^{1}H and ^{195}Pt NMR Prediction for Inclusion Compounds Formed by Cisplatin and Oxidized Carbon Nanostructures

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Supplementary Material

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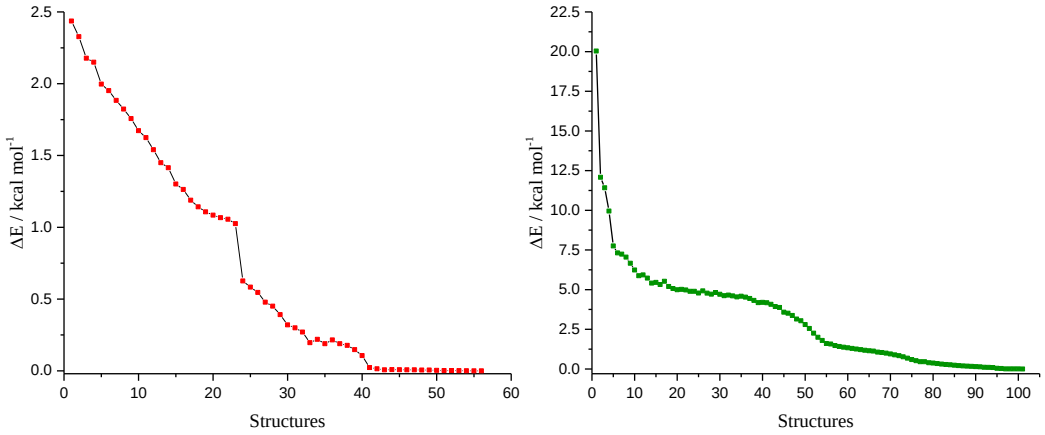

Figure S1. B3LYP/LANL2DZ/def2-SVP/IEF-PCM(UFF) potential energy curve for the geometry optimization process of cDDP@CNTox (a) and cDDP@CNCox (b) complexes.

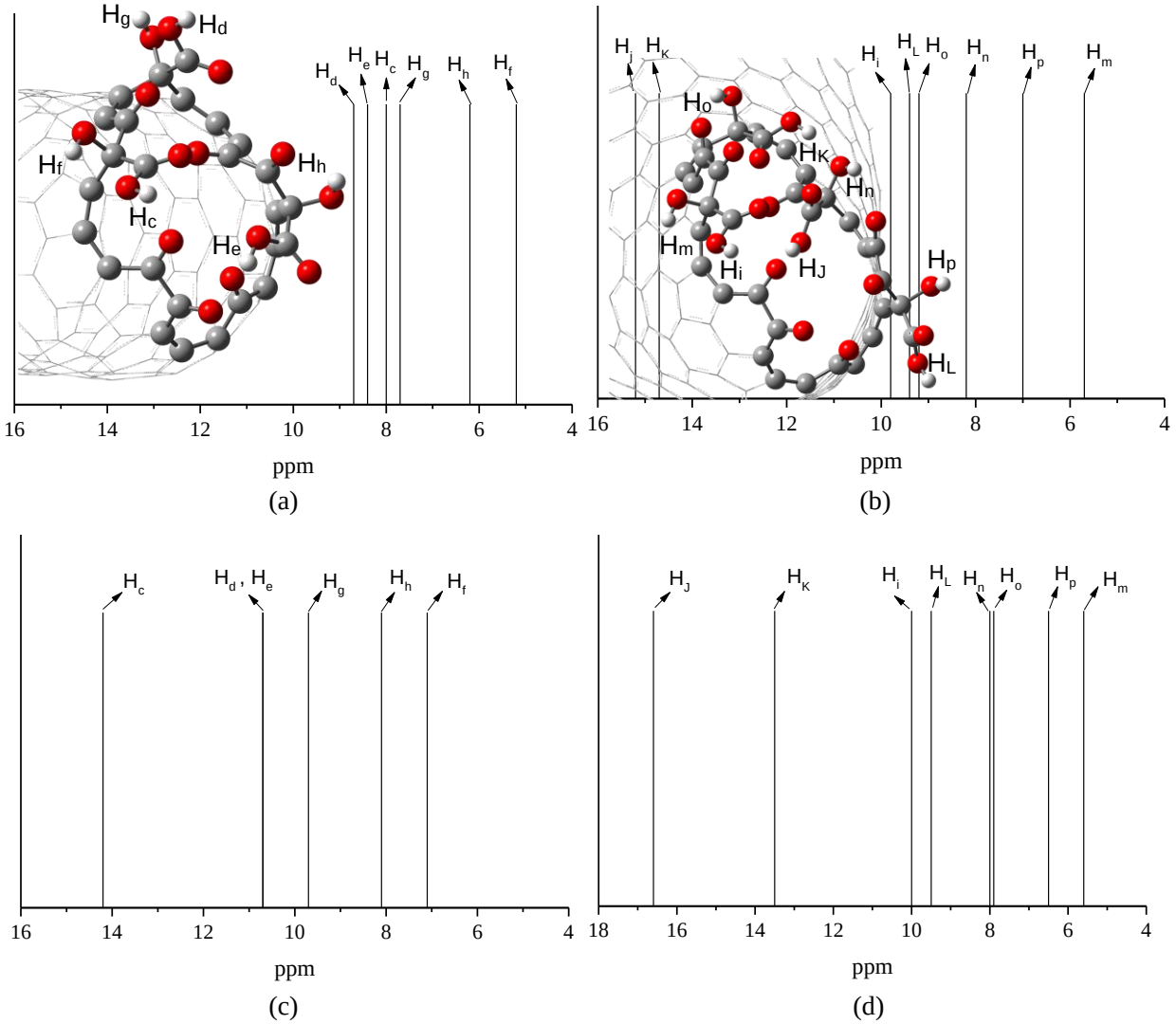

Figure S2. PBEPBE/NMR-DKH/IEF-PCM(UFF) ^{1}H NMR spectra for the oxidized region of free CNtox (a) and CNCox (b) nanostructures and its inclusion complexes (c-d), respectively. All values in ppm.

In order to verify if the simulation protocol provided the equilibration of the cDDP@CNTox complex, we analyzed the temporal variation of the macroscopic properties, such as temperature, kinetic and potential energy, density, volume and pressure, as shown in Figure S3. The evolution of the root-mean-square deviation (RMSD) calculated in relation to the first structure of the production run was also included in this figure.

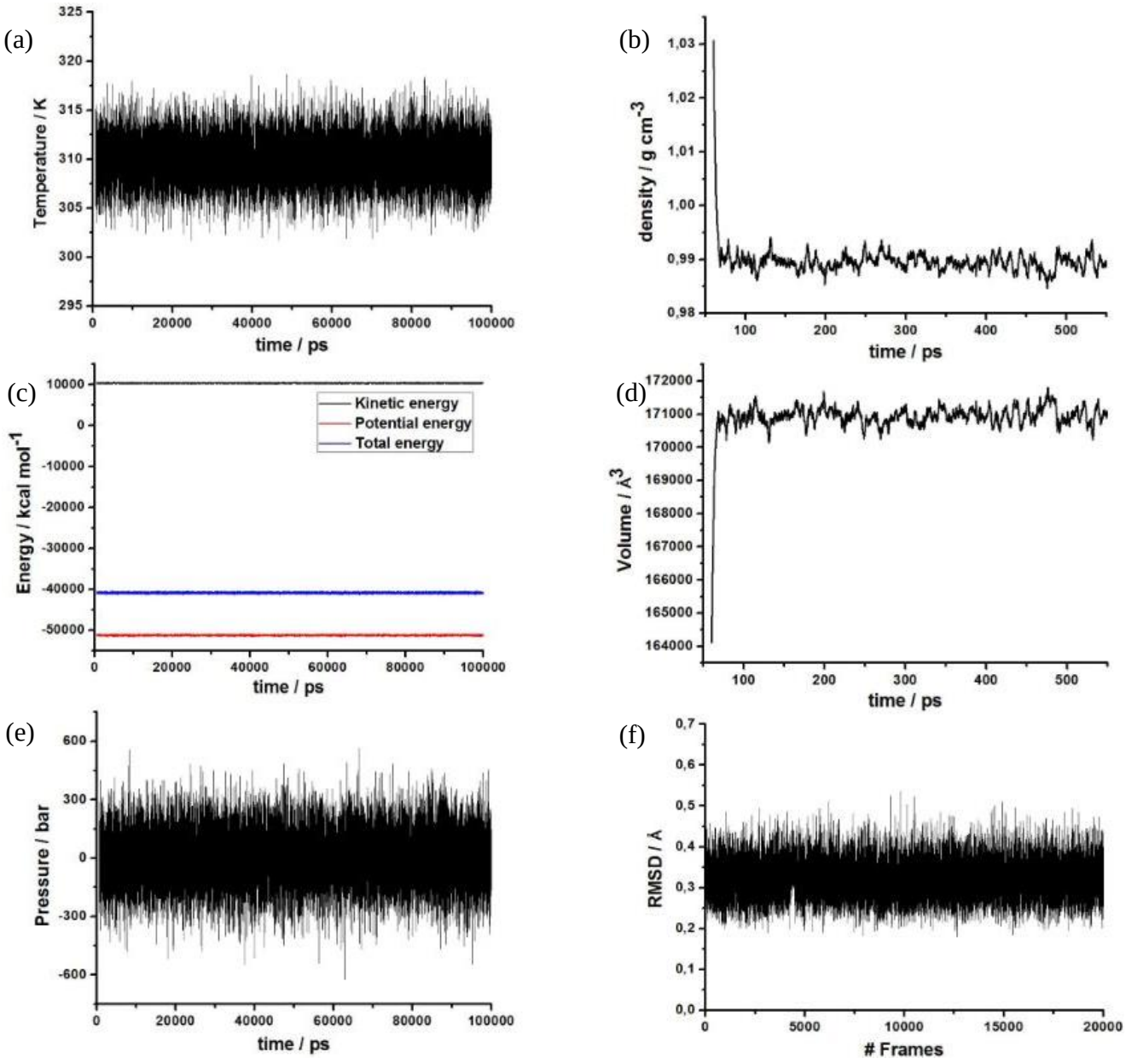

Figure S3. Analyzing the simulation of the cDDP@CNTox complex: the temporal variation of the temperature (a), total, kinetic, and potential energy (b), pressure (c) through the 100 ns production trajectory, density (d) and volume (e) during the last equilibration step (540 ps), and root mean square deviation (f) during the production run.

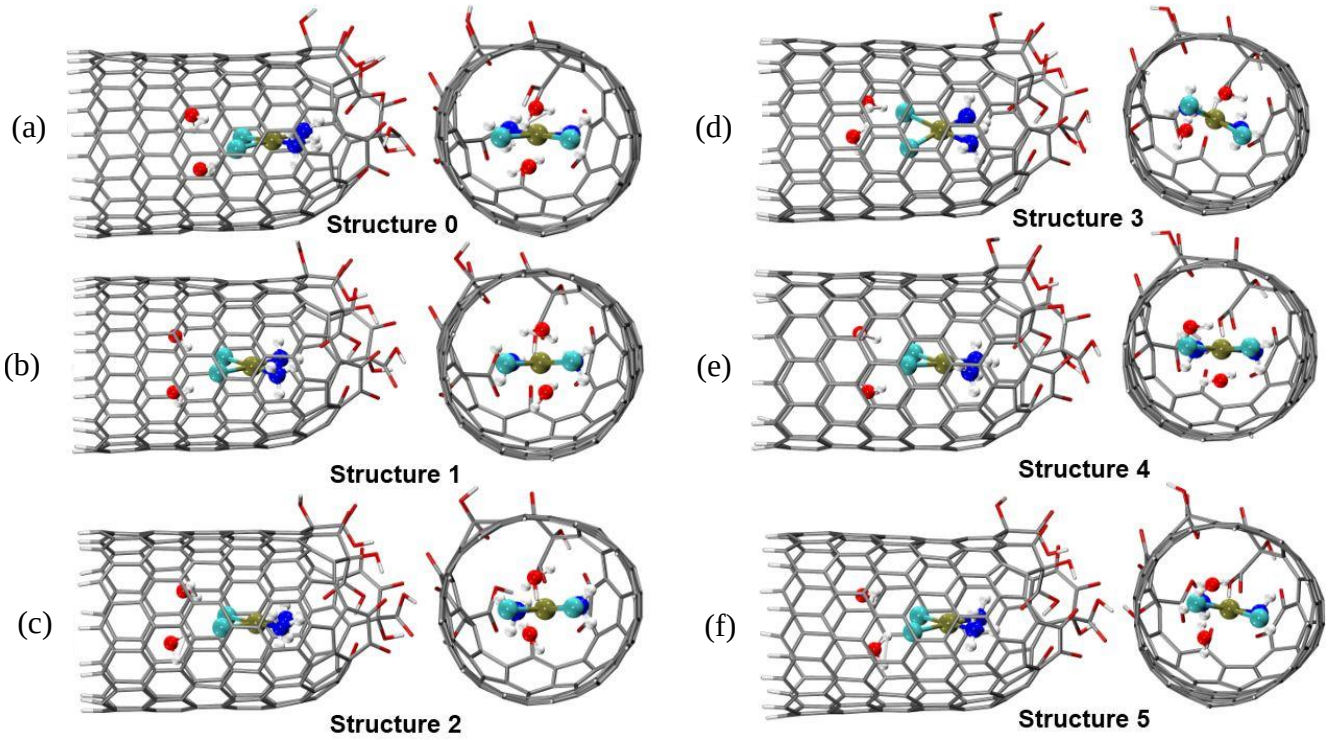

Figure S4. The snapshots of the first six structures (cDDP@CNTox) referring to the total set of 20 structures: Structure 0 (a), structure 1 (b), structure 2 (c), structure 3 (d), structure 4 (e), and structure 5 (f).

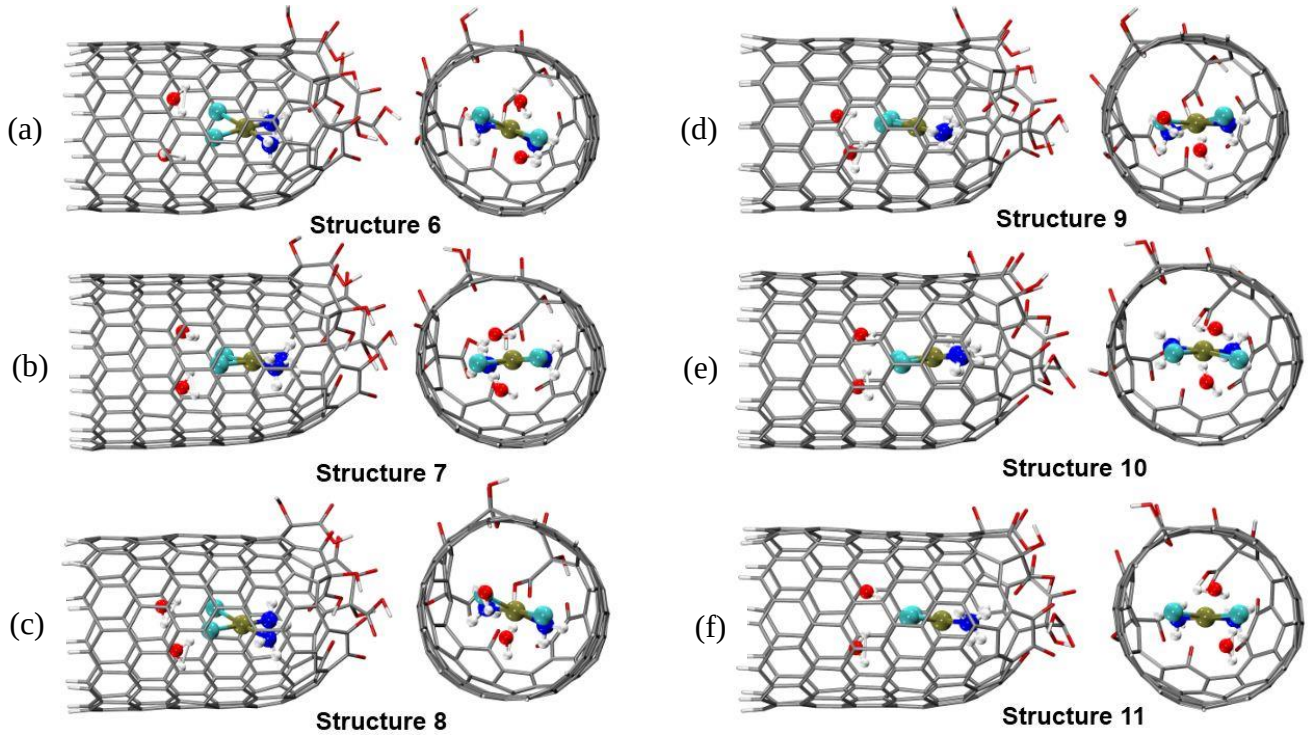

Figure S5. The snapshots of the structures (cDDP@CNTox) referring to the total set of 20 structures: Structure 6 (a), structure 7 (b), structure 8 (c), structure 9 (d), structure 10 (e), and structure 11 (f).

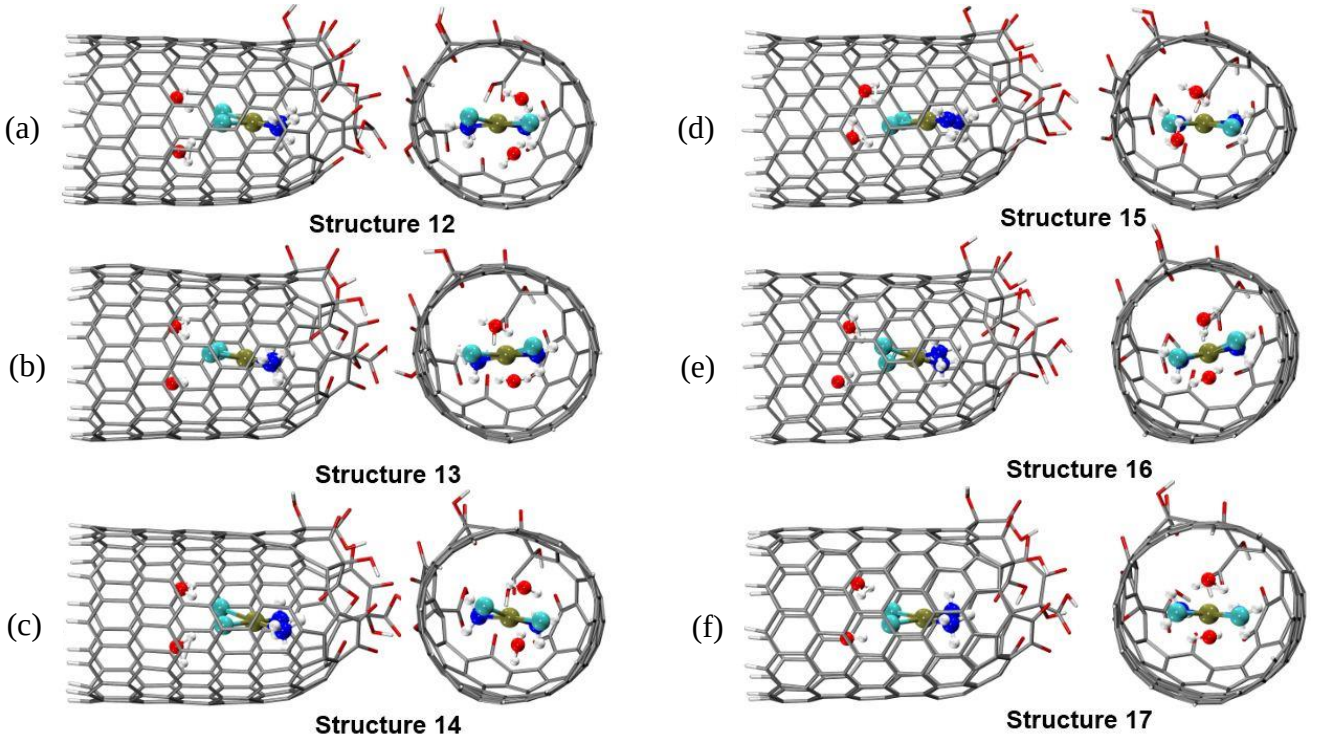

Figure S6. The snapshots of the structures (cDDP@CNTox) referring to the total set of 20 structures: Structure 12 (a), structure 13 (b), structure 14 (c), structure 15 (d), structure 16 (e), and structure 17 (f).

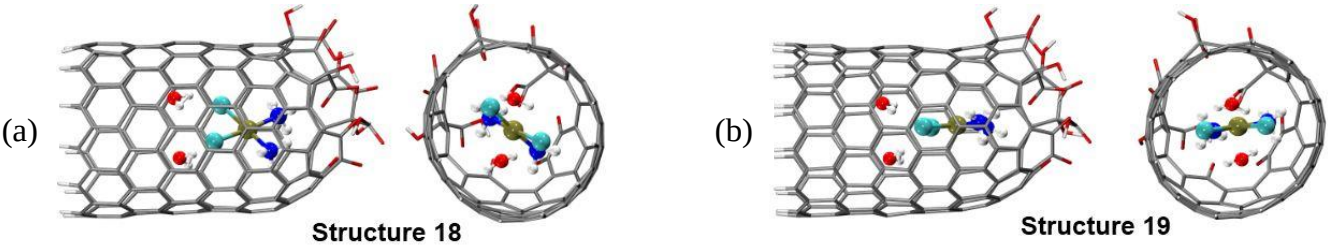

Figure S7. The snapshots of the last two structures (cDDP@CNTox) referring to the set of 20 structures: Structure 18 (a) and structure 19 (b).

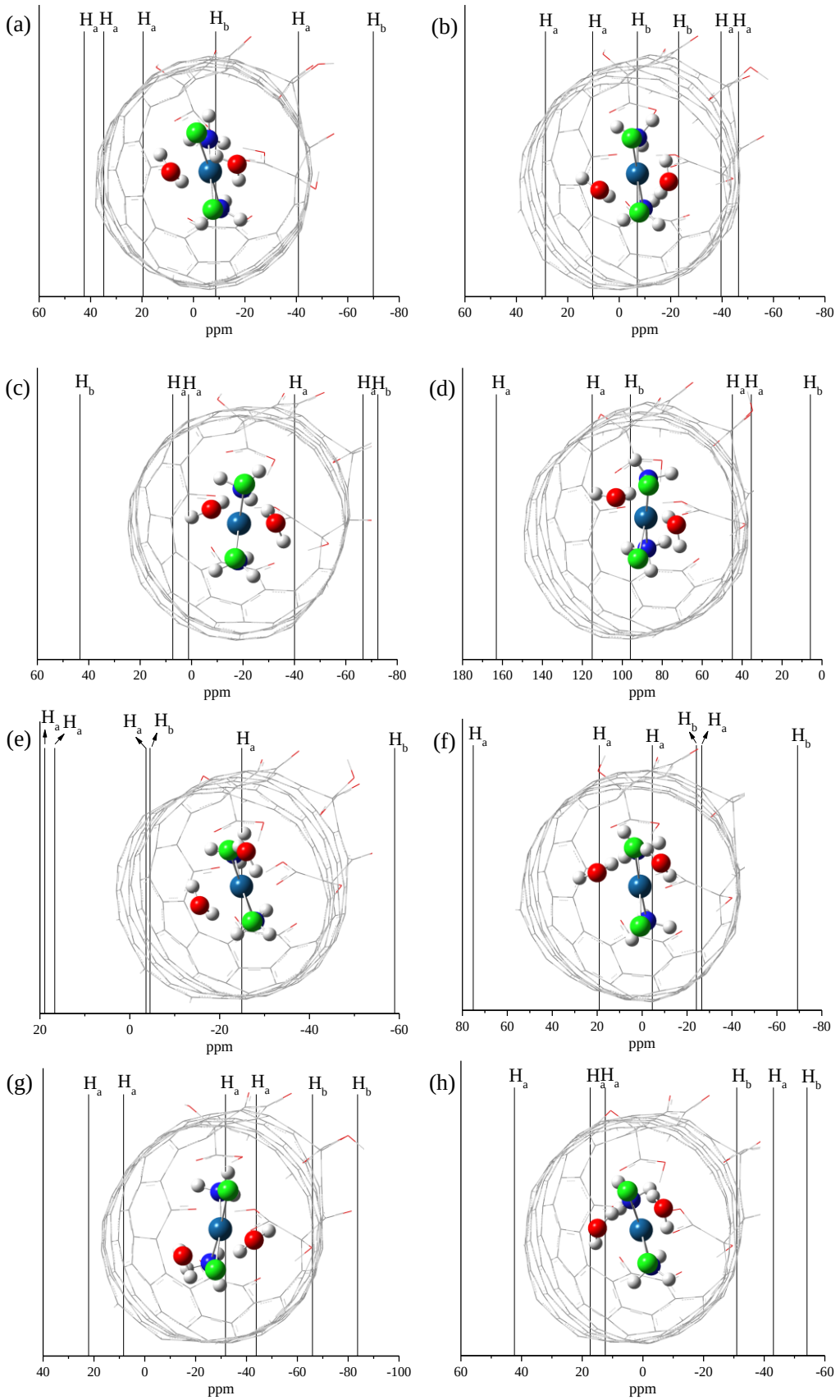

Figure S8. PBEPBE/NMR-DKH/IEF-PCM(UFF) ^{1}H NMR spectrum for cDDP in the geometry of structures 0 to 7 (a-h) obtained by MD simulation.

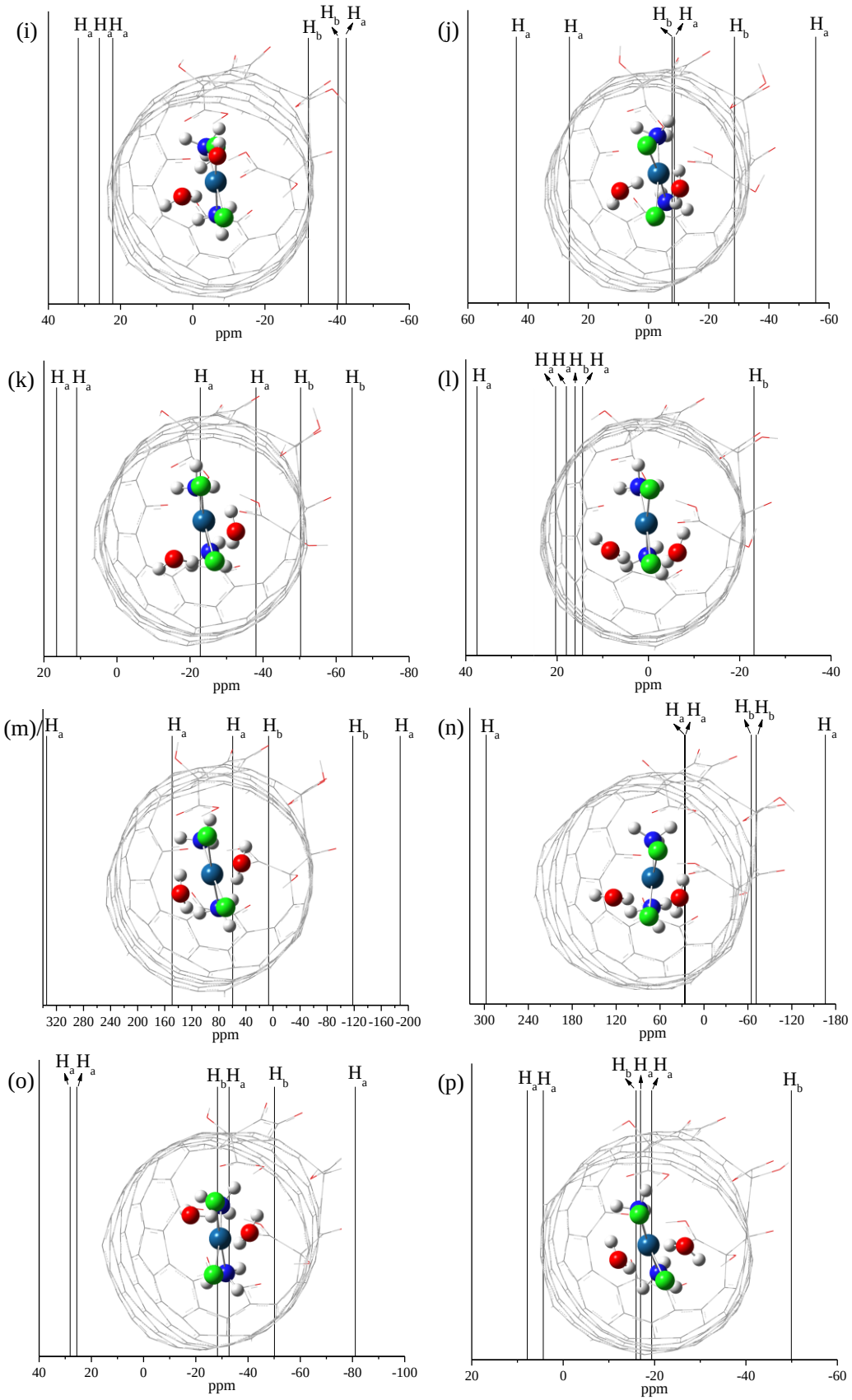

Figure S9. PBEPBE/NMR-DKH/IEF-PCM(UFF) ^{1}H NMR spectrum for cDDP in the geometry of structures 8 to 15 (i-p) obtained by MD simulation.

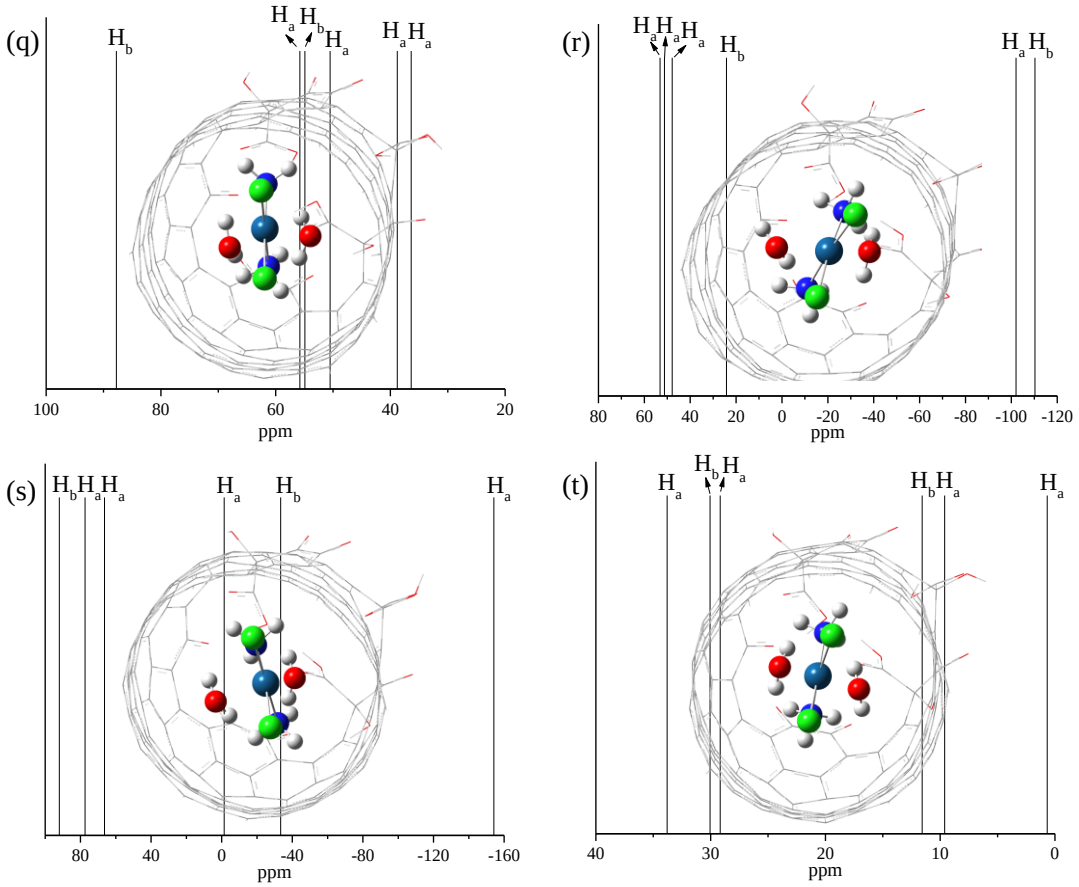

Figure S10. PBEPBE/NMR-DKH/IEF-PCM(UFF) ^{1}H NMR spectrum for cDDP in the geometry of structures 16 to 19 (q-r) obtained by MD simulation.

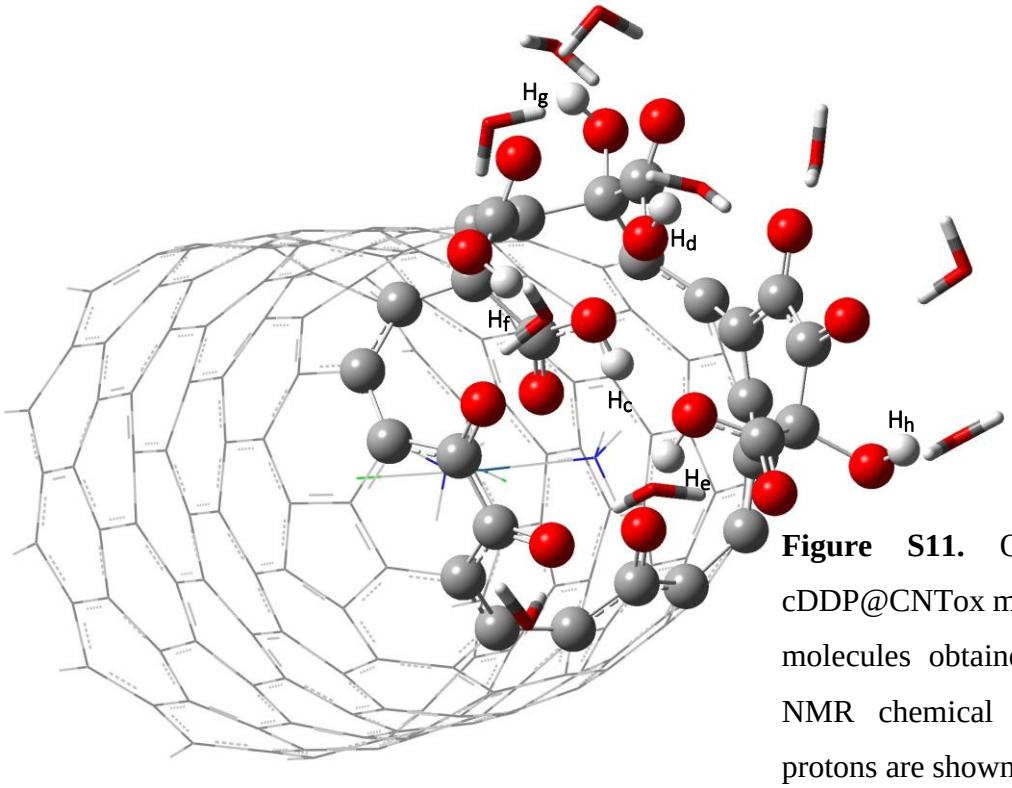

Figure S11. Oxidized region of the cDDP@CNTox model solvated with 10 water molecules obtained by MD simulation. ^{1}H NMR chemical shifts of the highlighted protons are shown in Table S4.

Table S1. Interatomic distance (*d*) between Pt (cisplatin) and C (nanostructures) atoms and its B3LYP/LANL2DZ/def2-SVP/IEF-PCM(UFF) ChelpG charges (in a.u.) in the inclusion complexes and isolated monomers geometries (in parenthesis).

cDDP@CNTox			cDDP@CNCox		
Atoms	*d* / Å	Charge	Atoms	*d* / Å	Charge
Pt	-	-0.2 (0.1)	Pt	-	-0.08 (0.1)
Pt --- C105	4.50	0.07 (0.05)	Pt --- C77	4.90	0.02 (0.06)
Pt --- C106	4.42	-0.07 (-0.08)	Pt --- C78	4.93	-0.04 (-0.04)
Pt --- C107	4.81	-0.06 (0.1)	Pt --- C79	5.10	0.001 (-0.03)
Pt --- C108	4.61	-0.09 (0.08)	Pt --- C80	4.92	-0.004 (0.02)
Pt --- C118	4.57	-0.02 (-0.01)	Pt --- C93	4.73	0.008 (-0.01)
Pt --- C120	4.75	-0.04 (-0.2)	Pt --- C95	4.95	-0.01 (0.03)
Average	**4.61**	**Σ= -0.2 (-0.06)**	**Average**	**4.92**	**Σ= -0.03 (0.03)**

Table S2. PBEPBE/NMR-DKH/IEF-PCM(UFF) ^{1}H, ^{15}N and ^{195}Pt NMR chemical shift values for the cisplatin in the geometry of structures 0 to 19 (Frames) obtained by MD simulation. All values in ppm.

cDDP Chemical shifts (δ) / ppm					cDDP Chemical shifts (δ) / ppm				
Frame	$^{1}H_a$	$^{1}H_b$	^{15}N	^{195}Pt	Frame	$^{1}H_a$	$^{1}H_b$	^{15}N	^{195}Pt
0	42.5, 34.9, 19.6, -40.8	-8.6, -70	165.3, 160.2	-2089	**10**	16.5, 11, -22.8, -38.1	-50.3, -64.4	172.8, 164	-2085
1	28.7, 10.3, -39.6, -46.4	-7, -23	168.9, 137.4	-2107	**11**	37.5, 20.3, 18, 14.4	16.1, -23.1	184.4, 181.2	-2076
2	43.4, 7.3, 1.2, -66.7	-40, -72.5	165.5, 161	-2092	**12**	34.5, 49.1, 59.6, -188	6.5, -118	227, 179	-2072
3	63.1, 115.1, 45, 35.4	96, 5.8	191.1, 186.4	-2081	**13**	97.7, 26.2, 26.1, -165.8	-64.6, -71.4	194.2, 171	-2083
4	19, 16.7, -25, -3.6	-4.5, -60	165.2, 159	-2098	**14**	28.1, 25.6, -32.7, -81	-28.3, -50.1	253.5, 231.5	-2096
5	75.2, 19, -4.5, 26.5	-24.2, -69.2	157.5, 155.2	-2105	**15**	7.8, 4.3, -16.9, -19.3	-16, -50	158, 155.7	-2102
6	22.1, 8.3, -31.7, -43.8	-66, -83.7	272.2, 102.1	-2095	**16**	55.8, 54.9, 38.8, 36.4	87.7, 50.5	163, 161.5	-2092
7	42.4, 17.4, 12.4, -43	-31, -54	178, 166.1	-2085	**17**	53.2, 51.2, 47.8, -102	24.2, -110.3	214.2, 203.8	-2047
8	31.7, 26, 22.2, -42.5	-32, -40.3	161.4, 155.1	-2087	**18**	77.4, 66.4, -1.4, -154.2	92, -33.4	213.7, 189.6	-2074
9	44, 26.2, -8.6, -55.6	-7.8, -28.5	188.1, 181.7	-2067	**19**	33.8, 29.2, 11.6, 0.7	30, 9.6	169.6, 165	-2083

Table S3. Intermolecular distance between the two water molecules and of cisplatin molecule for the selected structures (Frames) of the MD simulation.

Frames	^{195}Pt NMR δ / ppm	$d_{Pt\text{---}O}$ / Å	Frames	^{195}Pt NMR δ / ppm	$d_{Pt\text{---}O}$ / Å
0	-2089	4.08 / 4.34	10	-2085	4.22 / 4.79
1	-2107	4.41 / 4.46	11	-2076	4.40 / 4.56
2	-2092	4.21 / 4.73	12	-2072	4.24 / 4.25
3	-2081	4.20 / 4.84	13	-2083	4.31 / 4.33
4	-2098	4.21 / 4.82	14	-2096	3.86 / 4.58
5	-2105	4.32 / 4.79	15	-2102	4.10 / 4.52
6	-2094	4.32 / 4.72	16	-2092	4.03 / 4.30
7	-2085	4.08 / 4.09	17	-2047	4.13 / 4.38
8	-2087	3.88 / 4.67	18	-2074	4.18 / 4.30
9	-2067	3.98 / 4.25	19	-2083	4.10 / 4.19

Table S4. PBEPBE/NMR-DKH/IEF-PCM(UFF) ^{1}H NMR chemical shift values for the oxidized region of isolated CNTox in the inclusion complex geometry and its cDDP@CNTox model obtained by MD simulation. All values in ppm. The protons indicated are shown in Figure S11.

Structure	Chemical shifts (δ) / ppm					
	Carboxyls			Hydroxyls		
	H_c	H_d	H_e	H_f	H_g	H_h
CNTox	8.4	9.5	7.3	12.6	3.8	11.7
cDDP@CNTox	-1.3	-0.6	7.1	3.3	11.6	14.4

CARTESIAN COORDINATES OF INCLUSION COMPLEXES MODELS

cDDP@CNTox

C	8.25181900	-3.81099400	1.39777700
C	7.59272300	-4.10591300	0.18235200
C	5.42953300	-4.15151700	1.40850000
C	6.15955800	-4.28668200	0.19406000
C	4.01106300	-4.34047800	1.41852600
C	3.33220000	-4.69615200	0.21710100
C	1.18823100	-4.74604200	1.44304100
C	1.92081900	-4.90849200	0.22801800
C	-0.22451600	-4.95365200	1.45714800
C	-0.90706000	-5.34267400	0.25349200
C	-3.08206600	-5.00074500	1.38433400
C	-2.35574100	-5.40608500	0.24905300
C	8.09116700	-2.46010300	3.44553400
C	7.50832700	-3.34261700	2.50615800
C	5.26764900	-2.78570100	3.43038000
C	6.07350600	-3.50898400	2.50425300
C	3.84805400	-2.96109800	3.43536500
C	3.23490600	-3.87750900	2.52490600
C	1.01619400	-3.32749800	3.47355300
C	1.82182800	-4.06465300	2.53661200
C	-0.39677700	-3.51452500	3.50174700
C	-0.98461900	-4.46672900	2.58415700
C	-3.23889000	-3.66120900	3.23395900
C	-2.38131600	-4.54989000	2.52491100
C	7.82745700	-0.27000000	4.53119400
C	7.28826800	-1.50984500	4.11642300
C	5.00758300	-0.60804100	4.51374300
C	5.85357500	-1.67783200	4.10501400
C	3.58927900	-0.78227300	4.52368700
C	3.01947600	-2.02842700	4.12311400
C	0.75650900	-1.14038800	4.58235100
C	1.60365500	-2.20751800	4.13967200
C	-0.65264400	-1.32163700	4.62137100
C	-1.24046900	-2.57154700	4.18981800
C	-3.49995200	-1.56033200	4.31753100
C	-2.67262700	-2.67638400	4.06672000
C	7.53094700	2.17106600	4.40255500
C	7.00191100	0.87587900	4.60955000
C	4.71254400	1.81947400	4.41273500
C	5.56829700	0.69915500	4.60593800
C	3.29271800	1.64943400	4.43893800
C	2.73277800	0.35369000	4.64991200
C	0.46801500	1.32241600	4.52293300
C	1.31789900	0.18193700	4.68047600

C	-0.94567000	1.15704300	4.57011800
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C	-3.75008600	0.70779600	4.28582100
C	-2.88290300	-0.32196400	4.66922300
C	7.25922100	4.24118200	3.09477600
C	6.71171100	3.19814000	3.87821000
C	4.44196800	3.89112000	3.13948600
C	5.27855700	3.01863900	3.89286300
C	3.02175200	3.73263200	3.17844700
C	2.44333300	2.69422900	3.96793800
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C	1.02743100	2.53699800	4.01191300
C	-1.22550800	3.27462400	3.31635100
C	-1.80073900	2.21047200	4.09504500
C	-3.98488700	2.74582200	3.11984300
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C	7.07200700	5.39442200	0.92693900
C	6.47584900	4.86521200	2.09562400
C	4.25390600	5.04041000	0.99144200
C	5.04297100	4.68684400	2.12350100
C	2.83340000	4.88418300	1.02854800
C	2.20240400	4.38638700	2.20869500
C	0.00584800	4.59724300	1.10358700
C	0.78599600	4.24014700	2.25220600
C	-1.40592300	4.43598500	1.12758000
C	-2.02321900	3.93034500	2.30606000
C	-4.23926500	3.80973300	1.06742000
C	-3.39223600	3.64981400	2.22900000
C	7.02083500	5.28450900	-1.52934900
C	6.35060700	5.40592200	-0.28987900
C	4.20621500	4.90499600	-1.44749600
C	4.91870700	5.21979100	-0.25423200
C	2.78799600	4.73295800	-1.41139700
C	2.08078600	4.90708200	-0.18416900
C	-0.05917000	4.40986600	-1.34147900
C	0.66489100	4.75380500	-0.14834700
C	-1.47030700	4.26486900	-1.31513400
C	-2.18153300	4.47946100	-0.07504300
C	-4.19611400	4.55119600	-1.47837700
C	-3.60730700	4.31726300	-0.08510000
C	7.13990300	3.92943700	-3.57582200
C	6.38402500	4.63975200	-2.61540800
C	4.32809500	3.52500700	-3.46048100
C	4.95449700	4.43756900	-2.56581300
C	2.90966700	3.33043300	-3.40995300
C	2.11754300	4.07275400	-2.48578600
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C	0.70130200	3.88489500	-2.43843600
C	-1.34411500	2.73477300	-3.22795300

C	-2.14949300	3.53941300	-2.37197400
C	-4.17148900	2.32009500	-3.02770500
C	-3.59769700	3.41818200	-2.36713200
C	7.40729400	1.73866800	-4.65699500
C	6.58248900	2.80156200	-4.22074700
C	4.59540900	1.34211800	-4.53727100
C	5.15326300	2.59636600	-4.15682100
C	3.17949700	1.14533600	-4.49015600
C	2.32260300	2.20489400	-4.05816800
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C	-1.04641000	0.55610400	-4.36112700
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C	7.75143000	-0.69421200	-4.52639000
C	6.89998500	0.42018000	-4.71161600
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C	-0.69256100	-1.90951100	-4.40644300
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C	3.83963200	-3.36735600	-3.17465400
C	2.99157700	-2.51248400	-3.93600700
C	1.02545300	-3.82012800	-3.19580700
C	1.58365300	-2.72901700	-3.93616200
C	-0.38043300	-4.04768300	-3.21359400
C	-1.23965200	-3.15801100	-3.95508600
C	-3.20909300	-4.30816200	-3.02224900
C	-2.67564700	-3.29362100	-3.83863800
C	8.24761800	-3.91869300	-1.05765400
C	7.49946100	-3.56417600	-2.20469100
C	5.43158800	-4.29369100	-1.02965600
C	6.06895800	-3.76083300	-2.18717600
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C	3.24300700	-4.20233500	-2.18127600
C	1.19996700	-4.96493900	-1.00960300
C	1.83599300	-4.43333800	-2.18372800
C	-0.20540400	-5.19584100	-1.00394000
C	-0.95190000	-4.91800400	-2.21247800

C	-3.05397900	-5.34422400	-0.97342600
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C	-5.22039500	2.30217700	2.58978600
C	-5.45584300	3.03431200	1.36275900
C	-5.66318800	5.03593700	-1.42224300
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C	-5.63445600	1.94668400	-3.22671100
C	-5.01966500	-0.51301400	-3.52307100
C	-6.10729800	0.41457200	-3.04330500
C	-4.81570200	-1.95122300	-3.45474300
C	-5.29002900	-2.99814400	-2.58302700
C	-4.46425200	-4.11597500	-2.36066200
C	-4.35378900	-4.77480400	-1.04725000
C	-4.39901700	-4.37532900	1.34978200
C	-5.07664200	-4.34308300	0.09450300
C	-4.47583800	-3.51650100	2.54720700
C	-5.24521600	-2.27341900	2.69656400
C	-4.76053400	-1.32342900	3.71084100
C	-4.96609200	0.15520300	3.68793600
C	-5.80704600	1.04536300	2.97067800
C	-7.94891800	-0.42170600	2.43829100
C	-7.29164100	0.97693800	2.59852500
C	-7.64421100	1.89383600	1.37155900
C	-6.47191700	-2.97356900	-1.67423800
C	-6.38159400	-3.72352500	-0.26750900
O	-8.81764000	2.07754500	1.13170200
O	-7.52870800	-2.44823400	-1.94872600
C	-6.39327500	0.18628600	-1.55267900
O	-5.51078400	0.00513100	-0.73215200
O	-7.67914700	0.19565300	-1.28384100
H	-7.84943300	-0.08175300	-0.34609600
O	-7.25216500	0.23531300	-3.82959500
H	-7.99158300	0.67899400	-3.38430100
O	-3.60913000	5.79542600	-1.93949800
H	-3.90925100	5.92924600	-2.85264200
O	-6.18062400	5.15467600	-2.64520200
H	-7.03219500	5.62038900	-2.56897300
O	-6.15449100	5.53125700	-0.43809400
O	-6.44702600	2.70457700	-3.68535000
O	-6.77179400	2.86314300	-0.63586900
O	-7.40456900	-3.80194400	0.37801500
O	-6.11545400	-1.94466100	1.87127600
O	-7.92635200	1.60061300	3.71403200
H	-8.84734900	1.77496400	3.45438500
O	-8.24024000	-0.75312200	1.15612300
O	-8.30647700	-1.07179400	3.38101400
H	-8.29826200	-1.72891400	1.09056200
H	8.61510600	2.30574000	4.40031200
H	8.91243100	-0.14190500	4.53836000

H	8.34315100	4.37697100	3.07891300
H	8.15532100	5.53392600	0.90127200
H	8.10257400	5.43372300	-1.56320800
H	8.22054400	4.08372100	-3.61962500
H	8.48799700	1.89250200	-4.70144600
H	8.83319500	-0.54506700	-4.56097600
H	9.14751000	-2.61382600	-3.24156400
H	9.33127800	-3.78016900	-1.06783300
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Pt	-1.25953200	-0.42532100	0.01648500
N	-2.94718800	0.69603000	0.49695800
H	-2.72682600	1.69338400	0.43078400
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N	-2.47352300	-2.01883600	-0.53931900
H	-1.87467500	-2.75394200	-0.92622500
H	-2.98869500	-2.41706100	0.25230100
H	-3.22538000	0.51615000	1.46660400
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Cl	0.12278700	1.38361200	0.63765100

cDDP@CNCox

C	1.32295400	10.02790600	4.01665500
C	1.80763000	11.34255800	3.66794400
C	-1.50916100	6.14834600	2.71931700
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C	-0.06904500	8.07119900	3.35390600
C	0.41403700	9.84302600	1.71885100
C	0.51582800	9.34024900	3.04258400
C	1.10127900	11.05672000	1.34573800
C	1.69905200	11.83647000	2.40200100
C	-4.48057600	2.35219300	1.58936800
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C	-2.38153500	5.96135700	0.43040500
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C	-1.62150800	7.11760200	0.06933400
C	-0.97711600	7.89802700	1.07450000
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C	-0.24040500	9.06928500	0.71330900
C	0.84165900	10.47111800	-1.02202400
C	1.27176200	11.36731300	0.00291900
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C	-6.48368500	0.72288700	1.50294700
C	-6.23128900	3.18637800	-0.95848800
C	-5.23361100	1.36155000	0.79017600
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C	-1.75227500	6.41890700	-2.27186700
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C	0.15949700	8.46257300	-2.93245200
C	-0.45107400	8.43996400	-1.65101400
C	1.12615400	9.48458200	-3.25137400
C	1.34823300	10.54097400	-2.32717600
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C	-8.04076000	1.37038100	-3.88812300
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C	-6.78846100	2.27231000	-3.87299100
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C	-3.02567500	4.38179900	-2.89465700
C	-1.09414600	5.18341600	-4.27104400
C	-1.01293100	6.36463800	-3.49413000
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C	-0.02164500	7.34803300	-3.79869700
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C	-4.10559700	-0.15265400	-4.87354000
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C	-3.04217000	0.76745000	-5.01610400
C	-3.15248600	2.06958200	-4.46157100
C	-0.94200400	2.61093900	-5.43354500
C	-2.08881800	2.98169100	-4.66735400
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C	-0.04759700	4.88256000	-5.19144600
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C	-2.19583400	-3.36765900	-4.98625400
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C	4.63823700	-0.42771000	-6.21565000
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C	-4.64770900	-5.58573100	2.84575800
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C	-2.29056800	-6.63980500	0.30071500
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C	1.52026000	-4.29470800	4.56422700
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C	9.59140800	-3.73846500	-2.06386800
C	12.01011700	-3.31665600	-2.25120500
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C	0.40074800	-1.15871800	6.21784400
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C	-8.12771300	-3.19151500	2.90007100
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H	-8.04088000	-0.77872200	-6.19564200
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H	-9.93968300	-2.58420800	-4.36137900
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H	-8.14557000	1.36824500	2.23201900
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H	-7.25983000	-1.77770200	-0.51395100
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H	-7.32558000	3.15344200	0.60234900
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O	-6.81890400	-5.70331100	1.75832300
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H	1.84905100	12.25178500	-0.27716000
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H	2.72136600	10.05981400	-4.59789400
H	3.82448400	8.47273600	-6.12965500
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H	6.80320100	4.86996700	-7.63312800
H	8.49014900	3.03992900	-7.60651700
H	10.21897600	1.30661500	-7.09623400
H	11.94245800	-0.26148300	-6.17586600
H	12.49726900	-1.94557300	-4.50925200
H	12.87788300	-3.02552600	-2.84306300
H	13.20991200	-3.75071700	-0.54204600
H	12.19415800	-4.01853700	1.73527100
H	11.07775100	-3.74281600	3.94549700
H	9.87717100	-2.85208800	5.91973500
H	8.64487500	-1.39661900	7.48202700
H	7.45070300	0.49145900	8.51952900
H	6.35259200	2.65680800	9.01292800
H	5.39533100	4.95582800	9.00065400
H	4.60579800	7.28842900	8.55810500
H	4.00177700	9.58801700	7.76947600
H	2.92748200	10.96184300	6.07296600
Pt	-2.39775500	-1.84236100	-0.31011000
N	-3.88727600	-2.82457700	0.76705900
H	-3.55379600	-2.98460300	1.72135900
H	-4.77233200	-2.30374400	0.80990700
N	-3.80160700	-1.31110400	-1.73934900
H	-4.36418100	-2.09511000	-2.07661700
H	-4.43528700	-0.59340500	-1.36091100
H	-4.09661500	-3.74085000	0.35782800
H	-3.31418200	-0.90585500	-2.54238300
Cl	-0.76885400	-0.72587100	-1.64733600
Cl	-0.86537400	-2.40304200	1.43027800