Electronic Supplementary Information (ESI)

belonging to the article

Halogen bonding in cadmium(II) MOFs: influence on the structure and on the nitroaldol reaction in aqueous medium

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Computational models

The structures of all model clusters (Fig. S2) were taken from the experimental X-ray structures of **3** or **4**. In **5N3$_{I}$**$_{...I}$, the chains were terminated by the benzoate ligands in the units A, C and D. In the units C, D and E, the iodine atoms and carboxylate groups of the H_3L^3 ligand were substituted by the hydrogen atoms and the pyrimidine moiety was substituted by the propenyl one.

In **2N3$_{I}$**$_{...I}$, in the unit A, the chain was terminated by two acetate ligands and one of the carboxylate groups of H_3L^3 was replaced by the COOH group. In the unit B, the chain was terminated by one acetate ligand and two carboxylate groups of H_3L^3 were replaced by the COOH groups.

In **2N4$_{I}$**$_{...I}$, in the unit A, one H_2L^4 ligand was replaced by the acetate ligand, one μ-H_2L^4 ligand was replaced by the acetic acid and one μ-H_2L^4 ligand was replaced by the H_3L^4 one. In the unit B, one H_2L^4 ligand was replaced by the acetate ligand and two μ-H_2L^4 ligands were replaced by the acetic acid molecules.

In **3N3$_{I}$**$_{...O}$, in the unit A, two H_3L^3 ligands were substituted by the acetate ligands. In the third ligand, one of the carboxylate groups was replaced for the COOH group. In the unit B, one H_3L^3 ligand was substituted by the acetate ligand and in another ligand, two I atomd were replaced for two H atoms. In the unit C, two H_3L^3 ligands were substituted by the acetate ligands and in the third ligand, triiododicarboxylatophenyl moiety was replaced for the iodovinil one.

In **2N4$_{I}$**$_{...O}$, in both units A and B, two H_2L^4 ligands were replaced by the acetate ligands, one μ-H_2L^4 ligand was replaced by the acetic acid and one μ-H_2L^4 ligand was replaced by the H_3L^4 one.

The C–H and O–H bond lengths were fixed at their idealized values of 1.09 and 1.00 Å, respectively in all clusters. Atomic coordinates are given in Table S1.

Calculations of the interaction energies

Because of the rigid structures of complexes and existence of the multiple intermolecular interactions, the direct calculations of the interaction energies are not possible. Therefore, the following procedures were applied to estimate E_{int} values.

The E_{int} of the I···I bond in **2N3$_{I}$**$_{...I}$ (E_{int}(**2N3$_{I}$**$_{...I}$)) was estimated as the total energy difference between the structures **2N3$_{I}$**$_{...I}$**M2** and **2N3$_{I}$**$_{...I}$**M1**. In **2N3$_{I}$**$_{...I}$**M1**, one of the I atoms forming the I···I bond was replaced with the hydrogen atom while, in **2N3$_{I}$**$_{...I}$**M2**, one of the non-interacting I atoms was replaced for H (Fig. S4). The C–H bond was fixed at 1.09 Å.

The E_{int} of the I···I bonds in **2N4$_{I}$**$_{...I}$ were estimated using the following equations:

$$E_{int}(\mathbf{2N4_{I1}}_{\cdots}\mathbf{_{I5}}) = [(E_{M4} - E_{M2}) + (E_{M4} - E_{M3}) - (E_{M4} - E_{M1})]/2$$

$$E_{int}(\mathbf{2N4_{I5}}_{\cdots}\mathbf{_{I5'}}) = [(E_{M4} - E_{M1}) + (E_{M4} - E_{M3}) - (E_{M4} - E_{M2})]/2$$

$$E_{int}(\mathbf{2N4_{I1}}_{\cdots}\mathbf{_{I5'}}) = [(E_{M4} - E_{M1}) + (E_{M4} - E_{M2}) - (E_{M4} - E_{M3})]/2$$

where E_{M1}, E_{M2}, E_{M3} and E_{M4} are total energies of the model structures **2N4$_{I}$**$_{...I}$**M1**, **2N4$_{I}$**$_{...I}$**M2**, **2N4$_{I}$**$_{...I}$**M3** and **2N4$_{I}$**$_{...I}$**M4** (Fig. S4). In **2N4$_{I}$**$_{...I}$**M1**, **2N4$_{I}$**$_{...I}$**M2** and **2N4$_{I}$**$_{...I}$**M3**, one of the interacting atoms (I5', I1 and I5, respectively) was substituted for the H atom. In **2N4$_{I}$**$_{...I}$**M4**, one of the non-interacting I atoms was substituted for the H atom. The C–H bonds were fixed at 1.09 Å.

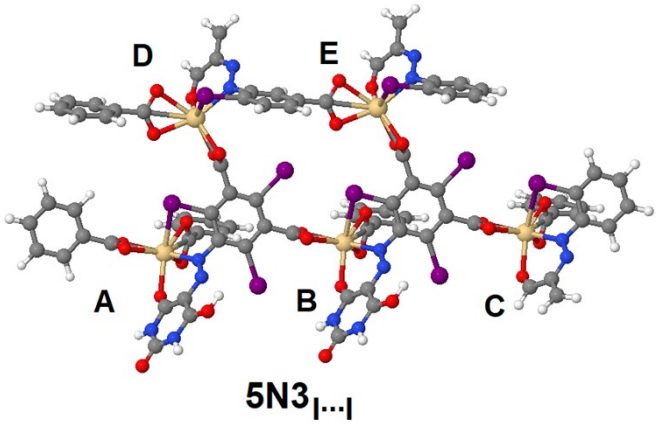
The E_{int} of the I···O bond in $\mathbf{3N3_{I\cdots O}}$ was estimated as $E_{int}(\mathbf{3N3_{I\cdots O}}) = E(\mathbf{3N3_{I\cdots O}M2}) - E(\mathbf{3N3_{I\cdots O}M1}) + E_{int}(\mathbf{2N3_{I\cdots I}})$, where $E(\mathbf{3N3_{I\cdots O}M1})$ and $E(\mathbf{3N3_{I\cdots O}M2})$ are total energies of model structures $\mathbf{3N3_{I\cdots O}M1}$ and $\mathbf{3N3_{I\cdots O}M2}$ (Fig. S4). Addition of the $E_{int}(\mathbf{2N3_{I\cdots I}})$ term is accounted for by the existence of the I···I interaction in structure $\mathbf{3N3_{I\cdots O}M1}$. Structures $\mathbf{3N3_{I\cdots O}M1}$ and $\mathbf{3N3_{I\cdots O}M2}$ were constructed by substitution of the I atom participating in the I···O interaction ($\mathbf{3N3_{I\cdots O}M1}$) or another non-coordinated I atom ($\mathbf{3N3_{I\cdots O}M2}$) by the H atom. The C–H bond was fixed at 1.09 Å.

The E_{int} of the I···O bond in $\mathbf{2N4_{I\cdots O}}$ was estimated as $E_{int}(\mathbf{2N4_{I\cdots O}}) = E(\mathbf{2N4_{I\cdots O}M2}) - E(\mathbf{2N4_{I\cdots O}M1})$, where $E(\mathbf{2N4_{I\cdots O}M1})$ and $E(\mathbf{2N4_{I\cdots O}M2})$ are total energies of model structures $\mathbf{2N4_{I\cdots O}M1}$ and $\mathbf{2N4_{I\cdots O}M2}$ (Fig. S4). Structures $\mathbf{2N4_{I\cdots O}M1}$ and $\mathbf{2N4_{I\cdots O}M2}$ were constructed by substitution of the I atoms participating in the I···O interactions ($\mathbf{2N4_{I\cdots O}M1}$) or another two non-coordinated I atoms ($\mathbf{2N4_{I\cdots O}M2}$) by the H atom. The C–H bond was fixed at 1.09 Å.

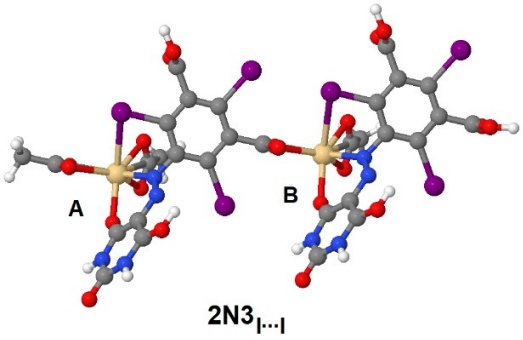
Initial geometry and optimization of $\mathbf{3_M}$

In the model structure $\mathbf{3_M}$, two fragments A and B are not directly connected via the $–CO_2$ bridge and they are bound only through the I···I interaction. Initial geometry of $\mathbf{3_M}$ was constructed from the structure of $\mathbf{2N3_{I\cdots I}}$ through the following steps: 1) elimination of the $\{CdAc_2\}$ moiety in fragment A, 2) cleavage of the C1–C2 bond, 3) rotation around the I1···I3 bond, 4) in fragment A, the H atom was placed at the position of the C1 atom and the C–H distance of set to 1.09 Å, 5) in fragment B, the CH_3 group was places at the position of the C2 atom, 6) reflection of the fragment B relative to the C–I1···I3 plane (Table S2). Such a construction allowed the disconnection of the fragments A and B through the $–CO_2$ bridge meanwhile keeping the I1···I3 bond and all other bond and dihedral angles within each fragment A and B unchanged.

Structure of $\mathbf{3_M}$ was partially optimized. All Cd–O, Cd–N and Cd–I bonds as well as the I3···I1–C, Cd–I···I, one I3–CdC_{Ac} angles and one I3$CdOC_{Ac}$ torsion angle were frozen to prevent the formation of other undesired intermolecular interactions during the optimization.



$\mathbf{5N3_{I\cdots I}}$



$\mathbf{2N3_{I\cdots I}}$

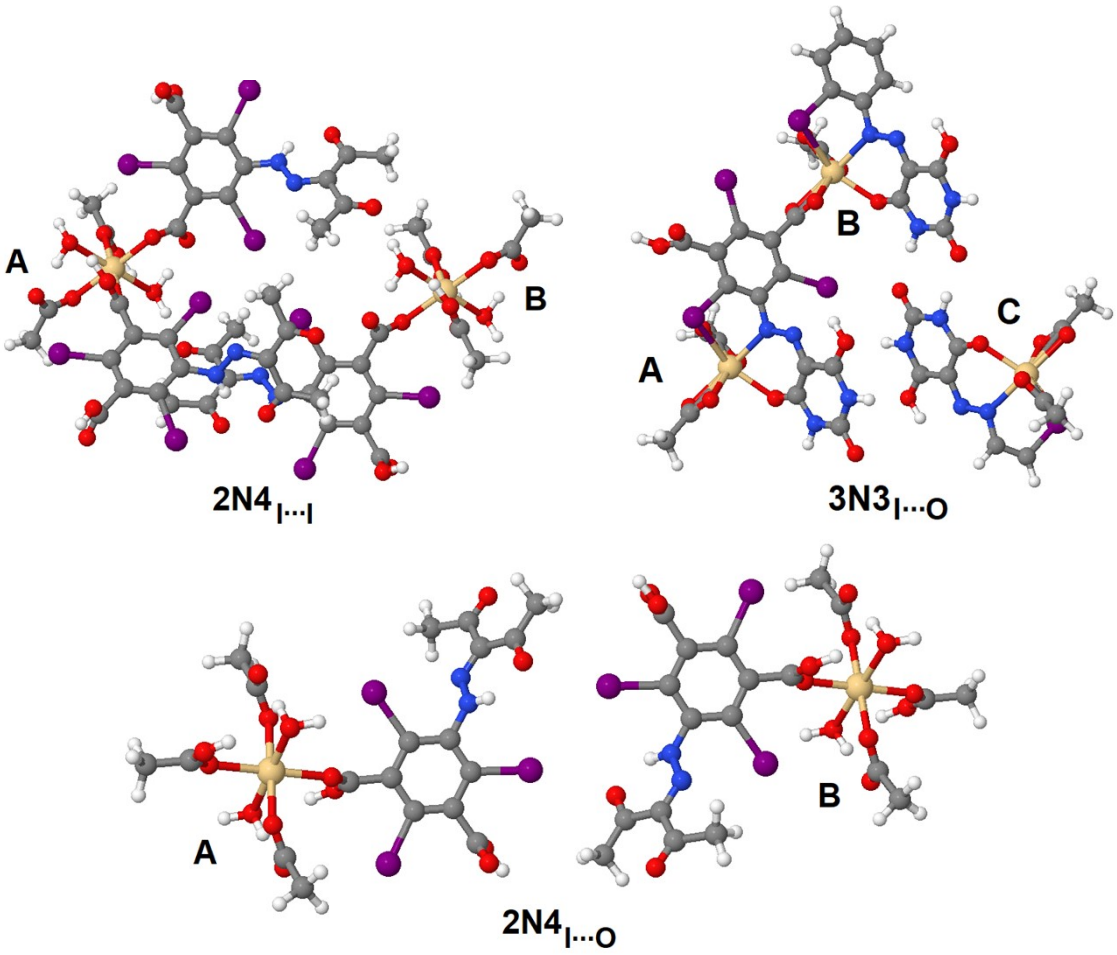


Fig. S1. Computational models.

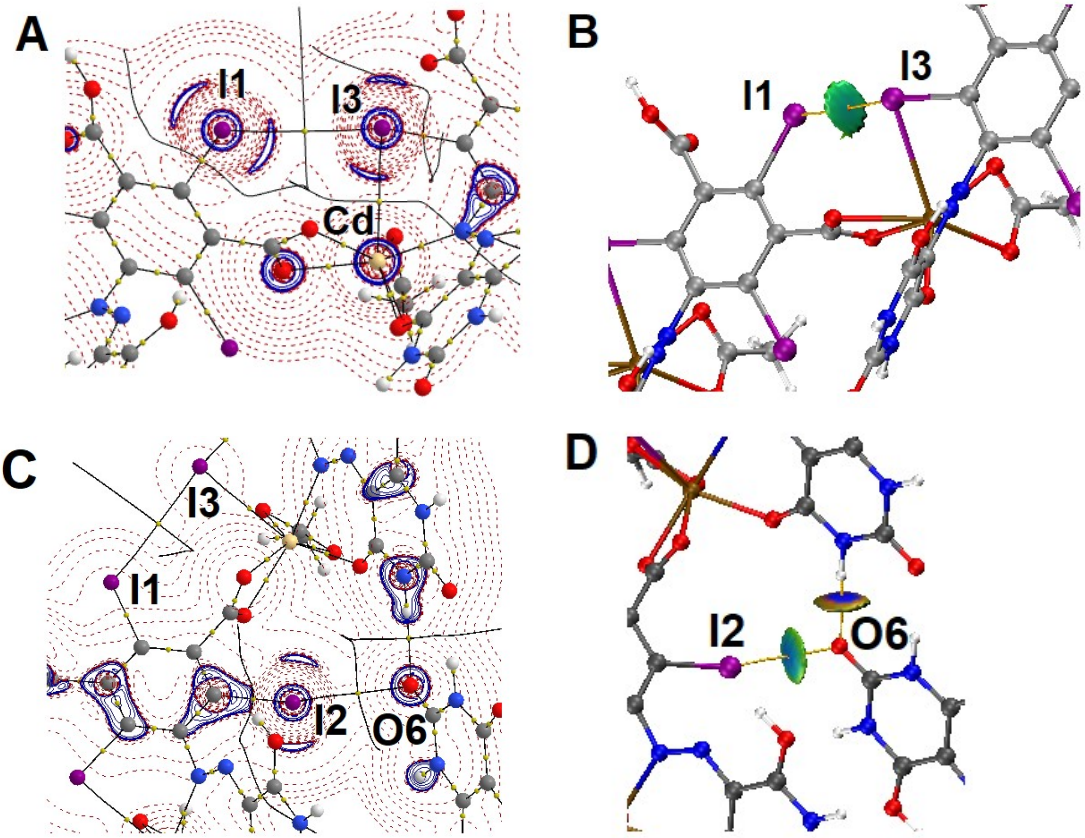


Fig. S2. Contour line diagram of the Laplacian distribution $\nabla^2\rho(r)$ in the plane formed by Cd and interacting I and/or O atoms, selected bond paths, zero flux surfaces (A, C) and the sign(λ_2)$\rho(r)$ function mapped on the δg_{inter} isosurface of 0.005 a.u. and blue-cyan-green-yellow-red color scale –0.02 < sign(λ_2)$\rho(r)$ < 0.02 for the I···I and I···O contacts (B, D) for **2N3$_{I\cdots I}$** (A, B) and **3N3$_{I\cdots O}$** (C, D).

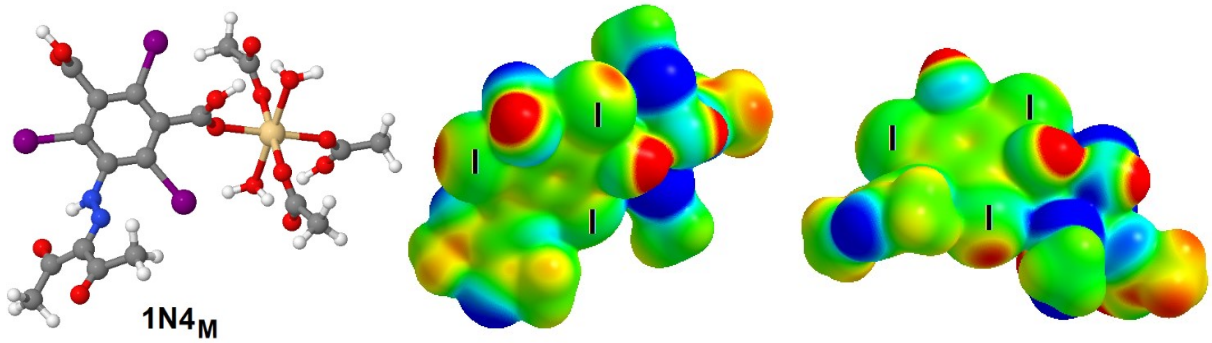
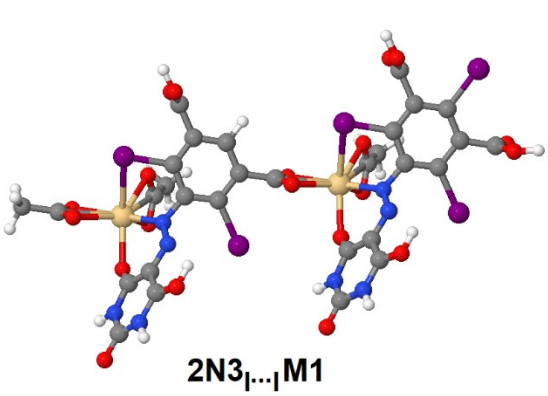
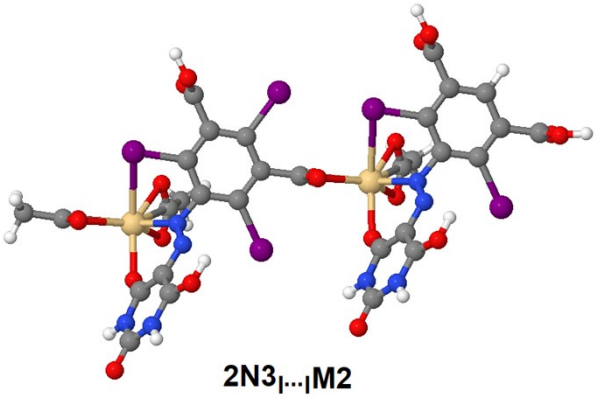


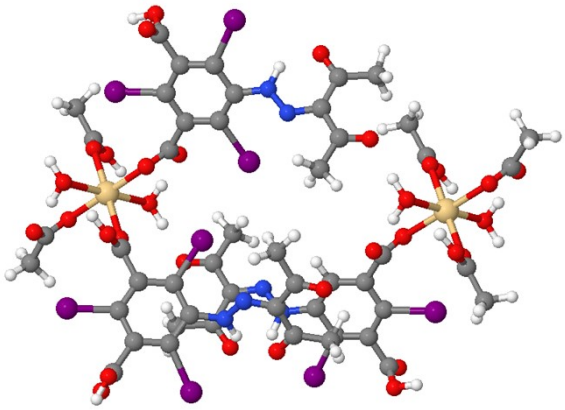
Fig. S3. Structure and ESP distribution mapped on the 0.002 a.u. isosurface of electron density for the [Cd(H_3L^4)(H_2O)$_2$(Ac)$_2$(HAc)] model complex (**1N4$_M$**) with blue-cyan-green-yellow-red color scale –0.05 < ESP < 0.05 a.u.



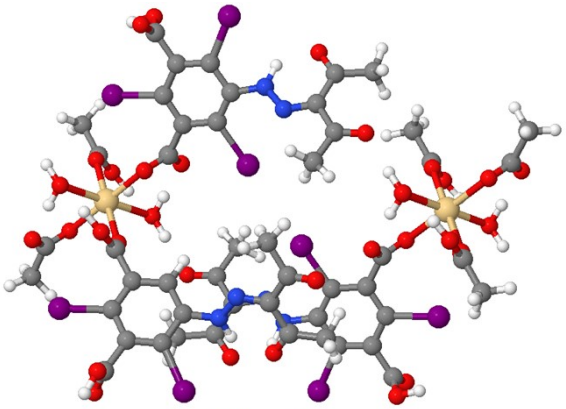
$2N3_{I\cdots I}M1$



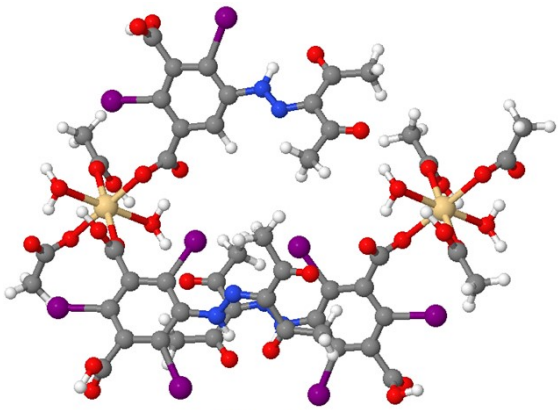
$2N3_{I\cdots I}M2$



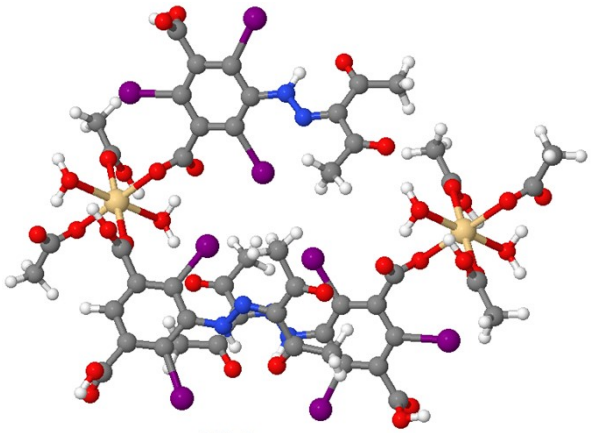
$2N4_{I\cdots I}M1$



$2N4_{I\cdots I}M2$



$2N4_{I\cdots I}M3$



$2N4_{I\cdots I}M4$

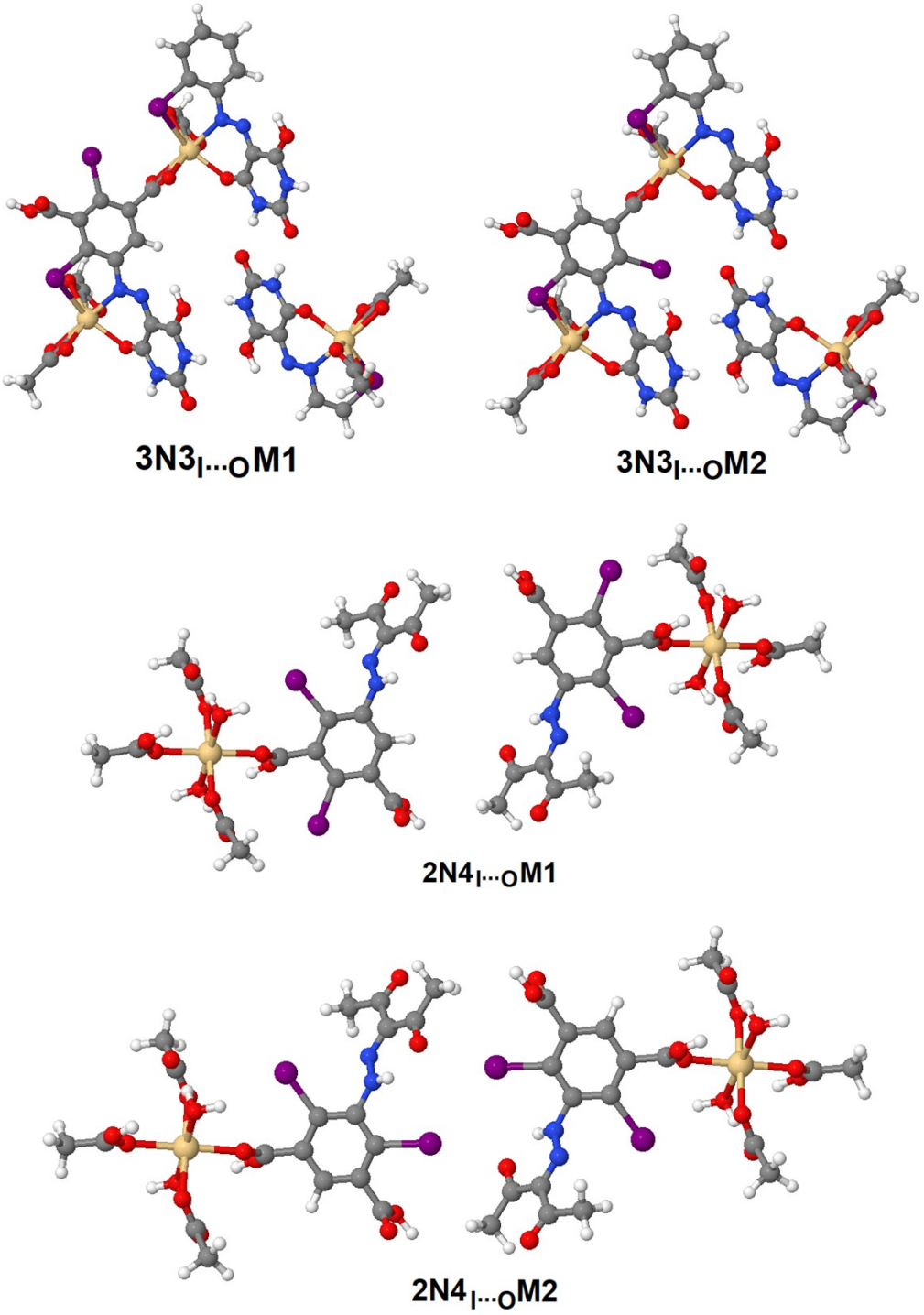


Fig. S4. Model structures used for the calculations of interaction energies.

Table S1. Calculated electron density, ρ_b, its Laplacian, $\nabla^2\rho_b$, potential and kinetic energy densities, V_b and G_b, second eigenvalue of the hessian matrix, $\lambda_{2,b}$, ratio of the first and third eigenvalues of the hessian matrix, $\lambda_{1,b}/\lambda_{3,b}$, at BCPs (in a.u.), second order NBO perturbation energies, E(2), and interaction energies, E_{int} (in kcal/mol).

	I···I						I···O	
	$2N3_{I\cdots I}$	**$5N3_{I\cdots I}$**	**$2N4_{I\cdots I}$**			**3_M**	**$3M3_{I\cdots O}$**	**$2N4_{I\cdots O}$**
			I1···I5	I5···I5'	I1···I5'			
ρ_b	0.0086	0.0085	0.0084	0.0063	0.0051	0.0123	0.0124	0.0121
$\nabla^2\rho_b$	0.0305	0.0304	0.0291	0.0245	0.0199	0.0395	0.0475	0.0452
V_b	–0.0052	–0.0051	–0.0049	–0.0038	–0.0025	–0.0082	–0.0090	–0.0085
G_b	0.0064	0.0064	0.0061	0.0049	0.0037	0.0090	0.0104	0.0099
$\lambda_{2,b}$	–0.0050	–0.0050	–0.0046	–0.0032	–0.0027	–0.0071	–0.0085	–0.0086
$\lambda_{1,b}/\lambda_{3,b}$	–0.129	–0.129	–0.125	–0.113	–0.124	–0.138	–0.138	–0.144
E(2)	2.6[a]	–	3.5[a]	1.7[a]	–	4.1[a]	1.7[b]	1.7[b]
E_{int}	–3.2	–	–2.9	–1.3	–3.7	–5.4	–4.7	–3.3

[a] For the LP(I) → σ*(I–C) transition(s). [b] Overall for the LP(O) → σ*(I–C) and σ(O–C) → σ*(I–C) transitions.

Table S2. Cartesian atomic coordinates (in Å) of the calculated structures.

$5N3_{I\cdots I}$

Cd	10.29399	-1.86492	-0.05112
I	5.83564	-3.90074	-0.40757
I	1.61510	-0.26433	2.03585
O	0.86360	-4.10366	-1.02650
O	8.17721	-1.11475	-0.46468
N	2.86115	-2.78916	0.54926
O	3.81257	2.50117	1.66757
O	8.36351	-2.16096	1.43248
C	5.25327	-2.16767	0.59781
O	4.06187	1.66926	3.65202
C	3.59121	-0.68113	1.52990
N	0.42457	-6.17160	-0.34590
H	-0.27579	-6.20214	-1.05904
N	2.99017	-3.93918	1.07311
C	6.24833	-1.22209	0.92121
C	3.89942	-1.91337	0.93946
O	-0.10035	-8.29596	0.25730
C	4.56609	0.27039	1.82765
C	5.87922	-0.01532	1.51766
C	2.14112	-4.97331	0.78592
C	1.13199	-4.99367	-0.21439
C	7.68939	-1.53642	0.60330
C	4.15006	1.58542	2.44442
N	1.55658	-7.24229	1.31941
H	1.71069	-8.06174	1.87147
C	0.59137	-7.30203	0.40717
C	2.37082	-6.14431	1.57658
I	7.35937	1.35931	2.09013
O	3.25584	-6.27421	2.45894
H	3.82301	-5.45062	2.46414
Cd	1.10078	-1.89495	-0.64467

Cd	2.93614	3.79698	3.38950
I	10.80830	-0.23428	2.62940
O	10.05681	-4.07362	-0.43293
N	12.05436	-2.75912	1.14282
O	11.19175	-1.60870	-2.18198
O	11.47577	0.08622	-0.86337
I	-3.35757	-3.93078	-1.00115
I	-7.57813	-0.29436	1.44228
O	-8.32961	-4.13369	-1.62006
O	-1.01600	-1.14479	-1.05824
N	-6.33206	-2.81920	-0.04430
O	-5.38063	2.47114	1.07403
O	-0.82969	-2.19099	0.83892
C	-3.93994	-2.19771	0.00425
O	-5.13133	1.63923	3.05846
C	-5.60201	-0.71116	0.93633
N	-8.76865	-6.20163	-0.93946
H	-9.46901	-6.23216	-1.65260
N	-6.20304	-3.96923	0.47954
C	-2.94490	-1.25211	0.32765
C	-5.29380	-1.94339	0.34591
O	-9.29354	-8.32600	-0.33626
C	-4.62712	0.24034	1.23409
C	-3.31399	-0.04536	0.92409
C	-7.05209	-5.00336	0.19236
C	-8.06123	-5.02371	-0.80794
C	-1.50384	-1.56645	0.00974
C	-5.04313	1.55538	1.85086
N	-7.63664	-7.27234	0.72584
H	-7.48252	-8.09177	1.27790
C	-8.60184	-7.33207	-0.18640
C	-6.82240	-6.17434	0.98303
I	-1.83383	1.32926	1.49657
O	-5.93736	-6.30425	1.86538
H	-5.37020	-5.48066	1.87058
Cd	-8.09243	-1.92500	-1.23823
Cd	-6.25707	3.76693	2.79594
O	1.99855	-1.63874	-2.77555
O	2.28257	0.05618	-1.45692
O	-8.39517	2.96507	2.79132
O	-8.16920	4.80501	3.92799
C	-11.28383	4.47955	3.17732
C	-12.97720	3.68847	4.70954
C	-10.31124	3.79082	3.93135
C	-12.64142	4.46147	3.59073
C	-12.02509	2.98247	5.44406
C	-10.70719	3.04450	5.04243
C	-8.86476	3.87057	3.50962
I	-5.76670	3.65603	5.93533
O	-6.43998	5.50609	1.37387
N	-4.46626	5.08775	3.40622
O	0.79803	2.99512	3.38489
O	1.02401	4.83504	4.52155

C	-2.09063	4.50958	3.77087
C	-3.78400	3.71852	5.30310
N	-4.30417	6.34284	3.29634
C	-1.11803	3.82086	4.52491
C	-3.44822	4.49151	4.18429
C	-2.83189	3.01252	6.03762
C	-1.51399	3.07454	5.63599
C	-5.12829	7.12268	2.53117
C	-6.14330	6.67347	1.64386
C	0.32845	3.90061	4.10317
I	3.42652	3.68608	6.52890
O	2.75323	5.53611	1.96742
N	4.72697	5.11779	3.99978
O	-10.20921	-1.17483	-1.65180
O	-10.02291	-2.22103	0.24536
C	-13.13315	-2.22775	-0.58931
C	-14.79522	-0.74120	0.34277
C	-12.13810	-1.28216	-0.26591
C	-14.48699	-1.97344	-0.24766
C	-13.82033	0.21031	0.64052
C	-12.50719	-0.07541	0.33052
C	-10.69703	-1.59650	-0.58382
O	-7.19467	-1.66877	-3.36911
O	-6.91064	0.02615	-2.05049
C	-5.64174	1.82819	-6.59055
C	-7.33511	1.03710	-5.05831
C	-4.66914	1.13945	-5.83652
C	-6.99933	1.81009	-6.17712
C	-6.38301	0.33111	-4.32380
C	-5.06510	0.39314	-4.72542
C	-6.82849	-0.49816	-3.14202
C	7.10259	4.53962	4.36444
C	5.40922	3.74855	5.89667
N	4.88904	6.37287	3.88989
C	8.07518	3.85090	5.11846
C	5.74500	4.52155	4.77786
C	6.36132	3.04256	6.63117
C	7.67923	3.10458	6.22955
C	4.06492	7.15272	3.12472
C	3.04988	6.70350	2.23742
C	12.74468	1.88826	-5.40343
C	11.05131	1.09720	-3.87119
C	13.71729	1.19953	-4.64939
C	11.38709	1.87019	-4.99002
C	12.00342	0.39120	-3.13669
C	13.32133	0.45321	-3.53831
C	11.55791	-0.43809	-1.95491
C	14.44647	-2.13763	1.19138
C	12.78441	-0.65108	2.12346
N	12.18337	-3.90916	1.66666
C	15.44153	-1.19204	1.51477
C	13.09262	-1.88331	1.53301
C	13.75930	0.30041	2.42121

C	15.07243	0.01472	2.11122
C	11.33433	-4.94328	1.37949
C	10.32519	-4.96363	0.37919
C	3.55148	1.85823	-5.99699
C	1.85811	1.06716	-4.46475
C	4.52407	1.16950	-5.24295
C	2.19389	1.84015	-5.58358
C	2.81019	0.36116	-3.73025
C	4.12811	0.42318	-4.13187
C	2.36472	-0.46812	-2.54846
H	-6.72618	7.44776	1.14498
C	-4.94929	8.53759	2.63541
H	-9.95422	2.49573	5.60811
H	-12.31566	2.39533	6.31523
H	-14.02154	3.63690	5.01746
H	-13.39963	5.03171	3.05400
H	-10.99357	5.02451	2.27905
H	-12.86309	-3.15179	-1.10049
H	-15.26322	-2.71440	-0.43889
H	-15.83577	-0.51780	0.57823
H	-14.08980	1.15770	1.10736
H	-11.73657	0.66129	0.55749
H	-4.31213	-0.15562	-4.15974
H	-3.61753	1.18949	-6.11888
H	-5.35148	2.37315	-7.48881
H	-7.75752	2.38033	-6.71385
H	-8.37944	0.98553	-4.75040
H	2.46704	7.47779	1.73855
C	4.24391	8.56764	3.22897
H	-3.12244	2.42538	6.90880
H	-1.80037	5.05455	2.87262
H	-0.76102	2.52577	6.20167
H	4.88108	-0.12559	-3.56618
H	5.57567	1.21953	-5.52531
H	3.84174	2.40320	-6.89524
H	1.43569	2.41036	-6.12032
H	0.81378	1.01560	-4.15682
H	9.71928	-5.86794	0.32260
C	11.47758	-6.12725	2.16854
H	14.71654	-3.06169	0.68022
H	16.48956	-1.40172	1.30084
H	15.84306	0.75141	2.33819
H	14.07429	-0.09556	-2.97263
H	14.76889	1.24958	-4.93175
H	13.03494	2.43322	-6.30169
H	10.62890	2.44042	-5.52674
H	10.00698	1.04563	-3.56327
H	13.48985	1.24781	2.88803
H	6.07076	2.45541	7.50234
H	8.43220	2.55582	6.79525
H	9.12679	3.90092	4.83610
H	7.39285	5.08459	3.46618
H	-5.61447	9.28906	2.21008

H	-4.12659	9.03139	3.15248
H	3.57874	9.31908	2.80364
H	5.06662	9.06144	3.74604
H	12.38646	-6.43126	2.68776
H	10.69482	-6.86522	2.34375

$2N3_{I\cdots I}$

I	6.17508	-3.26757	0.28726
I	1.32817	-3.47629	3.95750
O	1.36640	-2.50899	-0.91549
O	8.20189	-2.06671	3.06178
N	3.00537	-3.41309	1.25188
O	3.25342	-2.00121	6.55174
O	8.26026	-4.24016	3.02748
C	5.29502	-3.31448	2.17850
O	3.34079	-4.15607	6.75478
C	3.38433	-3.34472	3.65816
N	1.06491	-4.04408	-2.49186
H	0.46521	-3.38521	-2.94600
N	3.18797	-4.41816	0.49683
C	6.13820	-3.22203	3.30516
C	3.89021	-3.41474	2.35385
O	0.69413	-5.53174	-4.16569
C	4.21015	-3.22561	4.77542
C	5.57414	-3.16540	4.58067
C	2.49365	-4.59274	-0.66945
C	1.62372	-3.65645	-1.29072
C	7.63240	-3.17600	3.10081
C	3.58597	-3.13374	6.14828
N	2.08776	-6.08234	-2.51089
H	2.25711	-6.96027	-2.95876
C	1.25439	-5.24486	-3.12039
C	2.74478	-5.84944	-1.30725
I	6.82039	-3.12347	6.26983
O	3.52252	-6.74371	-0.89002
H	3.99556	-6.40053	-0.07856
Cd	1.32256	-1.83454	1.23477
I	-2.82027	-2.19113	-1.38408
I	-7.66720	-2.39986	2.28618
O	-7.62895	-1.43257	-2.58681
O	-0.79346	-0.99029	1.39045
N	-5.98998	-2.33668	-0.41944
O	-5.74192	-0.92481	4.88043
O	-0.73508	-3.16374	1.35616
C	-3.70033	-2.23806	0.50717
O	-5.65455	-3.07965	5.08346
C	-5.61102	-2.26829	1.98683
N	-7.93045	-2.96766	-4.16318
H	-8.53015	-2.30878	-4.61731
N	-5.80738	-3.34174	-1.17451
C	-2.85717	-2.14560	1.63384
C	-5.10515	-2.33832	0.68254
O	-8.30120	-4.45532	-5.83701
C	-4.78520	-2.14920	3.10408

C	-3.42120	-2.08898	2.90933
C	-6.50170	-3.51632	-2.34079
C	-7.37164	-2.58004	-2.96204
C	-1.36297	-2.09958	1.42949
C	-5.40936	-2.05733	4.47696
N	-6.90760	-5.00592	-4.18224
H	-6.73824	-5.88384	-4.63009
C	-7.74096	-4.16843	-4.79172
C	-6.25058	-4.77302	-2.97856
I	-2.17495	-2.04705	4.59850
O	-5.47282	-5.66730	-2.56135
H	-4.99979	-5.32411	-1.74989
Cd	-7.67279	-0.75812	-0.43656
O	2.44536	0.11152	0.63108
O	2.38550	-0.28317	2.76013
O	-9.78881	0.08612	-0.28088
O	-9.73044	-2.08732	-0.31517
C	-11.85251	-1.06919	-0.03749
C	-10.35830	-1.02317	-0.24184
O	-6.55000	1.18794	-1.04024
O	-6.60985	0.79326	1.08880
C	-5.83977	2.91058	0.40815
C	-6.33899	1.50876	0.14658
C	3.15557	1.83418	2.07948
C	2.65636	0.43234	1.81790
H	-12.35330	-1.01172	-1.00392
H	-12.16057	-0.22696	0.58205
H	-12.12300	-2.00212	0.45700
H	-4.93381	2.86672	1.01263
H	-6.60498	3.47526	0.94076
H	-5.62041	3.40099	-0.54023
H	4.06153	1.79032	2.68395
H	2.39036	2.39885	2.61209
H	3.37492	2.32459	1.13110
H	-6.10020	-3.12784	5.97734
H	2.89515	-4.20427	7.64866
H	9.25574	-4.32692	3.06550

$2N4_{I\cdots I}$

Cd	7.05103	0.72553	0.50643
I	6.66856	-3.34768	1.76445
H	7.52947	-0.59230	-3.01628
I	1.31860	-0.90244	0.31703
I	1.86588	-6.87580	1.40501
O	6.89884	0.16252	-3.19670
O	5.01490	-6.13316	3.13271
O	6.48581	1.58086	-1.47627
O	5.41928	-0.81299	0.10992
O	8.70970	-0.59543	-0.65939
O	4.13097	-0.25353	1.86144
O	-1.58107	-5.14146	1.65059
N	-0.22229	-3.58741	-0.24497
C	6.43660	1.22005	-2.67718
C	-2.23635	-3.11378	-1.34834

N	0.52656	-4.11570	0.68680
H	0.10543	-4.73382	1.35055
C	5.73713	2.14779	-3.63842
O	-3.43662	-3.07808	-1.41663
C	2.69485	-4.94262	1.17243
O	5.31991	-6.72554	1.01025
C	4.51031	-1.04421	0.98999
C	-1.52277	-3.80423	-0.25434
C	3.86452	-2.41196	0.96362
C	2.49581	-2.60602	0.72226
C	4.86716	-5.95940	1.92847
C	-2.23801	-4.59858	0.78722
C	4.62131	-3.52855	1.32847
C	1.89623	-3.85142	0.79173
C	4.04098	-4.80332	1.45244
C	-1.42352	-2.35642	-2.37634
H	-2.05489	-2.11259	-3.23075
H	-0.58418	-2.97108	-2.70161
H	-1.04771	-1.43556	-1.93039
C	-3.74903	-4.66368	0.82971
H	-4.06339	-5.25770	1.68787
H	-4.11375	-5.12892	-0.08605
H	-4.15435	-3.65516	0.91161
H	5.90725	-5.77102	3.40209
H	9.22325	0.26143	-0.70491
H	9.25202	-1.22480	-0.10279
O	7.20323	1.28855	4.20956
O	7.61628	-0.12980	2.48912
O	8.68280	2.26407	0.90295
O	5.39237	2.04650	1.67222
O	9.97111	1.70460	-0.84858
C	7.66549	0.23101	3.69003
C	8.36495	-0.69671	4.65126
C	9.59177	2.49528	0.02286
C	10.23755	3.86302	0.04924
H	4.87883	1.18964	1.71778
H	4.85005	2.67585	1.11565
H	6.57260	2.04335	4.02912
Cd	-6.52712	0.09646	-1.79633
H	-6.04867	-1.22137	-5.31904
O	-6.67930	-0.46657	-5.49947
O	-7.09235	0.95177	-3.77902
O	-8.15888	-1.44208	-2.19285
O	-4.86846	-1.22450	-2.96214
O	-9.44720	-0.88261	-0.44131
C	-7.14158	0.59097	-4.97993
C	-7.84103	1.51870	-5.94118
C	-9.06786	-1.67329	-1.31276
C	-9.71363	-3.04102	-1.33914
H	-4.35492	-0.36764	-3.00769
H	-4.32614	-1.85386	-2.40556
I	-2.69238	-0.21151	1.10524
I	-6.14464	4.16967	-3.05435

I	-0.79467	1.72442	-1.60694
I	-8.06850	-2.09237	3.04987
I	-3.14891	-4.49086	5.44572
I	-1.34198	7.69779	-2.69491
O	-6.37493	0.65946	1.90680
O	-4.49098	6.95514	-4.42264
O	-5.96188	-0.75887	0.18636
O	-4.89537	1.63499	-1.39980
O	-8.18578	1.41742	-0.63053
O	-3.60704	1.07550	-3.15135
N	-1.05387	-1.31550	3.71543
C	-3.81538	-1.36124	2.44576
O	-6.70674	-4.87847	4.83545
C	-5.99442	-2.13425	3.16867
O	0.28489	-3.77791	3.77586
O	2.10498	5.96344	-2.94050
N	0.74624	4.40943	-1.04494
C	-5.91266	-0.39808	1.38726
C	2.76027	3.93578	0.05844
N	-0.00263	4.93769	-1.97669
H	0.41849	5.55580	-2.64046
O	-6.34672	-3.15160	6.18986
C	-5.21320	-1.32580	2.34850
C	-3.99100	-3.06307	4.15775
O	3.96055	3.90007	0.12674
O	2.06095	-0.13997	4.62666
C	-2.17092	5.76463	-2.46234
N	-1.79381	-2.36347	3.48536
H	-1.36909	-3.26309	3.38390
O	-4.79599	7.54754	-2.30017
C	-3.98638	1.86620	-2.27990
C	2.04668	4.62624	-1.03556
C	-5.38254	-2.99843	4.07875
C	-3.34061	3.23394	-2.25352
C	0.92900	-2.77502	4.00643
C	-1.97190	3.42800	-2.01219
C	0.22209	-1.43109	3.94324
C	0.95235	-0.15759	4.18138
C	-4.34324	6.78140	-3.21836
C	2.76194	5.42057	-2.07713
C	-4.09738	4.35054	-2.61836
C	-1.37230	4.67342	-2.08164
C	-3.51705	5.62532	-2.74235
C	0.23295	1.11676	3.81923
H	-0.09313	1.06672	2.78035
H	-0.63465	1.23965	4.46752
H	0.90805	1.96259	3.94924
C	-3.19805	-2.22978	3.38023
C	1.94743	3.17841	1.08643
H	2.57881	2.93457	1.94083
H	1.10811	3.79310	1.41170
H	1.57163	2.25754	0.64048
C	4.27296	5.48567	-2.11961

H	4.58731	6.07968	-2.97777
H	4.63767	5.95093	-1.20385
H	4.67826	4.47715	-2.20152
C	-6.22645	-3.78580	5.04497
C	2.36142	-2.86200	4.28162
H	2.71411	-3.86846	4.05634
H	2.89367	-2.14202	3.65999
H	2.54324	-2.63968	5.33311
H	-5.38333	6.59300	-4.69200
H	-6.82209	-3.72254	6.85922
H	-8.69933	0.56057	-0.58500
H	-8.72811	2.04677	-1.18712
H	-7.00557	1.41427	1.72638
H	-8.33834	0.93312	-6.71438
H	-7.10992	2.18283	-6.40214
H	-8.58039	2.11068	-5.40174
H	-8.96480	-3.80073	-1.11517
H	-10.13386	-3.22537	-2.32783
H	-10.50752	-3.08239	-0.59344
H	9.74333	4.51214	-0.67360
H	11.29309	3.77140	-0.20679
H	10.14151	4.29093	1.04709
H	9.44385	-0.58246	4.54636
H	8.08544	-1.72684	4.43037
H	8.07111	-0.45137	5.67182
H	4.66648	1.94378	-3.62614
H	6.12578	1.98908	-4.64431
H	5.91359	3.18103	-3.33953

$3M3_{I\cdots O}$

Cd	-1.13904	2.93299	-2.24085
I	-1.35550	-1.61156	-0.38373
I	-6.60137	-2.47303	2.57355
O	-3.42662	-5.96032	1.01055
O	-2.75904	1.34568	-1.97522
N	-3.73632	-3.13391	1.35202
O	-8.04177	0.22171	0.76356
O	-1.80989	1.92679	-0.10710
C	-3.19680	-0.94543	0.33695
O	-7.25731	0.97710	2.63605
C	-5.31004	-1.27655	1.46196
N	-1.81310	-6.82779	2.26611
H	-2.08139	-7.72009	1.90302
N	-2.67345	-3.25188	2.03760
C	-3.59350	0.37189	0.02684
C	-4.05355	-1.77973	1.10129
O	-0.18603	-7.82104	3.49831
C	-5.72032	0.01548	1.13524
C	-4.85538	0.81877	0.42205
C	-2.13258	-4.47086	2.34480
C	-2.54112	-5.73504	1.84052
C	-2.64435	1.26304	-0.73570
C	-7.10059	0.47659	1.54150
N	-0.40182	-5.60027	3.57093

H	0.37774	-5.55474	4.19560
C	-0.75833	-6.80552	3.13776
C	-1.01433	-4.39737	3.23542
I	-5.42025	2.80639	0.04994
O	-0.52489	-3.34486	3.71643
H	-0.99772	-2.56122	3.31353
Cd	-5.29435	-4.72578	0.74995
I	-2.44605	5.18573	-0.41725
O	0.72870	1.69845	-1.98026
N	0.41900	4.52485	-1.63879
O	-0.88243	2.80569	-4.54958
O	-2.30463	4.29204	-3.87109
I	8.01067	-7.23879	-0.45974
O	4.83591	-3.75150	1.10325
N	5.14561	-6.57791	0.76179
H	4.80486	-8.57284	1.59953
C	6.71933	-8.43527	0.65185
N	3.22240	-2.88403	-0.15229
H	3.49069	-1.99173	0.21079
N	4.08275	-6.45993	0.07620
C	5.46285	-7.93209	1.01251
O	1.59532	-1.89077	-1.38450
H	7.04005	-9.44523	0.90723
C	3.54188	-5.24097	-0.23098
C	3.95042	-3.97678	0.27329
N	1.81111	-4.11154	-1.45712
H	1.03155	-4.15709	-2.08179
C	2.16762	-2.90629	-1.02395
C	2.42361	-5.31445	-1.12161
O	1.93418	-6.36696	-1.60262
H	2.40702	-7.15061	-1.19971
Cd	6.70364	-4.98604	1.36386
H	1.92042	6.36535	-3.03034
C	0.95851	6.71334	-2.65386
C	-1.15473	6.38221	-1.52885
N	2.34221	0.83097	-0.72470
H	2.07391	-0.06132	-1.08779
N	1.48185	4.40689	-0.95320
C	0.56182	8.03065	-2.96397
C	0.10175	5.87904	-1.88951
O	3.96928	-0.16227	0.50750
C	-1.56501	7.67425	-1.85557
C	-0.70006	8.47754	-2.56876
C	2.02273	3.18791	-0.64601
C	1.61418	1.92373	-1.15029
H	1.24750	8.67445	-3.51485
H	-2.56077	8.00691	-1.56248
N	3.75350	2.05849	0.58012
H	4.53305	2.10403	1.20480
C	3.39698	0.85325	0.14695
C	3.14099	3.26141	0.24461
H	-0.99332	9.50942	-2.76194
O	3.63043	4.31391	0.72562

H	3.15759	5.09755	0.32272
C	-1.76327	3.66411	-4.75751
C	-5.91857	-3.99466	-1.76670
C	-2.25562	3.82332	-6.17703
O	7.37450	-3.97985	-0.76991
O	8.32364	-3.39873	1.09822
C	8.20895	-3.31610	-0.14130
O	6.44705	-4.85874	3.67258
O	7.86924	-6.34509	2.99409
C	7.32787	-5.71716	3.88051
O	-6.91435	-6.31309	1.01559
O	-5.96520	-5.73198	2.88371
C	-6.79966	-6.39573	2.25511
O	-5.03775	-4.85308	-1.55877
O	-6.45994	-3.36673	-0.88028
C	-6.41094	-3.83544	-3.18622
H	-8.97767	0.56071	0.85911
C	-7.73995	-7.36871	3.03949
H	-7.29198	-8.36196	3.06879
H	-8.70717	-7.42092	2.53965
H	-7.87594	-7.00129	4.05662
H	-5.94505	-4.59067	-3.81919
H	-6.14921	-2.84270	-3.55233
H	-7.49370	-3.95812	-3.21110
C	7.75631	-5.99854	5.35813
H	8.53557	-6.76054	5.37161
H	6.89459	-6.34996	5.92560
H	8.13733	-5.08120	5.80688
C	9.14924	-2.34311	-0.92567
H	8.64332	-1.99671	-1.82685
H	10.06491	-2.86623	-1.20131
H	9.39476	-1.48835	-0.29546
H	-2.07715	2.90060	-6.72910
H	-1.72129	4.64313	-6.65709
H	-3.32359	4.04108	-6.16886

$2N4_{I\cdots O}$

Cd	9.72722	1.47655	-1.28779
H	10.83923	0.45098	-4.76438
O	11.70590	0.78793	-4.39649
O	11.76189	1.24973	-2.17707
O	9.52831	3.29270	-2.64758
O	8.92643	-0.01945	-3.01287
O	9.30257	4.80203	-1.00090
C	12.28115	1.07353	-3.30583
C	13.77901	1.22202	-3.39660
C	9.16095	4.42953	-2.17123
C	8.47978	5.38399	-3.12698
H	9.35109	-0.73486	-2.45802
H	7.94446	-0.20831	-3.02048
I	6.27263	-1.23049	0.70138
I	5.77992	4.76736	0.77177
I	0.79925	1.47492	0.99138
O	7.74854	2.16518	1.82090

O	7.69256	1.70338	-0.39852
O	9.92614	-0.33959	0.07199
O	10.52801	2.97256	0.43728
O	10.15188	-1.84893	-1.57469
N	3.27459	-1.76706	1.90158
C	5.06761	0.47004	0.89133
O	2.24435	4.71538	0.22202
C	4.90126	2.88665	0.86461
O	1.04529	-2.33960	0.30101
C	7.17330	1.87958	0.73024
O	2.45122	4.28179	2.39349
C	5.67544	1.73109	0.82102
C	2.89753	1.53670	0.99633
O	2.34862	-4.72606	3.41853
N	2.97518	-0.86391	1.01086
H	2.26182	-1.04606	0.33414
C	10.29350	-1.47642	-0.40436
C	3.51167	2.78899	0.95933
C	10.97467	-2.43088	0.55139
C	1.34927	-3.14180	1.16003
C	2.57591	-2.85933	2.01173
C	3.02878	-3.81115	3.06090
C	4.39867	-3.57768	3.64530
H	5.13387	-3.53671	2.84163
H	4.40349	-2.63439	4.19144
H	4.64591	-4.39356	4.32452
C	3.65777	0.37494	1.00114
C	2.68440	4.03572	1.12363
C	0.58219	-4.37421	1.32697
H	-0.10041	-4.49395	0.48565
H	1.26499	-5.22297	1.36554
H	0.01139	-4.32375	2.25420
H	1.81973	5.05091	2.49185
H	10.10336	3.68797	-0.11757
H	11.50999	3.16142	0.44489
H	8.61521	2.50213	2.18879
Cd	-10.88938	-1.45321	2.29907
I	-7.43478	1.25383	0.30989
H	-9.77737	-2.47879	-1.17752
I	-6.94207	-4.74402	0.23950
I	-1.96141	-1.45158	0.01989
O	-8.91070	-2.14183	-0.80962
O	-8.85471	-1.68004	1.40979
O	-11.08829	0.36293	0.93928
O	-11.69017	-2.94922	0.57399
O	-11.31404	1.87227	2.58597
N	-4.43675	1.79040	-0.89030
C	-6.22977	-0.44670	0.11994
O	-3.40651	-4.69204	0.78926
C	-6.06341	-2.86331	0.14666
O	-2.20744	2.36294	0.71027
C	-8.33546	-1.85624	0.28103
O	-3.61337	-4.25845	-1.38222

C	-6.83759	-1.70775	0.19026
C	-4.05968	-1.51336	0.01494
O	-3.51077	4.74940	-2.40726
N	-4.13734	0.88725	0.00042
H	-3.42398	1.06940	0.67713
C	-11.45565	1.49976	1.41563
C	-4.67383	-2.76565	0.05194
C	-12.13682	2.45422	0.45988
C	-2.51143	3.16514	-0.14875
C	-3.73806	2.88267	-1.00046
C	-4.19094	3.83449	-2.04962
C	-5.56082	3.60103	-2.63403
H	-6.29603	3.56005	-1.83036
H	-5.56564	2.65773	-3.18017
H	-5.80806	4.41690	-3.31324
C	-4.81993	-0.35160	0.01013
C	-3.84656	-4.01238	-0.11236
C	-1.74435	4.39755	-0.31570
H	-1.06175	4.51729	0.52562
H	-2.42714	5.24631	-0.35427
H	-1.17355	4.34709	-1.24292
H	-2.98189	-5.02757	-1.48058
H	-11.26551	-3.66463	1.12884
H	-12.67214	-3.13808	0.56638
O	-12.86806	-0.76459	5.40776
O	-12.92405	-1.22639	3.18834
O	-10.69047	-3.26936	3.65885
O	-10.08859	0.04279	4.02414
O	-10.46472	-4.77869	2.01217
C	-13.44330	-1.05019	4.31710
C	-14.94117	-1.19868	4.40788
C	-10.32311	-4.40619	3.18250
C	-9.64194	-5.36064	4.13825
H	-10.51325	0.75820	3.46929
H	-9.10662	0.23166	4.03175
H	-12.00139	-0.42764	5.77565
H	-15.21723	-2.23192	4.19745
H	-15.41625	-0.54031	3.68061
H	-15.27263	-0.93114	5.41118
H	-13.21668	2.31800	0.51845
H	-11.79974	2.25248	-0.55685
H	-11.88481	3.47982	0.72947
H	-9.03968	-6.07222	3.57343
H	-10.39564	-5.89846	4.71336
H	-8.99973	-4.79891	4.81654
H	14.04597	1.62001	-4.37559
H	14.24958	0.24845	-3.25950
H	14.12410	1.90493	-2.62033
H	7.40654	5.19363	-3.12719
H	8.87530	5.23586	-4.13182
H	8.66674	6.41012	-2.81051
H	11.75635	-2.97726	0.02365
H	10.24189	-3.13499	0.94551

H	11.41652	-1.86803	1.37359

3_M initial

I	-4.98536	4.36409	-2.68947
I	-0.20103	2.42624	0.52948
O	-1.60337	7.13153	-0.23001
O	-6.81351	1.36144	-1.74614
N	-2.10514	4.43298	-1.04682
O	-5.72056	0.97926	-3.58675
C	-3.89578	2.86918	-1.72432
C	-2.03144	2.08416	-0.40181
N	-0.82062	8.41556	-1.86430
H	-0.75042	9.14688	-1.18590
N	-1.85943	4.89629	-2.20379
C	-4.44623	1.57159	-1.67834
C	-2.64487	3.12820	-1.10588
O	-0.02254	9.82078	-3.45827
C	-2.58320	0.80562	-0.32871
C	-3.78247	0.57021	-0.96774
C	-1.39626	6.16915	-2.39892
C	-1.27754	7.19152	-1.41908
C	-5.74787	1.30169	-2.39205
N	-0.59756	7.74122	-4.03146
H	-0.35376	7.94559	-4.97953
C	-0.45497	8.72316	-3.14668
C	-1.05393	6.45588	-3.75898
I	-4.54183	-1.38722	-0.97076
O	-1.15426	5.66023	-4.72621
H	-1.58523	4.81814	-4.40192
Cd	-1.54361	5.26430	1.03105
I	2.76047	-3.21924	3.12790
I	7.99872	-1.77071	0.39486
O	7.13031	-5.66881	3.35017
O	-0.20403	5.93675	2.75380
N	5.84550	-3.52629	1.95016
O	7.32138	1.66894	0.96284
O	0.88893	5.55457	0.91319
C	3.99676	-1.89183	2.09682
O	6.59213	1.12804	-1.00383
C	6.08627	-1.27414	1.05115
N	6.53939	-7.68003	2.61661
H	7.19532	-8.05470	3.27187
N	5.17547	-4.47011	1.42680
C	3.51888	-0.58588	1.86238
C	5.29317	-2.26010	1.65185
O	6.00434	-9.78372	1.95287
C	5.63068	0.02685	0.84073
C	4.35416	0.35020	1.25063
C	5.48106	-5.78757	1.63579
C	6.43509	-6.30515	2.55302
C	0.86164	5.87700	2.10791
C	6.55539	1.03924	0.20607
N	4.93818	-8.05019	1.03540
H	4.39367	-8.68668	0.48916

C	5.82950	-8.57913	1.86792
C	4.69444	-6.69279	0.85419
I	3.62279	2.26841	0.81045
O	3.79048	-6.37039	0.04325
H	3.65879	-5.38025	0.09100
O	-3.61033	5.82907	1.93767
O	-2.97653	3.79192	2.31251
C	-4.85425	4.57025	3.49904
C	-3.74557	4.71531	2.48288
H	-5.47703	3.71476	3.23760
H	-4.42270	4.41679	4.48812
H	-5.46274	5.47454	3.50442
H	7.19526	1.73612	-1.51999
H	-6.49502	0.61576	-4.10447
C	2.16328	6.14690	2.82163
H	2.91347	6.46930	2.09959
H	2.50223	5.23641	3.31579
H	2.01438	6.92995	3.56508
H	2.50617	-0.30995	2.15632
H	-2.07849	0.01090	0.22063

3$_{M}$ optimized

53	6.915494	1.241873	-1.290105
53	1.351741	-0.249867	0.391572
8	5.619481	-2.711128	1.050746
8	6.398992	4.658475	-0.090117
7	4.350925	-0.554862	-0.332613
8	5.745681	4.537545	-2.237710
6	4.978039	1.787875	-0.782543
6	2.740946	1.213360	-0.061924
7	5.914771	-4.489180	-0.310063
1	6.179123	-5.028319	0.515965
7	4.694724	-1.140265	-1.377103
6	4.647132	3.140725	-0.694280
6	4.019852	0.821216	-0.461498
8	6.290603	-6.315527	-1.640825
6	2.407331	2.558268	0.008461
6	3.362278	3.520084	-0.300210
6	5.123211	-2.448421	-1.276535
6	5.531146	-3.171340	-0.079482
6	5.696596	4.189011	-0.944664
7	5.633100	-4.360201	-2.614732
1	5.679669	-4.804618	-3.531687
6	5.970301	-5.161694	-1.512572
6	5.242097	-3.073352	-2.510526
53	2.863057	5.526807	-0.142617
8	4.979114	-2.470121	-3.649787
1	4.734808	-1.543294	-3.426036
48	3.978850	-1.358294	1.798117
53	-4.545593	2.312961	0.858633
53	-7.411669	-2.910058	-0.560516
8	-9.984112	0.020151	0.045179
8	3.028170	-3.109391	2.913643
7	-7.124490	0.081706	0.079395

8	-4.390417	-4.766060	0.427819
8	2.887781	-3.264759	0.707081
6	-4.617889	0.290464	0.327939
8	-4.234426	-4.204705	-1.743389
6	-5.692969	-1.807624	-0.188226
7	-10.863523	2.084039	-0.314095
1	-11.789328	1.667776	-0.211845
7	-7.217987	1.266938	-0.303807
6	-3.383962	-0.352980	0.317212
6	-5.798300	-0.424396	0.058945
8	-11.824500	4.130191	-0.692950
6	-4.457651	-2.450374	-0.196694
6	-3.300966	-1.714833	0.050088
6	-8.473571	1.847699	-0.328693
6	-9.774431	1.190744	-0.167760
6	2.657219	-3.716336	1.861580
6	-4.368929	-3.933165	-0.437111
7	-9.551350	3.950251	-0.727513
1	-9.477191	4.950625	-0.906215
6	-10.844762	3.431100	-0.584386
6	-8.426591	3.204790	-0.608166
53	-1.442769	-2.619298	0.033008
8	-7.304544	3.878972	-0.766106
1	-6.555546	3.260204	-0.587464
8	5.511288	0.349719	2.180977
8	3.429613	0.781577	2.789375
6	5.038752	2.560379	2.952847
6	4.628215	1.142722	2.628388
1	5.599969	2.988074	2.106824
1	4.162878	3.178164	3.187680
1	5.719325	2.539346	3.818206
1	-4.187262	-5.175786	-1.829760
1	6.441646	5.216436	-2.325675
6	1.888179	-5.008155	2.013627
1	2.232391	-5.738727	1.268098
1	0.825284	-4.799989	1.811480
1	1.986978	-5.407763	3.030075
1	-2.472136	0.210712	0.523344
1	1.408104	2.854002	0.327991

$1N3_M$

I	2.27899	-0.52938	1.03050
I	-2.78955	2.36055	-0.70236
O	-2.45353	-2.16301	1.32433
O	4.11152	1.12624	-1.64536
N	-0.94531	0.19869	0.73380
O	-1.04821	3.70341	-3.49112
O	4.19533	2.36088	0.14268
C	1.27995	0.99917	0.01387
O	-0.95069	5.12164	-1.85673
C	-0.72008	2.13393	-0.72994
N	-2.63817	-2.56935	3.49990
H	-3.21500	-3.34794	3.25280
N	-0.70450	0.17526	1.98083

C	2.04909	1.90043	-0.75098
C	-0.13199	1.13629	0.05800
O	-2.88627	-3.08559	5.69633
C	0.03208	3.01130	-1.51026
C	1.40493	2.87976	-1.50871
C	-1.32175	-0.70387	2.82872
C	-2.16067	-1.79148	2.46445
C	3.55264	1.77522	-0.73823
C	-0.67864	4.04671	-2.35027
N	-1.59429	-1.35696	5.12519
H	-1.38750	-1.20473	6.09166
C	-2.39638	-2.37607	4.83296
C	-1.01728	-0.48290	4.20987
I	2.54131	4.28623	-2.57582
O	-0.25789	0.41019	4.66203
H	0.15915	0.89287	3.89190
Cd	-2.64056	-0.80656	-0.46603
O	-4.77115	-1.26519	-1.14777
O	-4.68734	-0.03056	0.64028
C	-6.83356	-0.49100	-0.25338
C	-5.32999	-0.61621	-0.24064
O	-1.50283	-2.37490	-1.75372
O	-1.69300	-0.41668	-2.65999
C	-0.90423	-2.16290	-4.02671
C	-1.37078	-1.58573	-2.71068
H	-7.27280	-1.33329	0.28114
H	-7.18924	-0.48913	-1.28371
H	-7.12474	0.43985	0.23321
H	-0.03790	-1.60462	-4.38150
H	-1.70763	-2.09159	-4.75988
H	-0.63061	-3.20883	-3.88809
H	-1.45145	5.85663	-2.31387
H	5.19105	2.44939	0.16855

$1N4_M$

Cd	9.72722	1.47655	-1.28779
H	10.83923	0.45098	-4.76438
O	11.70590	0.78793	-4.39649
O	11.76189	1.24973	-2.17707
O	9.52831	3.29270	-2.64758
O	8.92643	-0.01945	-3.01287
O	9.30257	4.80203	-1.00090
C	12.28115	1.07353	-3.30583
C	13.77901	1.22202	-3.39660
C	9.16095	4.42953	-2.17123
C	8.47978	5.38399	-3.12698
H	9.35109	-0.73486	-2.45802
H	7.94446	-0.20831	-3.02048
I	6.27263	-1.23049	0.70138
I	5.77992	4.76736	0.77177
I	0.79925	1.47492	0.99138
O	7.74854	2.16518	1.82090
O	7.69256	1.70338	-0.39852
O	9.92614	-0.33959	0.07199

O	10.52801	2.97256	0.43728
O	10.15188	-1.84893	-1.57469
N	3.27459	-1.76706	1.90158
C	5.06761	0.47004	0.89133
O	2.24435	4.71538	0.22202
C	4.90126	2.88665	0.86461
O	1.04529	-2.33960	0.30101
C	7.17330	1.87958	0.73024
O	2.45122	4.28179	2.39349
C	5.67544	1.73109	0.82102
C	2.89753	1.53670	0.99633
O	2.34862	-4.72606	3.41853
N	2.97518	-0.86391	1.01086
H	2.26182	-1.04606	0.33414
C	10.29350	-1.47642	-0.40436
C	3.51167	2.78899	0.95933
C	10.97467	-2.43088	0.55139
C	1.34927	-3.14180	1.16003
C	2.57591	-2.85933	2.01173
C	3.02878	-3.81115	3.06090
C	4.39867	-3.57768	3.64530
H	5.13387	-3.53671	2.84163
H	4.40349	-2.63439	4.19144
H	4.64591	-4.39356	4.32452
C	3.65777	0.37494	1.00114
C	2.68440	4.03572	1.12363
C	0.58219	-4.37421	1.32697
H	-0.10041	-4.49395	0.48565
H	1.26499	-5.22297	1.36554
H	0.01139	-4.32375	2.25420
H	1.81973	5.05091	2.49185
H	10.10336	3.68797	-0.11757
H	11.50999	3.16142	0.44489
H	8.61521	2.50213	2.18879
H	14.04597	1.62001	-4.37559
H	14.24958	0.24845	-3.25950
H	14.12410	1.90493	-2.62033
H	7.40654	5.19363	-3.12719
H	8.87530	5.23586	-4.13182
H	8.66674	6.41012	-2.81051
H	11.75635	-2.97726	0.02365
H	10.24189	-3.13499	0.94551
H	11.41652	-1.86803	1.37359

$2N3_{I\ldots I}M1$

I	8.23165	-0.30395	0.67886
I	3.08330	2.93577	0.60494
O	3.54610	-1.98119	0.06412
O	10.00893	2.52081	-0.77372
N	4.98993	0.39082	0.76415
O	4.77513	5.54890	-1.10440
O	10.07007	2.68126	1.39399
C	7.19011	1.50060	0.56807
O	4.84447	5.94579	1.02397

C	5.15773	2.80576	0.48424
N	3.38314	-3.43797	1.73253
H	2.82531	-3.99815	1.12015
N	5.23764	-0.25505	1.82956
C	7.93189	2.68385	0.37175
C	5.77536	1.56138	0.66339
O	3.15966	-5.00162	3.36267
C	5.88303	3.97585	0.26230
C	7.25880	3.89576	0.20887
C	4.64761	-1.45754	2.11002
C	3.83514	-2.23122	1.23784
C	9.43821	2.60677	0.33228
C	5.14157	5.27609	0.05633
N	4.40376	-3.19040	3.75691
H	4.61150	-3.54365	4.66910
C	3.62668	-3.94062	2.98187
C	4.95338	-1.95916	3.41540
I	8.35309	5.67664	0.01097
O	5.69179	-1.39963	4.26414
H	6.09231	-0.58317	3.84821
Cd	3.31502	0.09015	-0.79412
I	-0.58380	-2.83743	-0.18004
I	-5.73217	0.40231	-0.25396
O	-5.26936	-4.51464	-0.79476
O	1.19348	-0.01266	-1.63261
N	-3.82552	-2.14264	-0.09472
O	-4.04032	3.01546	-1.96326
O	1.25463	0.14781	0.53511
C	-1.62534	-1.03286	-0.29081
O	-3.97098	3.41234	0.16509
C	-3.65772	0.27230	-0.37465
N	-5.43232	-5.97143	0.87364
H	-5.99016	-6.53160	0.26125
N	-3.57781	-2.78852	0.97068
C	-0.88359	0.15040	-0.48715
C	-3.04010	-0.97206	-0.19549
O	-5.65578	-7.53507	2.50379
C	-2.93242	1.44238	-0.59657
C	-1.55664	1.36229	-0.65001
C	-4.16784	-3.99101	1.25113
C	-4.98032	-4.76467	0.37896
C	0.62274	0.07332	-0.52660
C	-3.67386	2.74263	-0.80255
N	-4.41170	-5.72389	2.89803
H	-4.20395	-6.07711	3.81021
C	-5.18877	-6.47408	2.12298
C	-3.86209	-4.49260	2.55652
O	-3.12365	-3.93309	3.40526
H	-2.72314	-3.11664	2.98933
Cd	-5.50044	-2.44332	-1.65301
O	4.48616	-0.58108	-2.68889
O	4.24097	1.56100	-2.48010
O	-7.62197	-2.54612	-2.49148

O	-7.56084	-2.38565	-0.32377
C	-9.69903	-2.38307	-1.34602
C	-8.19270	-2.46014	-1.38547
O	-4.32931	-3.11454	-3.54778
O	-4.57449	-0.97247	-3.33900
C	-3.74801	-1.76562	-5.39501
C	-4.22254	-1.94637	-3.97202
C	5.06743	0.76784	-4.53615
C	4.59292	0.58708	-3.11314
H	-10.11369	-3.39064	-1.31556
H	-10.05992	-1.86838	-2.23650
H	-10.01159	-1.83451	-0.45752
H	-2.89818	-1.08325	-5.41068
H	-4.55673	-1.35271	-5.99797
H	-3.44683	-2.73049	-5.80288
H	5.91726	1.45020	-4.55182
H	4.25871	1.18075	-5.13910
H	5.36860	-0.19703	-4.94402
H	-4.49284	4.26494	0.13887
H	4.32262	6.79839	0.99776
H	11.05845	2.81299	1.46956
H	-0.97913	2.27017	-0.82419

$2N3_{I...I}M2$

I	8.22386	-1.07357	0.70467
I	3.37695	2.59667	0.91339
O	3.41518	-2.27632	-0.05391
O	10.25067	1.70095	-0.49619
N	5.05415	-0.10895	0.85019
O	5.30220	5.19091	-0.56169
O	10.30904	1.66665	1.67726
C	7.34380	0.81767	0.75158
O	5.38957	5.39395	1.59317
C	5.43311	2.29733	0.78182
N	3.11369	-3.85269	1.48118
H	2.51399	-4.30683	0.82231
N	5.23675	-0.86400	1.85526
C	8.18698	1.94433	0.65913
C	5.93899	0.99302	0.85184
O	2.74291	-5.52652	2.96884
C	6.25893	3.41459	0.66271
C	7.62292	3.21984	0.60250
C	4.54243	-2.03028	2.02984
C	3.67250	-2.65155	1.09355
C	9.68118	1.73998	0.61310
C	5.63475	4.78745	0.57084
N	4.13654	-3.87172	3.51944
H	4.30589	-4.31959	4.39737
C	3.30317	-4.48122	2.68196
C	4.79356	-2.66808	3.28654
H	8.26992	4.09678	0.58073
O	5.57130	-2.25085	4.18081
H	6.04434	-1.43939	3.83763
Cd	3.37134	-0.12606	-0.72836

I	-0.77149	-2.74491	-0.37177
I	-5.61842	0.92535	-0.16304
O	-5.58017	-3.94764	-1.13033
O	1.25532	0.02962	-1.57261
N	-3.94120	-1.78027	-0.22622
O	-3.69314	3.51960	-1.63809
O	1.31370	-0.00467	0.60084
C	-1.65155	-0.85366	-0.32484
O	-3.60577	3.72263	0.51675
C	-3.56224	0.62600	-0.29461
N	-5.88167	-5.52401	0.40476
H	-6.48137	-5.97814	-0.25412
N	-3.75860	-2.53534	0.77884
C	-0.80839	0.27301	-0.41730
C	-3.05637	-0.67829	-0.22458
O	-6.25242	-7.19784	1.89242
C	-2.73642	1.74325	-0.41370
C	-1.37242	1.54850	-0.47392
C	-4.45292	-3.70162	0.95342
C	-5.32286	-4.32287	0.01714
C	0.68581	0.06866	-0.46332
C	-3.36058	3.11613	-0.50557
N	-4.85882	-5.54307	2.44302
H	-4.68946	-5.99092	3.32094
C	-5.69218	-6.15255	1.60553
C	-4.20180	-4.33939	2.21012
I	-0.12617	3.23767	-0.51585
O	-3.42404	-3.92218	3.10440
H	-2.95101	-3.11072	2.76121
Cd	-5.62401	-1.79739	-1.80478
O	4.49414	-0.72975	-2.67442
O	4.43428	1.39930	-2.27973
O	-7.74003	-1.64171	-2.64902
O	-7.68166	-1.67600	-0.47558
C	-9.80373	-1.39832	-1.49371
C	-8.30952	-1.60267	-1.53973
O	-4.50122	-2.40107	-3.75084
O	-4.56107	-0.27203	-3.35616
C	-3.79099	-0.95268	-5.47348
C	-4.29021	-1.21425	-4.07166
C	5.20435	0.71865	-4.39708
C	4.70514	0.45707	-2.99524
H	-10.30452	-2.36475	-1.55118
H	-10.11179	-0.77878	-2.33594
H	-10.07422	-0.90383	-0.56078
H	-2.88503	-0.34820	-5.42962
H	-4.55620	-0.42007	-6.03816
H	-3.57163	-1.90106	-5.96389
H	6.11031	1.32312	-4.35322
H	4.43914	1.25126	-4.96175
H	5.42370	-0.22973	-4.88749
H	-4.05142	4.61651	0.56494
H	4.94393	6.28783	1.64137

H	11.30452	1.70467	1.76402

$2N4_{I...I}M1$

Cd	6.94483	0.10498	1.92817
I	6.66910	-4.11826	1.28933
H	8.06711	0.39939	-1.68138
H	2.03881	-2.11959	0.01705
I	2.25487	-7.16392	-1.33386
O	7.41906	1.15973	-1.63777
O	5.02965	-7.22101	1.06409
O	6.63746	1.71810	0.41637
O	5.51318	-1.12182	0.65059
O	8.85871	-0.59952	0.62588
O	3.92773	-1.35500	2.22303
O	-1.30564	-5.69586	-0.99140
N	0.21677	-3.48631	-1.80052
C	6.80447	1.89862	-0.81420
C	-1.62780	-2.59075	-2.93793
N	0.84637	-4.35889	-1.05871
H	0.37254	-5.19961	-0.79668
C	6.19882	3.14568	-1.40748
O	-2.80171	-2.52954	-3.19245
C	2.96598	-5.31357	-0.59291
O	5.70753	-6.86090	-1.02387
C	4.49648	-1.70331	1.18202
C	-1.04656	-3.67886	-2.12494
C	3.96503	-2.93176	0.47708
C	2.66934	-3.00564	-0.05678
C	5.06092	-6.55460	0.03592
C	-1.85656	-4.83897	-1.65012
C	4.73484	-4.09793	0.46942
C	2.15933	-4.16371	-0.61722
C	4.23737	-5.30566	-0.05126
C	-0.72111	-1.46990	-3.39910
H	-1.22632	-0.88783	-4.16985
H	0.20177	-1.88951	-3.79949
H	-0.48878	-0.82378	-2.55256
C	-3.34654	-4.91592	-1.90167
H	-3.74758	-5.81696	-1.43755
H	-3.52745	-4.95056	-2.97599
H	-3.83260	-4.03651	-1.47922
H	5.83947	-7.00665	1.61020
H	9.30874	0.19630	1.03105
H	9.35139	-1.40515	0.95490
O	6.47060	-0.94976	5.49412
O	7.25223	-1.50813	3.43997
O	8.37649	1.33180	3.20577
O	5.03095	0.80951	3.23045
O	9.96194	1.56497	1.63333
C	7.08521	-1.68865	4.67054
C	7.69085	-2.93568	5.26382
C	9.39319	1.91329	2.67433
C	9.92464	3.14173	3.37926
H	4.58093	0.01367	2.82531

H	4.53828	1.61511	2.90145
H	5.82256	-0.18942	5.53771
Cd	-6.01847	0.50804	-2.74677
H	-4.89618	0.80244	-6.35632
O	-5.54422	1.56278	-6.31272
O	-6.32585	2.12114	-4.25857
O	-7.45013	-0.71877	-4.02437
O	-4.10459	-0.19646	-4.04906
O	-9.03559	-0.95195	-2.45191
C	-6.15885	2.30167	-5.48914
C	-6.76448	3.54872	-6.08243
C	-8.46684	-1.30026	-3.49292
C	-8.99827	-2.52870	-4.19785
H	-3.65457	0.59937	-3.64391
H	-3.61192	-1.00208	-3.72005
I	-2.67603	-0.99733	0.38071
I	-5.74274	4.73129	-2.10792
I	-0.52239	1.90343	-0.90475
I	-8.13849	-3.52380	0.40001
I	-3.49468	-6.71011	2.39443
I	-1.32852	7.77694	0.51526
O	-6.49270	-0.54672	0.81917
O	-4.10328	7.83404	-1.88271
O	-5.71108	-1.10507	-1.23497
O	-4.58682	1.73484	-1.46917
O	-7.93234	1.21255	-1.44449
O	-3.00135	1.96801	-3.04164
N	-1.39219	-3.10100	2.53546
C	-3.90857	-2.60587	0.90366
O	-6.87397	-6.80349	1.07061
C	-6.11154	-3.61197	0.84877
O	0.09743	-5.35824	1.79702
O	2.23200	6.30888	0.17279
N	0.70962	4.09937	0.98193
C	-5.87808	-1.28561	-0.00442
C	2.55417	3.20379	2.11934
N	0.08000	4.97191	0.24013
H	0.55382	5.81263	-0.02193
O	-6.85930	-5.81081	3.06071
C	-5.27244	-2.53264	0.58887
C	-4.22606	-4.87177	1.69288
O	3.72808	3.14256	2.37386
O	1.44564	-2.42071	4.37890
C	-2.03960	5.92662	-0.22568
N	-2.00777	-3.95355	1.76546
H	-1.50751	-4.72600	1.37423
O	-4.78116	7.47395	0.20526
C	-3.57010	2.31634	-2.00062
C	1.97292	4.29190	1.30636
C	-5.58877	-4.77980	1.40764
C	-3.03867	3.54478	-1.29568
C	0.62187	-4.54676	2.53206
C	-1.74297	3.61867	-0.76185

C	-0.16298	-3.30204	2.91225
C	0.42525	-2.24850	3.78163
C	-4.13456	7.16763	-0.85450
C	2.78294	5.45199	0.83152
C	-3.80847	4.71095	-1.28800
C	-1.23295	4.77675	-0.20137
C	-3.31099	5.91870	-0.76734
C	-0.31975	-0.94049	3.86386
H	-0.47370	-0.54679	2.85917
H	-1.28521	-1.10309	4.34297
H	0.26256	-0.22885	4.44916
C	-3.38394	-3.78796	1.48342
C	1.64747	2.08293	2.58050
H	2.15269	1.50085	3.35124
H	0.72460	2.50256	2.98090
H	1.41514	1.43680	1.73395
C	4.27291	5.52895	1.08308
H	4.67395	6.42998	0.61895
H	4.45382	5.56360	2.15741
H	4.75896	4.64954	0.66061
C	-6.51414	-5.90174	1.79578
C	1.99561	-4.74189	2.99021
H	2.45225	-5.55884	2.43150
H	2.56476	-3.82665	2.82746
H	1.99287	-4.98478	4.05281
H	-4.91310	7.61967	-2.42880
H	-7.39089	-6.61114	3.33797
H	-8.38238	0.41674	-1.84965
H	-8.42503	2.01816	-1.77351
H	-7.14076	0.21362	0.86277
H	-7.08958	3.34477	-7.10262
H	-6.02067	4.34543	-6.09049
H	-7.62095	3.85726	-5.48297
H	-8.24031	-3.31188	-4.18411
H	-9.24299	-2.27794	-5.23000
H	-9.89442	-2.88134	-3.68736
H	9.50405	4.03552	2.91844
H	11.01116	3.16690	3.29591
H	9.64161	3.10784	4.43130
H	8.76148	-2.78781	5.40509
H	7.52595	-3.77595	4.58939
H	7.22286	-3.14464	6.22580
H	5.15748	2.95559	-1.66735
H	6.75152	3.42695	-2.30384
H	6.24974	3.95580	-0.68004

$2N4_{I...I}M2$

Cd	7.15824	0.31454	0.43401
I	6.77577	-3.75867	1.69203
H	7.63668	-1.00329	-3.08870
I	1.42582	-1.31343	0.24461
I	1.97310	-7.28679	1.33259
O	7.00605	-0.24847	-3.26912
O	5.12211	-6.54415	3.06029

O	6.59302	1.16986	-1.54869
O	5.52649	-1.22398	0.03750
O	8.81691	-1.00642	-0.73181
O	4.23818	-0.66452	1.78902
O	-1.47385	-5.55245	1.57817
N	-0.11507	-3.99840	-0.31739
C	6.54381	0.80905	-2.74960
C	-2.12913	-3.52477	-1.42076
N	0.63378	-4.52669	0.61438
H	0.21265	-5.14481	1.27813
C	5.84434	1.73679	-3.71084
O	-3.32940	-3.48907	-1.48905
C	2.80207	-5.35361	1.10001
O	5.42712	-7.13653	0.93783
C	4.61752	-1.45520	0.91757
C	-1.41555	-4.21522	-0.32676
C	3.97174	-2.82295	0.89120
C	2.60303	-3.01701	0.64984
C	4.97437	-6.37039	1.85605
C	-2.13079	-5.00957	0.71480
C	4.72852	-3.93954	1.25605
C	2.00345	-4.26241	0.71931
C	4.14819	-5.21431	1.38002
C	-1.31630	-2.76741	-2.44876
H	-1.94767	-2.52358	-3.30317
H	-0.47696	-3.38207	-2.77403
H	-0.94049	-1.84655	-2.00281
C	-3.64181	-5.07467	0.75729
H	-3.95617	-5.66869	1.61545
H	-4.00653	-5.53991	-0.15847
H	-4.04713	-4.06615	0.83919
H	6.01446	-6.18201	3.32967
H	9.33046	-0.14956	-0.77733
H	9.35923	-1.63579	-0.17521
O	7.31044	0.87755	4.13714
O	7.72349	-0.54079	2.41670
O	8.79001	1.85307	0.83053
O	5.49958	1.63550	1.59980
O	10.07832	1.29360	-0.92100
C	7.77270	-0.17998	3.61761
C	8.47216	-1.10770	4.57884
C	9.69898	2.08428	-0.04956
C	10.34476	3.45202	-0.02318
H	4.98604	0.77864	1.64536
H	4.95726	2.26485	1.04323
H	6.67981	1.63235	3.95670
Cd	-6.41990	-0.31454	-1.86875
H	-5.94145	-1.63237	-5.39146
O	-6.57208	-0.87757	-5.57189
O	-6.98513	0.54077	-3.85144
O	-8.05166	-1.85308	-2.26527
O	-4.76124	-1.63550	-3.03456
O	-9.33998	-1.29361	-0.51373

C	-7.03436	0.17997	-5.05235
C	-7.73381	1.10770	-6.01360
C	-8.96064	-2.08429	-1.38518
C	-9.60641	-3.45201	-1.41156
H	-4.24770	-0.77864	-3.08011
H	-4.21892	-2.26486	-2.47798
H	-3.12328	-1.17343	1.67517
I	-6.03742	3.75867	-3.12677
I	-0.68745	1.31342	-1.67936
I	-7.96128	-2.50337	2.97745
I	-3.04169	-4.90185	5.37330
I	-1.23476	7.28679	-2.76733
O	-6.26771	0.24846	1.83438
O	-4.38376	6.54414	-4.49506
O	-5.85466	-1.16987	0.11394
O	-4.78815	1.22399	-1.47222
O	-8.07856	1.00642	-0.70295
O	-3.49982	0.66450	-3.22377
N	-0.94665	-1.72649	3.64301
C	-3.70816	-1.77224	2.37334
O	-6.59952	-5.28946	4.76303
C	-5.88720	-2.54524	3.09625
O	0.39211	-4.18890	3.70344
O	2.21220	5.55244	-3.01292
N	0.85346	3.99843	-1.11736
C	-5.80544	-0.80908	1.31484
C	2.86749	3.52478	-0.01398
N	0.10459	4.52669	-2.04911
H	0.52571	5.14480	-2.71288
O	-6.23950	-3.56259	6.11744
C	-5.10598	-1.73680	2.27608
C	-3.88378	-3.47406	4.08533
O	4.06776	3.48907	0.05432
O	2.16817	-0.55096	4.55424
C	-2.06370	5.35363	-2.53476
N	-1.68659	-2.77446	3.41294
H	-1.26187	-3.67408	3.31148
O	-4.68877	7.13654	-2.37259
C	-3.87916	1.45520	-2.35232
C	2.15390	4.21524	-1.10798
C	-5.27532	-3.40942	4.00633
C	-3.23339	2.82294	-2.32594
C	1.03622	-3.18601	3.93401
C	-1.86468	3.01700	-2.08461
C	0.32931	-1.84208	3.87082
C	1.05957	-0.56859	4.10896
C	-4.23602	6.37040	-3.29078
C	2.86916	5.00957	-2.14955
C	-3.99016	3.93954	-2.69078
C	-1.26508	4.26242	-2.15406
C	-3.40983	5.21432	-2.81477
C	0.34017	0.70576	3.74681
H	0.01409	0.65572	2.70793

H	-0.52743	0.82865	4.39510
H	1.01527	1.55159	3.87682
C	-3.09083	-2.64077	3.30781
C	2.05465	2.76741	1.01401
H	2.68603	2.52357	1.86841
H	1.21533	3.38210	1.33928
H	1.67885	1.84654	0.56806
C	4.38017	5.07467	-2.19203
H	4.69452	5.66868	-3.05019
H	4.74488	5.53993	-1.27627
H	4.78547	4.06615	-2.27394
C	-6.11923	-4.19679	4.97255
C	2.46864	-3.27299	4.20920
H	2.82133	-4.27945	3.98392
H	3.00089	-2.55301	3.58757
H	2.65046	-3.05067	5.26069
H	-5.27611	6.18200	-4.76442
H	-6.71487	-4.13353	6.78680
H	-8.59211	0.14957	-0.65742
H	-8.62089	1.63577	-1.25954
H	-6.89835	1.00327	1.65396
H	-8.23112	0.52212	-6.78680
H	-7.00270	1.77183	-6.47456
H	-8.47317	1.69968	-5.47416
H	-8.85758	-4.21172	-1.18759
H	-10.02664	-3.63637	-2.40025
H	-10.40030	-3.49339	-0.66586
H	9.85054	4.10114	-0.74602
H	11.40030	3.36040	-0.27921
H	10.24872	3.87993	0.97467
H	9.55106	-0.99345	4.47394
H	8.19265	-2.13783	4.35795
H	8.17832	-0.86236	5.59940
H	4.77369	1.53278	-3.69856
H	6.23299	1.57808	-4.71673
H	6.02080	2.77003	-3.41195

$2N4_{I...I}M3$

Cd	7.05103	0.56719	0.73403
I	6.66856	-3.69064	0.52307
H	7.52947	0.53367	-3.02695
I	1.31860	-0.89783	-0.00074
I	1.86588	-6.88306	-1.02138
O	6.89884	1.30467	-2.93833
O	5.01490	-6.77611	0.85612
O	6.48581	2.04906	-0.83655
O	5.41928	-0.74294	-0.16477
O	8.70970	-0.27537	-0.81327
O	4.13097	-0.81627	1.67247
O	-1.58107	-5.33731	-0.19743
N	-0.22229	-3.22866	-1.44716
C	6.43660	2.12074	-2.08844
C	-2.23635	-2.40621	-2.32200
N	0.52656	-4.04377	-0.75227

H	0.10543	-4.85163	-0.33995
C	5.73713	3.32129	-2.67440
O	-3.43662	-2.34931	-2.37396
C	2.69485	-4.98692	-0.57876
O	5.31991	-6.60685	-1.34095
C	4.51031	-1.26121	0.58314
C	-1.52277	-3.42920	-1.53012
C	3.86452	-2.53745	0.09057
C	2.49581	-2.63726	-0.20261
C	4.86716	-6.20096	-0.21607
C	-2.23801	-4.53188	-0.82306
C	4.62131	-3.71150	0.05152
C	1.89623	-3.83132	-0.56328
C	4.04098	-4.95179	-0.26799
C	-1.42352	-1.34294	-3.02897
H	-2.05489	-0.82158	-3.74846
H	-0.58418	-1.80928	-3.54485
H	-1.04771	-0.63013	-2.29496
C	-3.74903	-4.60758	-0.80539
H	-4.06339	-5.45928	-0.20216
H	-4.11375	-4.73156	-1.82506
H	-4.15435	-3.68789	-0.38350
H	5.90725	-6.52795	1.23312
H	9.22325	0.54538	-0.56298
H	9.25202	-1.05716	-0.50550
O	7.20323	-0.17029	4.40641
O	7.61628	-0.91468	2.30462
O	8.68280	1.87733	1.63285
O	5.39237	1.40977	2.28132
O	9.97111	1.95065	-0.20440
C	7.66549	-0.98637	3.55650
C	8.36495	-2.18690	4.14247
C	9.59177	2.39560	0.88492
C	10.23755	3.67183	1.37750
H	4.87883	0.58900	2.03106
H	4.85005	2.19152	1.97356
H	6.57260	0.60070	4.49501
Cd	-6.52712	0.76364	-1.64500
H	-6.04867	0.73013	-5.40599
O	-6.67930	1.50112	-5.31738
O	-7.09235	2.24550	-3.21559
O	-8.15888	-0.54649	-2.54383
O	-4.86846	-0.07892	-3.19230
O	-9.44720	-0.61983	-0.70656
C	-7.14158	2.31719	-4.46747
C	-7.84103	3.51773	-5.05345
C	-9.06786	-1.06477	-1.79589
C	-9.71363	-2.34099	-2.28847
H	-4.35492	0.74184	-2.94204
H	-4.32614	-0.86069	-2.88454
I	-2.69238	-0.51815	0.97625
I	-6.14464	5.02148	-1.43404
H	-1.36377	3.06954	-0.81266

I	-8.06850	-2.95068	2.16031
I	-3.14891	-6.02396	3.59134
I	-1.34198	8.21389	0.11041
O	-6.37493	0.02615	2.02736
O	-4.49098	8.10695	-1.76712
O	-5.96188	-0.71822	-0.07443
O	-4.89537	2.07377	-0.74618
O	-8.18578	1.60621	-0.09771
O	-3.60704	2.14709	-2.58346
N	-1.05387	-2.44829	3.05144
C	-3.81538	-2.05702	1.84269
O	-6.70674	-6.17946	2.88530
C	-5.99442	-3.03067	2.25762
O	0.28489	-4.78288	2.26603
O	2.10498	6.66813	-0.71355
N	0.74624	4.55952	0.53619
C	-5.91266	-0.78992	1.17745
C	2.76027	3.73705	1.41103
N	-0.00263	5.37459	-0.15869
H	0.41849	6.18246	-0.57102
O	-6.34672	-5.01997	4.74866
C	-5.21320	-1.99046	1.76342
C	-3.99100	-4.24176	2.86938
O	3.96055	3.68014	1.46300
O	2.06095	-1.65532	4.30977
C	-2.17092	6.31777	-0.33222
N	-1.79381	-3.35438	2.47682
H	-1.36909	-4.16504	2.07378
O	-4.79599	7.93769	0.42996
C	-3.98638	2.59205	-1.49412
C	2.04668	4.76005	0.61916
C	-5.38254	-4.15400	2.81725
C	-3.34061	3.86828	-1.00154
C	0.92900	-3.91932	2.82570
C	-1.97190	3.96809	-0.70839
C	0.22209	-2.63483	3.22598
C	0.95235	-1.51958	3.88531
C	-4.34324	7.53180	-0.69489
C	2.76194	5.86270	-0.08791
C	-4.09738	5.04232	-0.96248
C	-1.37230	5.16216	-0.34770
C	-3.51705	6.28263	-0.64299
C	0.23295	-0.19822	3.98086
H	-0.09313	0.11007	2.98752
H	-0.63465	-0.30447	4.63208
H	0.90805	0.55213	4.39232
C	-3.19805	-3.19280	2.42375
C	1.94743	2.67376	2.11799
H	2.57881	2.15241	2.83747
H	1.10811	3.14014	2.63388
H	1.57163	1.96095	1.38398
C	4.27296	5.93841	-0.10557
H	4.58731	6.79011	-0.70882

H	4.63767	6.06241	0.91409
H	4.67826	5.01873	-0.52748
C	-6.22645	-5.22435	3.45590
C	2.36142	-4.09518	3.05455
H	2.71411	-4.96390	2.49863
H	2.89367	-3.20601	2.71665
H	2.54324	-4.24590	4.11866
H	-5.38333	7.85877	-2.14410
H	-6.82209	-5.78542	5.18237
H	-8.69933	0.78546	-0.34799
H	-8.72811	2.38798	-0.40549
H	-7.00557	0.79715	2.11598
H	-8.33834	3.23192	-5.98031
H	-7.10992	4.29947	-5.25947
H	-8.58039	3.88952	-4.34408
H	-8.96480	-3.13149	-2.33784
H	-10.13386	-2.17607	-3.28059
H	-10.50752	-2.63491	-1.60188
H	9.74333	4.52903	0.92027
H	11.29309	3.67331	1.10558
H	10.14151	3.73265	2.46153
H	9.44385	-2.04366	4.08297
H	8.08544	-3.07935	3.58258
H	8.07111	-2.30540	5.18539
H	4.66648	3.12539	-2.73265
H	6.12578	3.51619	-3.67392
H	5.91359	4.18999	-2.04015

$2N4_{I...I}M4$

Cd	7.07815	-0.22945	1.41474
I	6.74780	-4.15030	-0.26983
H	7.88157	1.01090	-2.07684
I	1.44246	-1.22634	-0.25622
I	2.12174	-6.51540	-3.21065
O	7.23979	1.71948	-1.78352
O	5.09495	-7.12623	-1.15160
O	6.64019	1.71156	0.40339
O	5.54060	-1.11734	-0.01161
O	8.87126	-0.53100	-0.18186
O	4.09824	-1.78377	1.57459
O	-1.39537	-5.26598	-2.20141
N	0.05073	-2.88876	-2.53628
C	6.69932	2.20698	-0.74807
C	-1.88596	-1.77206	-3.24368
N	0.74258	-3.90867	-2.10132
H	0.29340	-4.79899	-2.02688
C	6.04427	3.55085	-0.94520
O	-3.07758	-1.67379	-3.37392
C	2.89472	-4.90310	-2.07863
O	5.58828	-6.22475	-3.12461
C	4.57409	-1.83897	0.43485
C	-1.23608	-3.01960	-2.79194
C	3.98322	-2.85580	-0.51668
C	2.64593	-2.81874	-0.94043

C	5.03650	-6.21672	-1.97111
C	-2.00161	-4.28087	-2.56711
C	4.74944	-3.96289	-0.89069
C	2.08902	-3.80436	-1.73652
C	4.20848	-5.00644	-1.66242
C	-1.02292	-0.55004	-3.47368
H	-1.59338	0.19953	-4.02215
H	-0.13844	-0.83130	-4.04525
H	-0.71768	-0.13897	-2.51142
C	-3.50784	-4.32396	-2.70365
H	-3.86691	-5.32301	-2.45649
H	-3.78170	-4.08450	-3.73114
H	-3.95523	-3.59439	-2.02861
H	5.94929	-7.04171	-0.63880
H	9.35489	0.14339	0.37611
H	9.39073	-1.38290	-0.11525
O	6.91653	-2.17837	4.61301
O	7.51615	-2.17046	2.42608
O	8.61572	0.65845	2.84111
O	5.28506	0.07212	3.01132
O	10.05809	1.32487	1.25490
C	7.45702	-2.66588	3.57754
C	8.11206	-4.00973	3.77468
C	9.58224	1.38008	2.39463
C	10.17310	2.39690	3.34616
H	4.80144	-0.60229	2.45339
H	4.76559	0.92399	2.94472
H	6.27475	-1.46980	4.90630
Cd	-6.24326	1.07281	-1.88808
H	-5.43983	2.31316	-5.37965
O	-6.08161	3.02173	-5.08636
O	-6.68123	3.01380	-2.89943
O	-7.78082	0.18491	-3.31444
O	-4.45017	0.77126	-3.48466
O	-9.22320	-0.48152	-1.72823
C	-6.62212	3.50923	-4.05088
C	-7.27716	4.85310	-4.24803
C	-8.74734	-0.53672	-2.86797
C	-9.33819	-1.55353	-3.81949
H	-3.96655	1.44566	-2.92673
H	-3.93070	-0.08062	-3.41807
I	-2.64096	-1.11224	0.45034
I	-5.91290	4.99366	-0.20350
I	-0.60755	2.06970	-0.21713
H	-7.10235	-3.75458	0.38819
I	-3.28099	-7.16803	0.97838
I	-1.28686	7.35876	2.73731
O	-6.40490	-0.87612	1.31018
O	-4.26005	7.96961	0.67824
O	-5.80528	-0.86819	-0.87674
O	-4.70571	1.96070	-0.46171
O	-8.03635	1.37437	-0.29150
O	-3.26332	2.62712	-2.04795

N	-1.17420	-3.67083	1.87119
C	-3.82323	-2.82860	0.64098
O	-6.76280	-6.99313	-0.03515
C	-6.02261	-3.83596	0.51323
O	0.24539	-5.62716	0.45100
O	2.23027	6.10934	1.72806
N	0.78421	3.73215	2.06296
C	-5.86439	-1.36362	0.27470
C	2.72086	2.61543	2.77035
N	0.09233	4.75202	1.62799
H	0.54151	5.64235	1.55353
O	-6.57474	-6.54706	2.13551
C	-5.20935	-2.70748	0.47185
C	-4.07073	-5.22795	0.84068
O	3.91250	2.51714	2.90059
O	1.81349	-3.42501	3.58221
C	-2.05981	5.74648	1.60530
N	-1.85455	-4.30969	0.96142
H	-1.39030	-4.94367	0.34293
O	-4.75337	7.06813	2.65126
C	-3.73918	2.68234	-0.90819
C	2.07097	3.86297	2.31862
C	-5.45311	-5.09630	0.70473
C	-3.14833	3.69915	0.04334
C	0.83189	-5.02102	1.32417
C	-1.81104	3.66211	0.46707
C	0.08316	-3.93444	2.07824
C	0.74493	-3.12769	3.13796
C	-4.20160	7.06009	1.49779
C	2.83653	5.12424	2.09376
C	-3.91453	4.80624	0.41736
C	-1.25411	4.64773	1.26318
C	-3.37357	5.84981	1.18908
C	0.00993	-1.90226	3.61834
H	-0.23100	-1.26641	2.76643
H	-0.91010	-2.20463	4.11856
H	0.64104	-1.35264	4.31671
C	-3.25007	-4.10806	0.84875
C	1.85781	1.39341	3.00033
H	2.42828	0.64384	3.54879
H	0.97335	1.67469	3.57192
H	1.55259	0.98233	2.03807
C	4.34275	5.16732	2.23031
H	4.70181	6.16636	1.98315
H	4.61660	4.92787	3.25782
H	4.79013	4.43776	1.55526
C	-6.34113	-6.30097	0.86575
C	2.24033	-5.29664	1.59888
H	2.64654	-5.93140	0.81137
H	2.79314	-4.35779	1.63124
H	2.33021	-5.80529	2.55873
H	-5.11439	7.88507	0.16545
H	-7.08014	-7.40360	2.23992

H	-8.51998	0.69999	-0.84945
H	-8.55583	2.22625	-0.35811
H	-7.04669	-0.16756	1.60349
H	-7.68993	4.91181	-5.25512
H	-6.53688	5.64153	-4.11220
H	-8.07812	4.97724	-3.51924
H	-8.58192	-2.29648	-4.07278
H	-9.67194	-1.05071	-4.72717
H	-10.18644	-2.04599	-3.34410
H	9.71395	3.36956	3.16947
H	11.24822	2.46721	3.18099
H	9.98284	2.08653	4.37354
H	9.19093	-3.87916	3.85876
H	7.88901	-4.65119	2.92212
H	7.72969	-4.47015	4.68566
H	4.98424	3.41076	-1.15679
H	6.51674	4.06612	-1.78146
H	6.15839	4.14695	-0.03983

$3N3_{I...O}M1$

Cd	0.05660	3.30701	-1.25337
H	-2.06209	-1.01396	-0.38758
I	-7.15283	-1.97689	0.27801
O	-3.87997	-5.58605	-0.69439
O	-1.65565	1.92534	-1.86467
N	-4.09359	-2.82392	0.03094
O	-7.63885	1.11932	-1.39224
O	-1.41662	2.09722	0.28981
C	-3.06804	-0.60102	-0.31238
O	-7.54202	1.48314	0.74094
C	-5.46391	-0.81156	-0.07458
N	-2.90222	-6.83252	0.86211
H	-3.08124	-7.61901	0.27102
N	-3.36594	-3.17974	1.00948
C	-3.23032	0.78812	-0.49354
C	-4.20123	-1.41778	-0.06121
O	-1.91219	-8.20068	2.37875
C	-5.63450	0.55700	-0.28039
C	-4.51459	1.33480	-0.48738
C	-3.06187	-4.49103	1.25622
C	-3.34560	-5.60304	0.41820
C	-2.00804	1.64818	-0.70045
C	-7.03169	1.13161	-0.30266
N	-1.98295	-6.00547	2.77836
H	-1.48450	-6.15476	3.63233
C	-2.24023	-7.07694	2.03465
C	-2.34430	-4.69637	2.47770
I	-4.76319	3.41236	-0.66094
O	-1.99186	-3.79915	3.28360
H	-2.22839	-2.90968	2.89260
Cd	-5.43152	-4.09150	-1.35729
I	-1.66470	5.42161	0.38193
O	1.60816	1.81246	-0.59047
N	1.39454	4.57458	0.13486

O	1.12964	3.48557	-3.30982
O	-0.33391	5.03116	-2.90809
I	7.18319	-8.13163	1.70025
O	3.91033	-4.52247	2.67264
N	4.12395	-7.28460	1.94732
H	3.36130	-9.31802	2.23236
C	5.49426	-9.29695	2.05283
N	2.93258	-3.27600	1.11616
H	3.11160	-2.48951	1.70724
N	3.39631	-6.92877	0.96877
C	4.23160	-8.69074	2.03946
O	1.94255	-1.90783	-0.40049
H	5.62763	-10.36674	2.21371
C	3.09223	-5.61750	0.72205
C	3.37596	-4.50548	1.56006
N	2.01331	-4.10304	-0.80010
H	1.51486	-3.95377	-1.65407
C	2.27059	-3.03157	-0.05639
C	2.37464	-5.41215	-0.49945
O	2.02221	-6.30937	-1.30535
H	2.25875	-7.19885	-0.91433
Cd	5.46187	-6.01702	3.33555
H	3.42603	6.38455	-0.28366
C	2.42009	6.79749	-0.20846
C	0.02421	6.58694	0.02934
N	2.58591	0.56599	0.96603
H	2.40688	-0.22050	0.37494
N	2.12217	4.21877	1.11340
C	2.25781	8.18662	-0.38963
C	1.28688	5.98073	0.04271
O	3.57594	-0.80217	2.48267
C	-0.14638	7.95551	-0.17647
C	0.97355	8.73331	-0.38346
C	2.42626	2.90748	1.36014
C	2.14252	1.79547	0.52212
H	3.14082	8.80796	-0.53910
H	-1.15435	8.37005	-0.19253
N	3.50518	1.39304	2.88228
H	4.00362	1.24375	3.73625
C	3.24789	0.32157	2.13857
C	3.14384	2.70215	2.58162
H	0.84448	9.81188	-0.47357
O	3.49628	3.59936	3.38752
H	3.25973	4.48883	2.99651
C	0.44840	4.47363	-3.64988
C	-5.03971	-2.92488	-3.75379
C	0.52142	4.90191	-5.09696
O	6.93511	-4.80724	1.79236
O	7.17413	-4.63535	3.94684
C	7.52651	-4.35820	2.78262
O	4.38886	-6.19557	5.39200
O	5.85240	-7.74117	4.99027
C	5.07008	-7.18364	5.73205

O	-7.14378	-5.47317	-1.96858
O	-6.90475	-5.30129	0.18589
C	-7.49616	-5.75033	-0.80437
O	-4.35850	-3.91295	-3.41374
O	-5.82204	-2.36735	-3.01201
C	-4.96671	-2.49659	-5.20088
H	-8.51861	1.56104	-1.56790
C	-8.72396	-6.69498	-0.58933
H	-8.38868	-7.73213	-0.58893
H	-9.44268	-6.54575	-1.39509
H	-9.19610	-6.46537	0.36586
H	-4.35602	-3.20601	-5.75933
H	-4.52021	-1.50426	-5.26396
H	-5.97121	-2.47059	-5.62318
C	4.90792	-7.73176	7.18785
H	5.57272	-8.58351	7.33151
H	3.87600	-8.04567	7.34502
H	5.16202	-6.94808	7.90153
C	8.75431	-3.41354	2.56760
H	8.63845	-2.87564	1.62669
H	9.66818	-4.00682	2.53684
H	8.81193	-2.69986	3.38943
H	0.82400	4.05433	-5.71185
H	1.25044	5.70542	-5.20168
H	-0.45750	5.25492	-5.42119

$3N3_{I...O}M2$

Cd	-1.18266	2.90089	-1.83910
I	-1.39912	-1.64365	0.01802
I	-6.64499	-2.50512	2.97530
O	-3.47024	-5.99241	1.41230
O	-2.80266	1.31358	-1.57347
N	-3.77994	-3.16600	1.75377
O	-8.08539	0.18961	1.16531
O	-1.85351	1.89469	0.29465
C	-3.24042	-0.97753	0.73870
O	-7.30093	0.94500	3.03780
C	-5.35366	-1.30865	1.86371
N	-1.85672	-6.85988	2.66786
H	-2.12501	-7.75218	2.30477
N	-2.71707	-3.28397	2.43935
C	-3.63712	0.33979	0.42859
C	-4.09717	-1.81182	1.50304
O	-0.22965	-7.85313	3.90006
C	-5.76394	-0.01662	1.53699
C	-4.89900	0.78667	0.82380
C	-2.17620	-4.50295	2.74655
C	-2.58474	-5.76713	2.24227
C	-2.68797	1.23094	-0.33395
C	-7.14421	0.44449	1.94325
N	-0.44544	-5.63236	3.97268
H	0.33412	-5.58683	4.59735
C	-0.80195	-6.83761	3.53951
C	-1.05795	-4.42946	3.63717

H	-5.19226	1.81855	0.63062
O	-0.56851	-3.37695	4.11818
H	-1.04134	-2.59331	3.71528
Cd	-5.33797	-4.75787	1.15170
I	-2.48967	5.15363	-0.01550
O	0.68508	1.66635	-1.57851
N	0.37538	4.49275	-1.23704
O	-0.92605	2.77359	-4.14783
O	-2.34825	4.25994	-3.46934
I	7.96705	-7.27088	-0.05799
O	4.79229	-3.78359	1.50500
N	5.10199	-6.61000	1.16354
H	4.76124	-8.60493	2.00128
C	6.67571	-8.46736	1.05360
N	3.17878	-2.91612	0.24946
H	3.44707	-2.02382	0.61254
N	4.03913	-6.49202	0.47795
C	5.41923	-7.96418	1.41426
O	1.55170	-1.92286	-0.98275
H	6.99643	-9.47732	1.30898
C	3.49826	-5.27306	0.17077
C	3.90680	-4.00887	0.67504
N	1.76749	-4.14363	-1.05537
H	0.98793	-4.18918	-1.68004
C	2.12400	-2.93838	-0.62220
C	2.37999	-5.34654	-0.71986
O	1.89056	-6.39905	-1.20087
H	2.36340	-7.18270	-0.79796
Cd	6.66002	-5.01813	1.76561
H	1.87680	6.33325	-2.62859
C	0.91489	6.68124	-2.25211
C	-1.19835	6.35011	-1.12710
N	2.29859	0.79887	-0.32295
H	2.03029	-0.09341	-0.68604
N	1.43823	4.37479	-0.55145
C	0.51820	7.99855	-2.56222
C	0.05813	5.84694	-1.48776
O	3.92566	-0.19436	0.90925
C	-1.60863	7.64215	-1.45382
C	-0.74368	8.44544	-2.16701
C	1.97911	3.15581	-0.24426
C	1.57056	1.89163	-0.74854
H	1.20388	8.64235	-3.11310
H	-2.60439	7.97481	-1.16073
N	3.70988	2.02639	0.98187
H	4.48943	2.07193	1.60655
C	3.35336	0.82115	0.54870
C	3.09737	3.22931	0.64636
H	-1.03694	9.47732	-2.36019
O	3.58681	4.28181	1.12737
H	3.11397	5.06545	0.72447
C	-1.80689	3.63201	-4.35576
C	-5.96219	-4.02675	-1.36495

C	-2.29924	3.79122	-5.77528
O	7.33088	-4.01194	-0.36816
O	8.28002	-3.43082	1.49997
C	8.16533	-3.34819	0.26045
O	6.40343	-4.89083	4.07433
O	7.82562	-6.37718	3.39584
C	7.28425	-5.74925	4.28226
O	-6.95797	-6.34518	1.41734
O	-6.00882	-5.76407	3.28546
C	-6.84328	-6.42782	2.65686
O	-5.08137	-4.88517	-1.15702
O	-6.50356	-3.39882	-0.47853
C	-6.45456	-3.86753	-2.78447
H	-9.02129	0.52861	1.26086
C	-7.78357	-7.40080	3.44124
H	-7.33560	-8.39405	3.47054
H	-8.75079	-7.45301	2.94140
H	-7.91956	-7.03338	4.45837
H	-5.98867	-4.62276	-3.41744
H	-6.19283	-2.87479	-3.15058
H	-7.53732	-3.99021	-2.80935
C	7.71269	-6.03063	5.75988
H	8.49195	-6.79263	5.77336
H	6.85097	-6.38205	6.32735
H	8.09371	-5.11329	6.20863
C	9.10562	-2.37520	-0.52392
H	8.59970	-2.02880	-1.42510
H	10.02129	-2.89832	-0.79956
H	9.35114	-1.52044	0.10629
H	-2.12077	2.86850	-6.32735
H	-1.76491	4.61103	-6.25534
H	-3.36721	4.00898	-5.76711

$2N4_{I...O}M1$

Cd	10.95422	1.38526	0.01790
H	12.65955	0.36701	-3.21166
O	13.44682	0.71066	-2.69969
O	13.11385	1.17361	-0.50491
O	10.98053	3.19940	-1.35877
O	10.47567	-0.11735	-1.81740
O	10.46160	4.70752	0.22138
C	13.82219	1.00098	-1.52630
C	15.31197	1.16082	-1.35634
C	10.52773	4.33356	-0.95517
C	10.01546	5.28250	-2.01608
H	10.80304	-0.82933	-1.19618
H	9.51131	-0.31367	-1.99478
I	7.22734	-1.34728	1.38268
I	6.68537	4.64668	1.35674
H	2.75943	1.35394	0.89235
O	8.46162	2.05988	2.73547
O	8.79460	1.59693	0.54070
O	10.92792	-0.42886	1.39456
O	11.43277	2.88789	1.85319

O	11.44685	-1.93699	-0.18559
N	4.07072	-1.90621	2.04599
C	5.99504	0.34411	1.35811
O	3.29908	4.56766	0.20263
C	5.81791	2.75938	1.29899
O	2.15689	-2.49620	0.08421
C	8.08626	1.76955	1.56209
O	3.12967	4.13638	2.37780
C	6.59648	1.60972	1.39213
C	3.83175	1.39429	1.08366
O	2.91783	-4.87165	3.38436
N	3.92352	-1.00565	1.11537
H	3.33962	-1.19344	0.32556
C	11.38071	-1.56303	0.99096
C	4.43369	2.65120	1.15160
C	11.89299	-2.51197	2.05187
C	2.31332	-3.29578	0.98424
C	3.37165	-3.00372	2.03518
C	3.64287	-3.95172	3.14852
C	4.88897	-3.70765	3.96112
H	5.75201	-3.66137	3.29696
H	4.79205	-2.76417	4.49827
H	5.02079	-4.52141	4.67425
C	4.58825	0.23834	1.22207
C	3.58124	3.89166	1.16798
C	1.53809	-4.53392	1.01773
H	1.01255	-4.65913	0.07103
H	2.21015	-5.37746	1.17545
H	0.81486	-4.48749	1.83191
H	2.48500	4.90071	2.36396
H	11.10541	3.59987	1.23196
H	12.39714	3.08420	2.03056
H	9.24889	2.40352	3.24744
Cd	-9.94971	-1.69982	-0.01789
I	-6.22282	1.03272	-1.38268
H	-8.24438	-2.71808	-3.24744
I	-5.68085	-4.96124	-1.35674
H	-1.75491	-1.66850	-0.89235
O	-7.45711	-2.37443	-2.73546
O	-7.79008	-1.91149	-0.54069
O	-9.92340	0.11430	-1.39456
O	-10.42826	-3.20245	-1.85319
O	-10.44234	1.62243	0.18560
N	-3.06621	1.59165	-2.04598
C	-4.99053	-0.65867	-1.35811
O	-2.29457	-4.88222	-0.20262
C	-4.81339	-3.07394	-1.29899
O	-1.15237	2.18164	-0.08420
C	-7.08175	-2.08411	-1.56209
O	-2.12515	-4.45094	-2.37780
C	-5.59196	-1.92428	-1.39212
C	-2.82723	-1.70885	-1.08366
O	-1.91331	4.55709	-3.38436

N	-2.91902	0.69109	-1.11536
H	-2.33511	0.87888	-0.32556
C	-10.37619	1.24847	-0.99095
C	-3.42918	-2.96576	-1.15160
C	-10.88847	2.19741	-2.05187
C	-1.30881	2.98122	-0.98423
C	-2.36713	2.68916	-2.03517
C	-2.63836	3.63716	-3.14851
C	-3.88445	3.39310	-3.96111
H	-4.74750	3.34681	-3.29696
H	-3.78753	2.44961	-4.49827
H	-4.01627	4.20685	-4.67424
C	-3.58374	-0.55290	-1.22207
C	-2.57673	-4.20622	-1.16798
C	-0.53358	4.21936	-1.01773
H	-0.00804	4.34457	-0.07103
H	-1.20563	5.06290	-1.17545
H	0.18965	4.17293	-1.83190
H	-1.48049	-5.21527	-2.36396
H	-10.10089	-3.91443	-1.23196
H	-11.39262	-3.39876	-2.03056
O	-12.44231	-1.02522	2.69969
O	-12.10934	-1.48817	0.50491
O	-9.97601	-3.51396	1.35877
O	-9.47116	-0.19721	1.81740
O	-9.45708	-5.02208	-0.22138
C	-12.81767	-1.31554	1.52630
C	-14.30746	-1.47538	1.35635
C	-9.52322	-4.64812	0.95517
C	-9.01095	-5.59705	2.01608
H	-9.79852	0.51477	1.19618
H	-8.50680	-0.00088	1.99478
H	-11.65504	-0.68157	3.21166
H	-14.53519	-2.51075	1.10296
H	-14.65417	-0.82088	0.55667
H	-14.80977	-1.21003	2.28658
H	-11.96109	2.05301	-2.18111
H	-10.37878	1.99789	-2.99445
H	-10.69462	3.22498	-1.74437
H	-8.31464	-6.30422	1.56536
H	-9.84891	-6.14039	2.45275
H	-8.50021	-5.03023	2.79449
H	15.74160	1.56050	-2.27490
H	15.75887	0.19089	-1.13816
H	15.51221	1.84659	-0.53313
H	8.95994	5.08399	-2.20199
H	10.58024	5.13705	-2.93692
H	10.13712	6.31013	-1.67369
H	12.75834	-3.05257	1.66849
H	11.10824	-3.22149	2.31418
H	12.18145	-1.94550	2.93728

$2N4_{I...O}M2$

Cd	10.97967	1.38231	0.01789

H	12.68500	0.36406	-3.21167
O	13.47227	0.70771	-2.69970
O	13.13930	1.17066	-0.50492
O	11.00598	3.19644	-1.35878
O	10.50112	-0.12030	-1.81741
O	10.48705	4.70456	0.22137
C	13.84764	0.99803	-1.52631
C	15.33742	1.15787	-1.35635
C	10.55318	4.33060	-0.95518
C	10.04091	5.27954	-2.01609
H	10.82849	-0.83228	-1.19619
H	9.53676	-0.31662	-1.99479
I	7.25279	-1.35023	1.38267
H	6.29840	3.74644	1.32928
I	1.79205	1.31361	0.71521
O	8.48707	2.05692	2.73546
O	8.82005	1.59398	0.54069
O	10.95337	-0.43181	1.39455
O	11.45822	2.88493	1.85318
O	11.47230	-1.93994	-0.18560
N	4.09617	-1.90916	2.04598
C	6.02049	0.34116	1.35810
O	3.32453	4.56470	0.20262
C	5.84336	2.75642	1.29898
O	2.18234	-2.49915	0.08420
C	8.11171	1.76659	1.56208
O	3.15512	4.13342	2.37779
C	6.62193	1.60676	1.39212
C	3.85720	1.39133	1.08365
O	2.94328	-4.87460	3.38435
N	3.94897	-1.00860	1.11536
H	3.36507	-1.19639	0.32555
C	11.40616	-1.56598	0.99095
C	4.45914	2.64824	1.15159
C	11.91844	-2.51492	2.05186
C	2.33877	-3.29873	0.98423
C	3.39710	-3.00667	2.03517
C	3.66832	-3.95467	3.14851
C	4.91442	-3.71060	3.96111
H	5.77746	-3.66432	3.29695
H	4.81750	-2.76712	4.49826
H	5.04624	-4.52436	4.67424
C	4.61370	0.23539	1.22206
C	3.60669	3.88870	1.16797
C	1.56354	-4.53687	1.01772
H	1.03800	-4.66208	0.07102
H	2.23560	-5.38041	1.17544
H	0.84031	-4.49044	1.83190
H	2.51045	4.89775	2.36395
H	11.13086	3.59691	1.23195
H	12.42259	3.08124	2.03055
H	9.27434	2.40056	3.24743
Cd	-9.92426	-1.70278	-0.01789

I	-6.19737	1.02976	-1.38268
H	-8.21893	-2.72103	-3.24744
H	-5.24298	-4.06691	-1.32929
I	-0.73664	-1.63408	-0.71522
O	-7.43166	-2.37738	-2.73546
O	-7.76463	-1.91445	-0.54069
O	-9.89795	0.11134	-1.39456
O	-10.40281	-3.20541	-1.85319
O	-10.41689	1.61947	0.18560
N	-3.04076	1.58869	-2.04598
C	-4.96508	-0.66163	-1.35811
O	-2.26912	-4.88517	-0.20262
C	-4.78794	-3.07689	-1.29899
O	-1.12692	2.17868	-0.08420
C	-7.05630	-2.08706	-1.56209
O	-2.09970	-4.45389	-2.37780
C	-5.56651	-1.92724	-1.39212
C	-2.80178	-1.71180	-1.08366
O	-1.88786	4.55413	-3.38436
N	-2.89357	0.68813	-1.11536
H	-2.30966	0.87592	-0.32556
C	-10.35074	1.24551	-0.99095
C	-3.40373	-2.96871	-1.15160
C	-10.86302	2.19445	-2.05187
C	-1.28336	2.97826	-0.98423
C	-2.34168	2.68620	-2.03517
C	-2.61291	3.63420	-3.14851
C	-3.85900	3.39014	-3.96111
H	-4.72205	3.34385	-3.29696
H	-3.76208	2.44665	-4.49827
H	-3.99082	4.20389	-4.67424
C	-3.55829	-0.55586	-1.22207
C	-2.55128	-4.20917	-1.16798
C	-0.50813	4.21640	-1.01773
H	0.01741	4.34161	-0.07103
H	-1.18018	5.05994	-1.17545
H	0.21510	4.16997	-1.83190
H	-1.45504	-5.21822	-2.36396
H	-10.07544	-3.91738	-1.23196
H	-11.36717	-3.40171	-2.03056
O	-12.41686	-1.02818	2.69969
O	-12.08389	-1.49113	0.50491
O	-9.95056	-3.51691	1.35877
O	-9.44571	-0.20017	1.81740
O	-9.43163	-5.02503	-0.22138
C	-12.79222	-1.31850	1.52630
C	-14.28201	-1.47834	1.35635
C	-9.49777	-4.65107	0.95517
C	-8.98550	-5.60000	2.01608
H	-9.77307	0.51181	1.19618
H	-8.48135	-0.00384	1.99478
H	-11.62959	-0.68453	3.21166
H	-14.50974	-2.51371	1.10296

H	-14.62872	-0.82384	0.55667
H	-14.78432	-1.21299	2.28658
H	-11.93564	2.05005	-2.18111
H	-10.35333	1.99493	-2.99445
H	-10.66917	3.22202	-1.74437
H	-8.28919	-6.30717	1.56536
H	-9.82346	-6.14334	2.45275
H	-8.47476	-5.03318	2.79449
H	15.76705	1.55755	-2.27491
H	15.78432	0.18794	-1.13817
H	15.53766	1.84364	-0.53314
H	8.98539	5.08103	-2.20200
H	10.60569	5.13409	-2.93693
H	10.16257	6.30717	-1.67370
H	12.78379	-3.05552	1.66848
H	11.13369	-3.22444	2.31417
H	12.20690	-1.94845	2.93727