Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supplementary Information

Polar protic solvent-trapping polymorphism of the Hg^{II}-hydrazone coordination polymer: experimental and theoretical findings

Ghodrat Mahmoudi,*[a,b] Ali Akbar Khandar,[c] Jonathan White,[d] Mariusz P. Mitoraj,*[e] Himanshu Sekhar Jena, *[f] Pascal Van Der Voort,[f] Naseem Qureshi,[g] Alexander M. Kirillov,*[h] Koen Robeyns[i] and Damir A. Safin*[i]

[a]*Department of Chemistry, Faculty of Science, University of Maragheh, P.O. Box 55181-83111, Maragheh, Iran. Email: ghodratmahmoudi@gmail.com*

[b]*Inorganic Chemistry Department, RUDN University, Miklukho-Maklaya str. 6, 117198 Moscow, Russian Federation*

[c]*Department of Inorganic Chemistry, Faculty of Chemistry, University of Tabriz, P.O. Box 51666-16471, Tabriz, Iran*

[d]*BIO-21 Molecular Science and Biotechnology, University of Melbourne, Parkville, 3052 Victoria, Australia*

[e]*Department of Theoretical Chemistry, Faculty of Chemistry, Jagiellonian University, R. Ingardena 3, 30-060 Cracow, Poland. E-mail: mitoraj@chemia.uj.edu.pl*

[f]*COMOC–Center for Ordered Materials, Organometallics and Catalysis, Department of Inorganic and Physical Chemistry, Ghent University, Krijgslaan 281-S3, 9000 Ghent, Belgium. Email: himanshu.jena@ugent.be*

[g]*Department of Chemistry, Karakoram International University, Gilgit-Baltistan, Pakistan*

[h]*Centro de Química Estrutural, Complexo I, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001, Lisbon, Portugal. Email: kirillov@ist.utl.pt*

[i]*Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Place L. Pasteur 1, 1348 Louvain-la-Neuve, Belgium. E-mail: damir.a.safin@gmail.com*

Table S1 Selected bond lengths (Å°) and bond angles (°) in **HL-I**, **HL-II** and **1–5**.

	HL-I	**HL-II**	**1**	**2**	**3**	**4**	**5**
Bond lengths							
C=O	1.2224(15)	1.2216(15)	1.245(12)	1.259(3)	1.262(4)	1.257(10)	1.249(4)
C(O)–N	1.3596(16)	1.3544(17)	1.312(14)	1.334(3)	1.335(5)	1.328(11)	1.335(4)
N(C)–N(C)	1.3736(15)	1.3742(15)	1.367(11)	1.380(3)	1.373(4)	1.382(9)	1.372(4)
C(H)–N(N)	1.2859(16)	1.2876(17)	1.266(14)	1.280(3)	1.278(5)	1.269(11)	1.277(4)
Hg–O	–	–	2.434(7)	2.5674(18)	2.486(3)	2.480(6)	2.498(3)
Hg–N(N)	–	–	2.223(8)	2.2544(18)	2.242(3)	2.222(7)	2.231(3)
Hg–$N_{2\text{-Py}}$	–	–	2.441(10)	2.4420(19)	2.431(3)	2.510(7)	2.442(3)
Hg–$N_{4\text{-Py}}$	–	–	2.322(8)	2.4045(19)	2.393(3)	2.391(7)	2.409(3)
Hg–N_{azide}	–	–	2.135(13)	2.111(2)	2.140(3)	2.127(8)	2.137(3)
Bond angles							
O=C–N	123.55(12)	124.38(12)	129.4(9)	127.2(2)	128.7(4)	128.4(8)	128.5(3)
C(O)–N–N	118.54(10)	120.85(11)	111.3(7)	112.24(17)	111.6(3)	111.8(7)	111.9(2)
C(H)–N–N	116.94(10)	115.89(11)	120.0(8)	116.83(18)	118.9(3)	117.5(7)	118.6(3)
O–Hg–N	–	–	68.2(3)	65.79(6)	67.81(10)	68.0(2)	67.60(9)
O–Hg–$N_{2\text{-Py}}$	–	–	140.2(3)	134.72(6)	138.63(10)	137.1(2)	137.56(8)
O–Hg–$N_{4\text{-Py}}$	–	–	91.1(3)	86.11(6)	87.81(9)	89.7(2)	88.93(9)
O–Hg–N_{azide}	–	–	106.4(4)	92.69(7)	102.99(13)	109.5(3)	107.04(10)
N–Hg–$N_{2\text{-Py}}$	–	–	72.0(3)	70.78(6)	71.47(10)	70.1(2)	71.37(9)
N–Hg–$N_{4\text{-Py}}$	–	–	122.7(3)	97.97(6)	106.05(11)	99.5(2)	107.62(10)
N–Hg–N_{azide}	–	–	142.6(4)	150.08(8)	157.02(11)	160.0(3)	157.28(10)
$N_{2\text{-Py}}$–Hg–$N_{4\text{-Py}}$	–	–	110.5(3)	87.76(6)	96.64(10)	88.1(2)	93.40(10)
$N_{2\text{-Py}}$–Hg–N_{azide}	–	–	105.1(4)	132.46(7)	117.57(13)	113.1(3)	115.03(10)
$N_{4\text{-Py}}$–Hg–N_{azide}	–	–	93.8(4)	101.14(7)	94.20(12)	100.4(3)	94.04(11)
Hg–N_{azide}–N_{azide}			117.8(9)	119.57(17)	116.2(3)	116.8(6)	116.7(2)

Table S2 Hydrogen bond lengths (Å) and angles (°) for **HL-I**, **HL-II** and **1–5**

	D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠(DHA)
HL-I	N(3)–H(3A)···N(1)	0.91(2)	1.94(2)	2.680(2)	137.8(16)
HL-II	N(3')–H(3A')···N(1')	0.88(2)	1.92(2)	2.652(2)	140.4(17)
1[a]	O(2)–H(2O)···N(3)$^{\#1}$	1.00	2.35	3.02(2)	124
	O(2)–H(2P)···O(1)$^{\#2}$	1.03	2.46	3.49(2)	170
2[b]	O(2)–H(2B)···O(1)$^{\#1}$	0.81(3)	1.90(3)	2.700(3)	170(3)
	O(3)–H(3B)···O(2)$^{\#2}$	0.91(6)	1.89(6)	2.803(3)	175(4)
3[c]	O(2)–H(15)···N(5)$^{\#1}$	0.91(10)	1.96(9)	2.858(6)	170(7)
4[d]	O(2)–H(2)···N(5)$^{\#1}$	0.84	2.18	3.006(14)	167
5[e]	O(27)–H(27)···N(5)$^{\#1}$	0.84	1.96	2.753(8)	156

[a]Symmetry transformations used to generate equivalent atoms: #1 *x*, *y*, *z*; #2 1 – *x*, 2 – *y*, –*z*.

[b]Symmetry transformations used to generate equivalent atoms: #1 *x*, *y*, *z*; #2 3/2 – *x*, –1/2 + *y*, *z*.

[c]Symmetry transformations used to generate equivalent atoms: #1 *x*, *y*, *z*.

[d]Symmetry transformations used to generate equivalent atoms: #1 –1/2 + *x*, –1/2 – *y*, 1/2 + *z*.

[e]Symmetry transformations used to generate equivalent atoms: #1 2 – *x*, –*y*, 1 – *z*.

Table S3 $\pi\cdots\pi$ distances (Å) and angles (°) for **HL** and **2–5**[a]

	Cg(*I*)	Cg(*J*)	*d*[Cg(*I*)–Cg(*J*)]	α	β	γ	slippage
HL[b]	Cg(1)	Cg(2)$^{\#1}$	3.7074(11)	1.08(6)	23.7	24.4	1.489
	Cg(2)	Cg(1)$^{\#1}$	3.7074(11)	1.08(6)	24.4	23.7	1.532
	Cg(3)	Cg(4)$^{\#2}$	3.8972(11)	6.08(6)	26.0	31.2	1.708
	Cg(3)	Cg(4)$^{\#3}$	3.8850(11)	6.08(6)	27.8	29.1	1.813
	Cg(4)	Cg(3)$^{\#2}$	3.8972(11)	6.08(6)	31.2	26.0	2.018
	Cg(4)	Cg(3)$^{\#3}$	3.8850(11)	6.08(6)	29.1	27.8	1.891
2[c]	Cg(3)	Cg(4)$^{\#1}$	3.5773(13)	7.94(11)	23.6	18.3	1.431
	Cg(4)	Cg(3)$^{\#1}$	3.5773(13)	7.94(11)	18.3	23.6	1.124
3[d]	Cg(3)	Cg(4)$^{\#1}$	3.566(2)	12.37(19)	12.9	19.7	0.794
	Cg(4)	Cg(3)$^{\#2}$	3.566(2)	12.37(19)	19.7	12.9	1.201
	Cg(4)	Cg(5)$^{\#3}$	3.566(2)	12.37(19)	19.7	12.9	1.201
	Cg(5)	Cg(4)$^{\#3}$	3.566(2)	12.37(19)	12.9	19.7	0.794
4[e]	Cg(3)	Cg(4)$^{\#1}$	3.478(5)	4.4(4)	18.4	17.4	1.098
	Cg(4)	Cg(3)$^{\#1}$	3.478(5)	4.4(4)	17.4	18.4	1.039
5[f]	Cg(3)	Cg(4)$^{\#1}$	3.593(2)	13.33(17)	19.5	10.7	1.198
	Cg(4)	Cg(3)$^{\#1}$	3.593(2)	13.33(17)	10.7	19.5	0.669

[a]Cg(*I*)–Cg(*J*): distance between ring centroids; α: dihedral angle between planes Cg(*I*) and Cg(*J*); β: angle Cg(*I*) $\rightarrow$ Cg(*J*) vector and normal to plane *I*; γ: angle Cg(*I*) $\rightarrow$ Cg(*J*) vector and normal to plane *J*; slippage: distance between Cg(*I*) and perpendicular projection of Cg(*J*) on ring *I*.

[b]Symmetry transformations used to generate equivalent atoms: #1 –*x*, 1 – *y*, –*z*; #2 1 – *x*, –*y*, 1 – *z*; #3 2 – *x*, –*y*, 1 – *z*. Cg(1): N(1)–C(1)–C(2)–C(3)–C(4)–C(5); Cg(2): N(4)–C(10)–C(9)–C(8)–C(12)–C(11); Cg(3): N(1')–C(1')–C(2')–C(3')–C(4')–C(5'); Cg(4): N(4')–C(10')–C(9')–C(8')–C(12')–C(11').

[c]Symmetry transformations used to generate equivalent atoms: #1 2 – *x*, 1 – *y*, 1 – *z*. Cg(3): N(1)–C(1)–C(2)–C(3)–C(4)–C(5); Cg(4): N(4)–C(10)–C(9)–C(8)–C(12)–C(11).

[d]Symmetry transformations used to generate equivalent atoms: #1 1 – *x*, 1/2 + *y*, 3/2 – *z*; #2 1 – *x*, –1/2 + *y*, 3/2 – *z*; #3 1 – *x*, –*y*, 2 – *z*. Cg(3): N(1)–C(3)–C(2)c–C(1)c–C(5)c–C(4); Cg(4): N(4)–C(8)–C(9)–C(10)–C(11)–C(12); Cg(5): C(1)–C(2)–C(3)d–N(1)d–C(4)d–C(5).

[e]Symmetry transformations used to generate equivalent atoms: #1 1 – *x*, –*y*, 1 – *z*. Cg(3): N(1)–C(1)–C(2)–C(3)–C(4)–C(5); Cg(4): N(4)–C(10)–C(9)–C(8)–C(12)–C(11).

[f]Symmetry transformations used to generate equivalent atoms: #1 1 – *x*, –*y*, –*z*. Cg(3): N(1)–C(1)–C(2)–C(3)–C(4)–C(5); Cg(4): N(4)–C(10)–C(9)–C(8)–C(12)–C(11).

XYZ coordinates applied in the ETS-NOCV calculations

Compound 1

69

1 model

C	12.70303300	4.08725400	5.38224800
H	13.48144200	4.23790200	5.86778000
C	12.70602700	3.09198900	4.42551000
H	13.47695100	2.59806100	4.26472700
C	11.56236500	2.84255600	3.72029400
H	11.53242600	2.16217000	3.08830500
C	10.46660400	3.61802300	3.96544800
H	9.68370500	3.48713200	3.48150700
C	10.53097300	4.59847000	4.93651300
C	9.35737200	5.41345100	5.25807900
H	8.58944200	5.33071800	4.73911600
C	8.42178400	7.70527700	7.57749200
C	7.24369300	8.54865900	7.94203900
C	6.00572300	8.47827400	7.33074600
H	5.85153800	7.84357700	6.66851100
C	5.01924000	9.33030000	7.69210900
H	4.19292900	9.24015800	7.27502900
C	6.35151600	10.35643500	9.22511800
H	6.47426600	11.00101100	9.88416900
C	7.40087100	9.52293200	8.93220700
H	8.20772200	9.60566500	9.38749300
N	13.14762400	6.17163000	9.58807400
N	14.06375100	6.69642900	10.02107300
N	11.65367800	4.82938100	5.63695300
N	9.36336000	6.22719700	6.22755200
N	8.24514600	6.95944600	6.51250400
N	5.15546100	10.29469400	8.61223300
N	12.20305500	5.58138600	9.15348200
O	9.42323700	7.81270600	8.30977000
Hg	11.21163200	6.40291200	7.44998000
H	13.41707300	5.82094100	2.41333600
H	8.30652000	5.31096100	11.13859400
C	2.26636700	8.26094600	10.53685200
H	1.48795800	8.11029800	10.05132000
C	2.26337300	9.25621100	11.49359000

H	1.49244900	9.75013900	11.65437300
C	3.40703500	9.50564400	12.19880600
H	3.43697400	10.18603000	12.83079500
C	4.50279600	8.73017700	11.95365200
H	5.28569500	8.86106800	12.43759300
C	4.43842700	7.74973000	10.98258700
C	5.61202800	6.93474900	10.66102100
H	6.37995800	7.01748200	11.17998400
C	6.54761600	4.64292300	8.34160800
C	7.72570700	3.79954100	7.97706100
C	8.96367700	3.86992600	8.58835400
H	9.11786200	4.50462300	9.25058900
C	9.95016000	3.01790000	8.22699100
H	10.77647100	3.10804200	8.64407100
C	8.61788400	1.99176500	6.69398200
H	8.49513500	1.34718900	6.03493100
C	7.56852900	2.82526800	6.98689300
H	6.76167800	2.74253500	6.53160700
N	1.82177600	6.17657000	6.33102600
N	0.90564900	5.65177100	5.89802700
N	3.31572200	7.51881900	10.28214700
N	5.60604000	6.12100300	9.69154800
N	6.72425400	5.38875400	9.40659600
N	9.81393900	2.05350600	7.30686700
N	2.76634500	6.76681400	6.76561800
O	5.54616300	4.53549400	7.60933000
Hg	3.75776800	5.94528800	8.46912000
H	9.03702700	6.52725900	10.37288600
O	9.04600800	5.97776400	11.24843600
O	5.92339200	6.37043600	4.67066400
H	6.66288000	7.03723900	4.78050600
H	5.93237300	5.82094100	5.54621400
O	13.40809200	6.37043600	3.28888600
H	14.14758000	7.03723900	3.17904400

Compound 2

78

2 model

Hg	2.13277000	6.77947800	9.18537600
N	3.19675200	8.25437800	7.55562700
N	1.12337900	6.52665000	7.18552900

N	0.07598200	5.65510700	6.96812100
N	-3.28749700	2.00259400	7.42212500
N	2.03169200	6.82238100	11.29319500
N	2.47267800	7.77173300	11.89062100
N	2.85258900	8.62342600	12.56187000
O	0.59743700	4.72734400	9.03293000
C	2.58744700	8.20250600	6.34858100
C	2.98023900	9.00160200	5.28414200
H	2.54287100	8.93567500	4.44247800
C	4.02184600	9.89748800	5.47016700
H	4.30421100	10.46431700	4.76281800
C	4.64359800	9.94965000	6.70908500
H	5.35783100	10.55705000	6.86372600
C	4.20869000	9.10288300	7.71872400
H	4.65011100	9.12983400	8.55973800
C	1.48838300	7.25025600	6.19426500
H	1.04493600	7.16795600	5.35796700
C	-0.08712600	4.79979200	7.97841100
C	-1.20471600	3.82624200	7.75905100
C	-1.50719700	2.88964100	8.73746900
H	-1.00296500	2.85588000	9.54189600
C	-2.55039700	2.00491200	8.53079300
H	-2.74983200	1.37070700	9.21017400
C	-3.00238200	2.90905700	6.47183800
H	-3.52702100	2.91818500	5.67993200
C	-1.97828700	3.82885000	6.59867300
H	-1.80331100	4.45407200	5.90433300
H	0.62522500	-1.05193800	9.99394900
N	3.94890300	5.24215600	8.83877500
Hg	9.36917000	0.46527200	7.07552400
N	10.43315200	-1.00962800	8.70527300
N	8.35977900	0.71810000	9.07537100
N	7.31238200	1.58964300	9.29277900
N	9.26809200	0.42236900	4.96770500
N	9.70907800	-0.52698300	4.37027900
N	10.08898900	-1.37867600	3.69903000
O	7.83383700	2.51740600	7.22797000
C	9.82384700	-0.95775600	9.91231900
C	10.21663900	-1.75685200	10.97675800
H	9.77927100	-1.69092500	11.81842200
C	11.25824600	-2.65273800	10.79073300

H	11.54061100	-3.21956700	11.49808200
C	11.87999800	-2.70490000	9.55181500
H	12.59423100	-3.31230000	9.39717400
C	11.44509000	-1.85813300	8.54217600
H	11.88651100	-1.88508400	7.70116200
C	8.72478300	-0.00550600	10.06663500
H	8.28133600	0.07679400	10.90293300
C	7.14927400	2.44495800	8.28248900
C	6.03168400	3.41850800	8.50184900
C	5.72920300	4.35510900	7.52343100
H	6.23343500	4.38887000	6.71900400
C	4.68600300	5.23983800	7.73010700
H	4.48656800	5.87404300	7.05072600
C	4.23401800	4.33569300	9.78906200
H	3.70937900	4.32656500	10.58096800
C	5.25811300	3.41590000	9.66222700
H	5.43308900	2.79067800	10.35656700
H	-0.21275000	0.02608100	10.82975900
O	8.48308700	3.09756500	13.30548100
H	8.36527800	3.54992800	13.96811300
C	7.53743400	3.48327600	12.30690000
H	7.68505700	2.95440900	11.49483000
H	7.65032200	4.43523600	12.10136200
H	6.62854200	3.32534000	12.63797100
O	1.24668700	3.09756500	11.08586900
H	1.12887800	3.54992800	10.42323700
C	0.30103400	3.48327600	12.08445000
H	0.44865700	2.95440900	12.89652000
H	0.41392200	4.43523600	12.28998800
H	-0.60785800	3.32534000	11.75337900
O	1.73080200	0.34818300	10.83008500
H	1.62095400	1.24609700	10.94358600
C	0.53983500	-0.09997800	10.21558500
H	0.38352900	0.41295100	9.39554800

Compound 3

87

3 model

Hg	3.35526600	7.53389800	9.43404200
C	3.13665800	10.65006300	6.04079300
N	1.99457500	8.69064800	6.78839500

N	1.86252800	7.74497400	7.77450500
N	1.60961900	5.87245100	9.74951400
N	5.25856000	7.15410800	10.33532100
N	6.18965300	7.81159100	9.91688700
N	7.10252200	8.41983500	9.55285000
O	3.79343200	9.53494900	8.02570500
N	3.49453700	12.70071400	4.18992000
C	2.61339600	11.71449000	3.96815000
H	2.12959000	11.72028300	3.17452000
C	2.39514700	10.69206100	4.86499300
H	1.75905900	10.03602600	4.68646200
C	4.05565100	11.65076900	6.26953700
H	4.57068500	11.64787300	7.04364000
C	4.20392900	12.65871600	5.33224500
H	4.81915300	13.33502600	5.49961800
C	2.98535800	9.54363800	7.05619300
C	0.90605600	6.90067300	7.69639700
C	0.70403400	5.90720800	8.74248200
C	-0.38363100	5.05711400	8.71319200
C	-0.53417700	4.12012900	9.74254000
C	0.40019900	4.07668300	10.75654500
C	1.45886900	4.97311900	10.72028100
H	0.23244400	6.95136000	6.94600600
H	-0.97862600	5.15559200	8.01998600
H	-1.30331600	3.47568000	9.72161800
H	0.35000400	3.46119800	11.47904100
H	2.09981400	4.96732600	11.38140700
H	5.78632500	1.46268200	4.71435700
H	5.10484000	1.24400400	7.61550000
Hg	3.16445200	6.94810200	4.51376000
C	3.38306000	3.83193700	7.90700900
N	4.52514300	5.79135200	7.15940700
N	4.65719100	6.73702600	6.17329700
N	4.91010000	8.60954900	4.19828800
N	1.26115900	7.32789200	3.61248100
N	0.33006500	6.67040900	4.03091500
N	-0.58280400	6.06216500	4.39495200
O	2.72628600	4.94705100	5.92209700
N	3.02518100	1.78128600	9.75788200
C	3.90632300	2.76751000	9.97965200
H	4.39012800	2.76171700	10.77328200

C	4.12457200	3.78993900	9.08280900
H	4.76066000	4.44597400	9.26134100
C	2.46406700	2.83123100	7.67826500
H	1.94903300	2.83412700	6.90416200
C	2.31578900	1.82328400	8.61555700
H	1.70056600	1.14697400	8.44818400
C	3.53436100	4.93836200	6.89160900
C	5.61366300	7.58132700	6.25140500
C	5.81568400	8.57479200	5.20532000
C	6.90335000	9.42488600	5.23461000
C	7.05389600	10.36187100	4.20526200
C	6.11952000	10.40531700	3.19125700
C	5.06085000	9.50888100	3.22752100
H	6.28727500	7.53064000	7.00179700
H	7.49834400	9.32640800	5.92781600
H	7.82303500	11.00632000	4.22618400
H	6.16971400	11.02080200	2.46876100
H	4.41990400	9.51467400	2.56639600
H	6.18854700	0.32874100	6.94740000
H	6.58325400	1.27007100	8.13714800
O	0.96439600	12.30390700	8.72156100
C	0.17079200	12.21701500	7.55413000
H	-0.76685100	12.27349500	7.79821600
H	0.31768100	11.35678400	7.13011600
C	0.49134000	13.30026900	6.58894200
H	-0.06353500	13.21192900	5.81065400
H	1.41487900	13.23799600	6.33230200
H	0.33117100	14.15325900	7.00040200
H	0.73339400	13.01931800	9.23344500
O	1.82253600	9.41909300	1.74766000
C	1.02893200	9.50598500	0.58022900
H	0.09129000	9.44950500	0.82431500
H	1.17582100	10.36621600	0.15621500
C	1.34948100	8.42273100	-0.38495900
H	0.79460500	8.51107100	-1.16324700
H	2.27301900	8.48500400	-0.64159900
H	1.18931200	7.56974100	0.02650100
H	1.59153400	8.70368200	2.25954400
O	5.55532300	2.17809300	5.22624100
C	6.34892700	2.26498500	6.39367300
H	7.28656900	2.20850500	6.14958600

H 6.20203800 3.12521600 6.81768600

C 6.02837800 1.18173100 7.35886000

Compound 4

144

4 model

Hg 3.66195600 0.28433800 3.39737200

N 1.48826600 -0.89026400 3.84059800

N 2.88098400 0.86869100 5.39327900

N 3.53113000 1.79059600 6.19219800

N 6.62794000 5.35596900 7.82361200

N 4.84556000 -0.68315900 1.91972000

N 5.74877300 -1.36919500 2.31454800

N 6.63730700 -2.04372500 2.62022100

O 4.94420600 2.16597400 4.38247300

C 1.07315800 -0.66446200 5.07602700

C -0.01765500 -1.29584500 5.60748200

H -0.28336100 -1.11462800 6.50134400

C -0.72845000 -2.19473900 4.84908800

H -1.50556700 -2.61901700 5.19528600

C -0.28510800 -2.46656400 3.57545000

H -0.74360600 -3.09650900 3.03241700

C 0.83868800 -1.80785500 3.09262500

H 1.15659500 -2.00633100 2.21960400

C 1.83162700 0.32647800 5.85757800

H 1.53000500 0.56378600 6.72596800

C 4.53150600 2.38170900 5.54958900

C 5.24350500 3.42442600 6.36124400

C 6.29653500 4.13059700 5.80315900

H 6.56553700 3.95800900 4.90813900

C 6.95274800 5.08558100 6.55460600

H 7.66399000 5.57170300 6.15283100

C 5.62047100 4.64404500 8.36896100

H 5.39369800 4.80944100 9.27671800

C 4.90293900 3.69049800 7.68003900

H 4.18872100 3.22451200 8.09918100

Hg 7.83429400 6.90681200 9.18663700

H 1.60181100 3.94506500 7.00616800

N 5.66060400 8.08141400 9.62986300

N 7.05332300 6.32245900 11.18254400

N 7.70346900 5.40055400 11.98146200

N	10.80027900	1.83518100	13.61287700
N	9.01789900	7.87430900	7.70898500
N	9.92111200	8.56034500	8.10381300
N	10.80964600	9.23487500	8.40948600
O	9.11654500	5.02517600	10.17173800
C	5.24549700	7.85561200	10.86529200
C	4.15468400	8.48699500	11.39674700
H	3.88897800	8.30577800	12.29060900
C	3.44388900	9.38588900	10.63835300
H	2.66677200	9.81016700	10.98455100
C	3.88723100	9.65771400	9.36471500
H	3.42873200	10.28765900	8.82168200
C	5.01102700	8.99900500	8.88189000
H	5.32893400	9.19748100	8.00886900
C	6.00396600	6.86467200	11.64684300
H	5.70234400	6.62736400	12.51523300
C	8.70384500	4.80944100	11.33885400
C	9.41584400	3.76672400	12.15050900
C	10.46887400	3.06055300	11.59242400
H	10.73787600	3.23314100	10.69740300
C	11.12508600	2.10556900	12.34387000
H	11.83632900	1.61944700	11.94209500
C	9.79281000	2.54710500	14.15822600
H	9.56603700	2.38170900	15.06598300
C	9.07527800	3.50065200	13.46930300
H	8.36106000	3.96663800	13.88844600
H	0.31705800	4.89285800	6.98764300
Hg	0.51038300	7.47548800	2.39189300
N	2.68407300	6.30088600	1.94866700
N	1.29135500	8.05984100	0.39598600
N	0.64120900	8.98174600	-0.40293300
N	-2.45560100	12.54711900	-2.03434800
N	-0.67322100	6.50799100	3.86954500
N	-1.57643400	5.82195500	3.47471700
N	-2.46496800	5.14742500	3.16904400
O	-0.77186700	9.35712400	1.40679100
C	3.09918100	6.52668800	0.71323700
C	4.18999400	5.89530500	0.18178300
H	4.45569900	6.07652200	-0.71208000
C	4.90078900	4.99641100	0.94017700
H	5.67790600	4.57213300	0.59397900

C	4.45744700	4.72458600	2.21381500
H	4.91594500	4.09464100	2.75684800
C	3.33365100	5.38329500	2.69664000
H	3.01574400	5.18481900	3.56966100
C	2.34071200	7.51762800	-0.06831300
H	2.64233300	7.75493600	-0.93670300
C	-0.35916700	9.57285900	0.23967600
C	-1.07116600	10.61557600	-0.57197900
C	-2.12419600	11.32174700	-0.01389400
H	-2.39319800	11.14915900	0.88112600
C	-2.78040900	12.27673100	-0.76534100
H	-3.49165100	12.76285300	-0.36356600
C	-1.44813200	11.83519500	-2.57969600
H	-1.22135900	12.00059100	-3.48745300
C	-0.73060000	10.88164800	-1.89077400
H	-0.01638200	10.41566200	-2.30991700
H	1.64174000	6.69208400	6.34503400
N	1.71673700	9.02633100	3.75491700
Hg	4.68272200	14.09796200	8.18115700
N	6.85641200	15.27256400	7.73793100
N	5.46369300	13.51360900	6.18525000
N	4.81354800	12.59170400	5.38633200
N	3.49911700	15.06545900	9.65880900
N	2.59590500	15.75149500	9.26398200
N	1.70737100	16.42602500	8.95830800
O	3.40047100	12.21632600	7.19605600
C	7.27151900	15.04676200	6.50250200
C	8.36233300	15.67814500	5.97104800
H	8.62803800	15.49692800	5.07718500
C	9.07312800	16.57703900	6.72944100
H	9.85024500	17.00131700	6.38324300
C	8.62978500	16.84886400	8.00308000
H	9.08828400	17.47880900	8.54611300
C	7.50599000	16.19015500	8.48590400
H	7.18808300	16.38863100	9.35892500
C	6.51305100	14.05582200	5.72095100
H	6.81467200	13.81851400	4.85256200
C	3.81317100	12.00059100	6.02894000
C	3.10117300	10.95787400	5.21728500
C	2.04814300	10.25170300	5.77537100
H	1.77914100	10.42429100	6.67039100

C	1.39193000	9.29671900	5.02392400
H	0.68068800	8.81059700	5.42569900
C	2.72420700	9.73825500	3.20956800
H	2.95098000	9.57285900	2.30181200
C	3.44173900	10.69180200	3.89849100
H	4.15595600	11.15778800	3.47934800
C	1.19147900	4.72458600	6.55576300
O	7.37831000	9.98706900	6.38555900
H	7.88245600	10.65728400	6.43303100
C	6.10687800	8.23386700	3.32303800
H	5.55897600	7.43133400	3.19335800
H	6.98241300	8.10298800	2.90273700
H	5.66048600	9.00475800	2.91431600
C	6.29197600	8.48555700	4.81087900
H	5.41068100	8.63944800	5.23465300
H	6.70293700	7.69021600	5.23349500
C	7.15319800	9.65771400	5.02276600
H	8.02761900	9.48944200	4.59088700
H	6.74286600	10.43723500	4.57236100
C	2.05270100	5.89674300	6.76765100
H	2.93399600	5.74285200	6.34387600
H	2.78570100	6.95096600	8.38517100
H	0.46222100	3.72501600	5.14549900
H	1.36226400	6.27931200	8.67579200
H	2.68419200	5.37754200	8.66421400
C	2.23780000	6.14843300	8.25549200
O	0.96636800	4.39523100	5.19297100

Compound 5

75

5 model

C	3.78688600	10.65612800	-0.92512400
C	3.29275800	9.66358300	-3.05082100
H	2.81840700	9.69163900	-3.87344700
C	4.77701200	8.60418000	-1.65642100
H	5.36096800	7.87526500	-1.48274800
C	4.63126000	9.58460300	-0.68659100
H	5.10618100	9.52182400	0.13376400
N	4.12936600	8.64219300	-2.82660700
N	6.03156300	14.17251600	3.36935700
N	6.99435600	13.58669500	2.92445100

N	7.94655400	13.06355400	2.54917200
C	1.57717900	15.52482800	1.72900200
C	0.52798200	16.43518800	1.67325400
H	-0.07950500	16.42963300	0.94289300
C	0.38526900	17.35086400	2.70347300
H	-0.32246600	17.98444300	2.68959300
C	1.29346600	17.33016200	3.76007700
H	1.21025600	17.93990500	4.48380900
C	2.31505500	16.40561300	3.73201800
H	2.94196400	16.39907300	4.44577300
C	1.74760800	14.51768500	0.68256000
H	1.17053000	14.51885200	-0.07208400
C	3.66490300	11.74531700	0.10581900
C	3.09102200	10.67881200	-2.13445300
H	2.48482700	11.38470500	-2.32609500
N	2.46163200	15.51844400	2.74454600
N	2.66699500	13.63680200	0.77664200
N	2.75246700	12.67123000	-0.19487700
O	4.41696100	11.68727700	1.10153700
Hg	4.14919100	13.78107800	2.43664000
C	3.60378000	3.62447800	8.02137600
C	4.09790800	2.63193300	10.14707300
H	4.57225900	2.65998900	10.96969800
C	2.61365400	1.57253000	8.75267300
H	2.02969800	0.84361500	8.57900000
C	2.75940600	2.55295300	7.78284300
H	2.28448500	2.49017400	6.96248800
N	3.26130100	1.61054300	9.92285900
N	1.35910300	7.14086600	3.72689500
N	0.39631000	6.55504500	4.17180100
N	-0.55588800	6.03190400	4.54708000
C	5.81348700	8.49317800	5.36725000
C	6.86268400	9.40353800	5.42299800
H	7.47017100	9.39798300	6.15335900
C	7.00539800	10.31921400	4.39277900
H	7.71313200	10.95279300	4.40665900
C	6.09720000	10.29851200	3.33617500
H	6.18041000	10.90825500	2.61244300
C	5.07561100	9.37396300	3.36423400
H	4.44870200	9.36742300	2.65047800
C	5.64305900	7.48603500	6.41369200

H	6.22013600	7.48720200	7.16833600
C	3.72576300	4.71366700	6.99043300
C	4.29964400	3.64716200	9.23070500
H	4.90583900	4.35305500	9.42234700
N	4.92903400	8.48679400	4.35170600
N	4.72367100	6.60515200	6.31961000
N	4.63819900	5.63958000	7.29112900
O	2.97370500	4.65562700	5.99471500
Hg	3.24147500	6.74942800	4.65961200
H	1.16936400	9.85319800	0.06393700
C	0.86013000	9.11577500	0.64763200
H	0.04223700	9.41948600	1.11550200
O	1.86148500	8.82341300	1.60036100
H	1.57777600	8.24096700	2.13502100
H	1.37520100	7.51985700	-0.55562200
C	0.52682800	7.89723200	-0.21219200
H	0.00263000	8.20448700	-0.99380200
H	0.25932100	6.52900000	1.27167700
C	-0.23382700	6.80080100	0.45741000
H	-1.11067200	7.15844500	0.74605700
H	0.38356900	5.15522600	-0.64695100
C	-0.47661500	5.55536900	-0.40125000
H	-0.96311600	5.80834000	-1.21348700
H	-1.00558700	4.90591200	0.10745100