
С	1.272165000	2.642798000	-3.342907000
Н	0.909297000	2.164660000	-4.251420000
Н	1.909865000	4.446562000	-4.304824000
Н	2.327680000	4.186100000	-0.013724000
Н	4.002639000	2.433540000	-0.005530000
Н	4.691120000	1.617082000	4.175093000
Н	2.351759000	0.761009000	4.289975000
С	-2.641393000	1.274580000	-3.342372000
С	-3.907300000	1.825211000	-3.360842000
С	-4.483372000	2.210427000	-2.144054000
С	-3.749973000	2.079902000	-0.981059000
С	-2.434047000	1.577600000	-1.025603000
С	-1.682945000	2.314063000	1.126691000
С	-2.116142000	3.650638000	0.975876000
С	-2.102176000	4.509370000	2.057351000
С	-1.642778000	4.051322000	3.295020000
С	-1.174681000	2.750834000	3.363169000
Н	-0.765434000	2.350427000	4.292125000
Н	-1.621146000	4.690150000	4.177200000
Н	-2.424801000	4.006377000	-0.006282000
Н	-4.183435000	2.334915000	-0.014289000
Н	-4.443382000	1.915612000	-4.305105000
Н	-2.163716000	0.910180000	-4.250421000
Н	5.506131000	-2.589258000	-2.105617000
Н	2.429673000	-5.543205000	1.931584000
Н	-2.429673000	5.543205000	1.931584000
Н	-5.506131000	2.589258000	-2.105617000
Н	2.579547000	5.510277000	-2.104586000
Н	-5.541172000	-2.433932000	1.931015000
Н	-2.579547000	-5.510277000	-2.104586000
Н	5.541172000	2.433932000	1.931015000

## $Mo_2Co(dpa)_4(NCS)_2$

### $^{4}E$ E=-642.72 eV

S	0.000000000	0.00000000	-7.279164000
S	0.000000000	0.00000000	7.279576000
С	0.000000000	0.00000000	-5.670278000
С	0.000000000	0.00000000	5.668976000
N	0.000000000	0.00000000	-4.470100000
N	0.000000000	0.00000000	4.472429000
Mo	0.000000000	0.00000000	-2.228237000
Мо	0.000000000	0.00000000	-0.060879000
Со	0.000000000	0.00000000	2.528276000
N	-1.120801000	-1.916444000	-2.215646000
N	-1.926129000	1.101225000	-2.220788000
N	1.926129000	-1.101225000	-2.220788000
Ν	1.120801000	1.916444000	-2.215646000

	1 (000(0000)	1 11 5 0 2 1 0 0 0	0 0 0 0 1 1 0 0 0 0
Ν	-1.620068000	1.415031000	0.060419000
Ν	-1.420789000	-1.613240000	0.068253000
Ν	1.620068000	-1.415031000	0.060419000
N	1 420789000	1 613240000	0 068253000
10	1.420709000	1.013240000	0.000233000
Ν	-1.8/8451000	-1.0633/9000	2.282621000
N	1.076865000	-1.872484000	2.277129000
Ν	-1.076865000	1.872484000	2.277129000
N	1 878451000	1 063379000	2 282621000
N	1.070401000	1.0000070000	2.202021000
C	-1.256593000	-2.664043000	-3.338806000
С	-1.803516000	-3.931807000	-3.345157000
С	-2.197439000	-4.493055000	-2.123786000
C	-2 078614000	-3 744158000	-0 969401000
c	2.070014000	3./441300000	1 0000401000
C	-1.5//461000	-2.428433000	-1.026843000
С	-2.306636000	-1.636357000	1.124114000
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Н	-2.573261000	-5.516461000	-2.074781000
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