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Theoretical Study on Porphyrin Arch-Tapes of Carbonyl-Inserted Seven-Membered Ring with High Nonlinear Optical Properties

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It is well known that the NLO properties are induced by nonlinear charge displacements that are generated under a strong electric field of light. In the presence of weak and static electric field, the energy of a molecule is a function of the field strength. The energy of the perturbed system is described by expansion as follows:

$$E = E^0 - \mu_i F_i - \left(\frac{1}{2!}\right)\alpha_{ij}F_iF_j - \left(\frac{1}{3!}\right)\beta_{ijk}F_iF_jF_k - \left(\frac{1}{4!}\right)\gamma_{ijkl}F_iF_jF_kF_l + ... \quad (1)$$

where E^0 is the molecular energy in the absence of the applied electric field; μ_i is the component of the dipole moment along the *i* direction; F_i is the Cartesian component of the applied electric field along the *i* direction; α_{ij}, β_{ijk} and γ_{ijkl} are the polarizability, first, and second hyperpolarizability tensors, respectively.

The conceptual density functional theory (CDFT)[1,2] originally developed by Robert Parr is a theory framework aiming for unraveling reactivity of chemical systems. CDFT contains numerous concepts and quantities, some of them can be used to predict favorable reactive sites and reactive character, and some of them can compare reactivity among different chemical species. Due to the high popularity and important role of CDFT in quantum chemistry, as well as there are so many meaningful relevant quantities, this method has been used to calculate all global reactive parameters, which were finished by Multiwfn 3.3.8. To yield all below quantities, electronic energy (*E*) and electron density of *N*, *N*+1 and *N*-1 electron states must be available. Commonly *N* refers to the number of electrons carried by a chemical system at its most stable status. Geometry optimized for *N* electrons state is employed for all calculations.

In the section, Vertical ionization potential (VIP): E(*N*-1) − E(*N*), Vertical electron affinity (VEA): E(*N*) − E(*N*+1), Mulliken electronegativity (χ): (VIP+VEA)/2,

Chemical potential (μ): -χ, Hardness (η): VIP−VEA, which is also equivalent to fundamental gap.[2] Note that according to the convention employed by many CDFT papers, the prefix of 1/2 in original definition of is dropped. Softness (S): $1/\eta$, [3] and Electrophilicity index (ω):$\mu^2/(2\eta)$.[4]

Table S1 Frequencies values (cm^{-1}) of all the studied complexes calculated at the B3LYP/6-31G(d)/SDD level.

Complex	Frequencies
1	8.64/10.60/14.64/21.36/24.59/28.52/31.55/34.15/35.91/40.44/43.26/ 44.79/45.54/49.55/50.39/51.85/52.15/56.78/60.15/66.58/69.14/69.25/ 90.37/99.96/102.17/113.77/118.5/132.37/134.9/144.88/148.32/157.03/ 175.57/179.85/185.96/193.46/209.91/216.31/216.86/219.22/221.55/ 228.99/230.17/235.05/247.26/249.4/250.19/252.66/255.98/258.95/ 262.59/265.35/270.74/285.83/292.67/299.72/303.83/309.97/316.53/ 316.97/321.91/325.67/328.25/331.76/333.47/337.6/352.3/377.48/ 406.6/411.11/416.43/417.32/417.6/417.88/418.54/418.89/419.79/ 426.41/429.76/432.39/453.32/460.32/465.62/472.48/472.89/474.95/ 477.57/491.28/499.07/507.37/519.05/526.18/529.21/548.1/552.18/ 566.37/572.11/573.5/574.29/580.17/581.7/595.18/619.08/623.51/ 634.88/634.91/635.03/635.22/636.31/636.61/656.25/661.05/664.37/ 667.45/670.78/671.6/674.87/675.23/680.95/683.71/690.14/693.62/ 694.49/706.27/715.31/715.47/715.94/716.73/716.96/717.02/730.95/ 732.88/735.15/735.88/745.36/747.5/748.9/764.41/765.35/769.71/ 772.63/774.21/775.92/781.67/797.52/801.53/803.41/806.5/809.88/ 810.53/822.94/833.14/836.91/844.28/845.98/847.37/852.98/857.49/ 858.54/863.26/863.57/863.7/863.86/864.14/864.41/873.05/878.26/ 889.59/892.7/899.44/902.22/914.16/914.48/916.6/917.64/918.27/

	918.69/921.1/921.31/938.19/938.62/939.43/939.99/940.04/940.24/ 971.02/971.14/971.24/971.41/971.45/971.51/996.9/996.94/996.96/997/ 997.04/997.17/997.41/1017.31/1017.33/1017.36/1017.38/1017.47/ 1017.7/1025.82/1029.71/1030.95/1033.89/1034.56/1039.11/1041.91/ 1044.33/1046.34/1048.99/1050.71/1055.98/1063.06/1064.81/1068.88/ 1069.63/1076.05/1077.78/1084.59/1108.26/1108.73/1109/1109.22/ 1109.47/1109.53/1111.39/1111.92/1112.83/1112.89/1116.73/1119.62/ 1176.91/1192.77/1192.8/1192.8/1192.81/1192.82/1192.84/1210.54/ 1213.04/1213.85/1213.94/1212.97/1214.13/1214.36/1214.65/1232.36/ 1240.86/1243.04/1253.49/1258.87/1265.32/1270.93/1274.18/1276.33/ 1277.57/1281.39/1292.91/1304.7/1322.22/1325.86/1327.85/1327.99/ 1329.03/1329.72/1330.08/1337.15/1346.01/1347.38/1349.66/1359.72/ 1361.85/1363.38/1363.74/1363.89/1364.16/1364.21/1365.17/1375.75/ 1380.35/1386.01/1393.11/1396.89/1403.74/1406.87/1415.11/1416.12/ 1478.46/1487.26/1487.29/1487.35/1487.66/1487.7/1488.65/1495.2/ 1499.92/1504.3/1508.19/1520.4/1508.19/1520.4/1523.19/1529.96/ 1535.55/1540.89/1542.35/1543.85/1544.87/1546.16/1548/1554.57/ 1557.71/1563.24/1564.23/1567.43/1570.76/1575.11/1591.07/1593.34/ 1595.49/1606.79/1610.27/1612.86/1620.38/1633.12/1633.16/1633.25/ 1633.33/1634.05/1634.67/1658.84/1658.92/1659.02/1659.11/1659.21/ 1659.4/1665.15/3183.02/3183.04/3183.07/3183.11/3183.13/3183.16/ 3190.54/3190.74/3190.77/3190.78/3190.84/3190.89/3200.43/3200.6/

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2	7.43/10.21/14.78/18.41/26.04/30.23/32.21/33.45/38.38/45.05/45.69/47. 36/51.07/53.44/53.8/55.09/55.4/56.79/64.27/67.62/76.95/78.12/99.15/1 06.51/111.95/116.39/130.82/143.1/147.98/149.15/159.45/165.1/168.71 /191.29/193.17/196.69/200.57/211.24/218.93/222.65/224.53/233.79/23 3.97/239.19/242.31/249.54/250.07/255.1/259.57/261.91/266.37/268.53 /268.94/275.33/302.1/303.31/306.93/312.55/314.64/321.27/323.88/327 .75/330.39/335.94/337.33/353.53/357.34/376.94/377.12/403.83/414.74 /417.34/417.98/418.8/419.27/419.27/419.82/421.06/425.47/427.09/449 .74/455.54/459.4/464.55/471.31/474.72/484.69/499.56/503.89/505.55/ 520.35/523/528.91/544.75/545.81/567.11/571.78/575.47/577.22/581.35 /583.52597.44/627.62/634.67/634.73/634.98/635.17/636.09/637.41/655 .01/659.85/664.49/667.89/668.3670.32/672.06/673.02/680.28/685.01/6 85.31/692.26/697.67/714.28/715.17/715.52/716.21/716.47716.63/720.4 4/727.47/732.35/733.99/740.47/741.98/743.46/747.29/748.2/765.39/76 7.34/768.25/775.75/775.93/778.19/782.66/793.51/802.61/803.02/809.0 5/809.18/833.12/835.68/838.73/841.42/847.77/849.33/852.64/855.26/8 55.6/862.96/863.11/863.69/863.94/864.57/864.69/866.1/871.79/882.56 /889.41/897.47/902.77/914.32/915.15/917.03/917.04/917.39/917.42/92

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4	5.41/11.62/15.56/18.52/21.42/24.18/28.39/29.86/34.15/34.83/41.05/ /44.52/47.24/49.46/51.01/51.55/54.9/55.43/60.83/65.47/66.48/77.52 /84.76/88.02/108.71/110.88/125.95/140.63/142.14/143.72/146.75 /159.19/164.24/170.95/184.52/190.94/191.61/207.87/214.79/221 /222.8/226.9/229.93/233.62/235.68/240.71/248.19/251.63/254.27 /260.06/264.2/266.79/270.22/273.77/287.82/299.26/304.86/307.07 /313.18/319.28/320.06/326.96/329.09/330.63/333.94/339.62/352.57 /369.92/378.63/397.13/404.23/414.38/415.57/416.41/417.01/417.27 /418.64/419.87/420.86/421.77/441.26/450.65/459.34/463.85/465.16 /469.45/471.1/477.88/498.05/508.02/510.08/525.45/529.31/535.44 /542/549.72/557.26/568.01/569.81/573.99/580.91/582.06/584.95 /600.27/608.48/629.61/634.54/634.79/635.07/635.32/636.34/639.28 /650.4/655.58/661.88/662.7/665.65/669.01/670.73/672.55/674.44 /680.76/687.44/690.62/695.67/708.33/714.3/715.49/715.82/716.53 /716.92/716.98/717.33/731.45/731.69/738.67/741.74/745.4/747.51 /751.12/765.01/765.37/767.26/770.35/773.85/774.71/775.83/787.42 /801.5/801.95/808.72/809.16/824.23/837.81/838.7/839.15/845.68 /850.14/853.9/855.02/862.34/862.5/863.21/863.61/864.14/864.28 /866.02/874.59/882.65/892.25/893.74/897.28/906.66/907.62/910 /912.7/914.84/915.36/918.45/918.8/925.8/938.75/939.06/940.1

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6-anti	3.74/6.58/7.08/13.71/15.61/18.87/21.82/25.38/25.72/28.68/28.82/31.19 /34.78/35.48/39.86/44.16/46.29/46.4348.81/50.32/50.7/53.33/53.8/56.0 5/56.86/57.9/62.47/64.99/66.31/68.49/71.94/84.8/84.81/95.49/107.05 /109.07/114/117.07/118.88/128.48/136.18/142.06/147.41/148.84/150.0 6/163.05/165.42/168.59/172.15/177.28/185.07/191.7/191.99/198.67/20 7.1/210.09/214.52/216.13/221.68/224.53/226.46/226.86/232.6/232.78/ 239.87/242.23/244.04/250.55/251.98/252.99/257.11/258.88/261.44/265 .28/268.15/269.98/273.59/276.05/280.37/290.01/298.46/301.37/302.98 /313.73/314.61/317.18/320.05/320.3/326.64/327.48/328.43/329.96 /331.53/343.1/344.55/353.84/365.01/368.78/372.33/372.49/393.83 /399.48/401.52/408.35/415.67/415.76/416.38/416.77/416.8/419.1 /419.25/420.43/420.91/421.53/422.95/433.87/437.8/442.79/446.71 /454.95/455.5/464.84/465.87/470.41/470.71/470.82/479.57/491.51 /498.98/500.89/502.34/509.82/511.68/525.59/529.63/534.31/535.21 /546.17/548.11/557.87/562.02/565.63/569.02/577.22/579.06/579.08 /583/584.06/586.89/602.04/603.75/607.49/614.91/629.7/630.21 /634.47/634.54/634.69/635.06/635.29/635.77/637.46/639.9/651.01 /653.58/656.98/661.46/661.6/662.7/663.89/667.54/668.46/669.18 /672.28/672.56/680.44/681.47/685.29/689.87/693.6/695.53/705.68

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7-anti	3.55/5.65/7.17/11.18/13.49/19.32/20.99/25.67/26.25/27.01/31.3/34.15 /35.95/39.48/46.52/47.29/47.6/49.64/50.04/50.7/52.06/53.13/53.79 /55.05/56.6/57.68/59.84/62.19/64.42/69.12/73.84/83.95/85.35/90.96 /97.03/99.35/101.48/102.01/109.35/114.71/124.26/128.33/131.74 /140.35/144.46/145.18/154.89/159.43/160.77/163.7/170.33/173.26 /183.18/185.32/189.6/190.26/195.64/197.7/200.33/201.32/203.05 /204.24/205.19/206.4/207.27/211.42/214.08/217.53/219.27/222.35 /225.07/226.08/230.39/232.84/238.02/242.75/242.87/245.61/251.42 /258.43/261.05/267.06/271.13/281.27/288.16/290.2/296.01/298.84 /306.21/310.6/311.41/321.35/327.67/331.1/331.84/339.41/343.66 /351.43/354.03/357.89/383.64/384.78/390.15/395.14/403.8/409.81 /411.89/415.02/417.87/418.34/418.83/419.17/419.43/420.06/420.8 /428.43/430.67/435.32/438.91/442.19/442.96/450.56/450.8/453.97 /456.67/461.21/466.66/469.65/484.22/493.64/496.89/504.35/508.78 /515.78/524.14/529.25/531.55/542.5/547.67/548.94/552.4/569.59 /572.48/572.82/576.59/577.88/579.56/582.28/583.45/589.33/591.45 /609.26/617.28/621.73/622.73/634.42/634.52/634.7/634.94/635.11 /635.19/635.74/635.97/647.49/650.92/655.47/659.51/666.87/667.23

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	/3287.04/3289.35/3290.58/3291.25/3291.38/3300.86/3301/3301.42 /3302.9

Table S2. Selected values of selected bond lengths (Å), angles (deg) and symmetry of the molecular structures of complexes **1**−**7-anti**

Complex	**1**	**2**	**3**	**4**	**5-anti**	**6-anti**	**7-anti**
C1-B	-	1.492	-	1.465 (1.464)	1.492	1.464	1.461
C2-B	-	1.492	-	1.465 (1.457)	1.493	1.467	1.465
N3-M	1.925	1.915	1.961	1.903 (1.884)	1.904	1.888	1.989
N4-M	1.939	1.940	1.959	1.933 (1.911)	1.936	1.930	2.074
N1-M	1.936	1.937	1.956	1.924 (1.905)	1.904	1.888	1.989
N2-M	1.950	1.944	1.961	1.936 (1.928)	1.936	1.930	2.074
θ	-	96 (97)	25	94 (84)	151	152 (138)	104 (97)
Symmetry	C_1	C_1	C_2	C_1	C_2	C_1	C_1

[a]Previously reported experimental data is in parentheses.

Table S3. Total polarizability α (a.u.) and second hyperpolarizability γ (10^5 a.u.) of the studied complexes computed at various levels of theory.

Complex	Functionals	α	γ	γ_{xxxx}	γ_{yyyy}	γ_{zzzz}
1	CAM-B3LYP	1834.1	138.9	641.0	29.3	1.5
	M06-2X	1848.2	146.8	677.0	30.9	1.4
2	CAM-B3LYP	1940.1	167.5	742.5	36.1	3.8
	M06-2X	1956.8	172.7	764.0	38.3	4.0
3	CAM-B3LYP	1943.0	167.1	771.1	26.1	0.5
	M06-2X	1959.5	173.2	800.6	28.2	0.4
4	CAM-B3LYP	1983.4	182.5	789.4	26.9	4.0
	M06-2X	1997.5	187.4	807.9	28.2	4.1
5-anti	CAM-B3LYP	3365.4	1113.9	4984.6	45.2	55.2
	M06-2X	3416.1	1175.5	5276.9	48.4	57.1
6-anti	CAM-B3LYP	3723.1	1344.6	6844.3	44.1	67.7
	M06-2X	3764.8	1549.6	7054.7	47.3	69.6
7-anti	CAM-B3LYP	4668.7	1584.3	7846.9	64.0	27.5
	M06-2X	4551.7	2101.3	10240.5	68.7	27.8

Table S4. The energy (ΔE, eV), the absorption wavelength (λ, nm), oscillator strength (f_0,) and major contribution for complexes **1** and **6-anti** using TD-ωB97XD/CAM-B3LYP with 6-31G(d,p) basis set.

Complex	Method	State	λ	ΔE	f_o	MO transition
1	ωB97XD	Q	723 (736) [a]	1.715	0.566	[b]H→L (74%)
		Soret	440 (488)	2.817	2.128	H-1→L+1 (49%), H-2→L+2 (32%)
	CAM-B3LYP	Q	717 (736) [a]	1.729	0.576	[b]H→L (75%)
		Soret	445 (488)	2.785	2.073	H-1→L+1 (55%), H-2→L+2 (28%)
6-anti	ωB97XD	Q	1235 (1254)	1.004	1.706	H→L (88%)
		Soret	481 (617)	2.578	2.405	H-1→L+2 (47%),
	CAM-B3LYP	Q	1199 (1254)	1.034	1.209	H→L (92%)
		Soret	491 (617)	2.520	2.270	H-1->L+2 (54%)

[a]Previously reported experimental data is in parentheses. [b]H = HOMO, H-1 = HOMO-1, and L = LUMO.

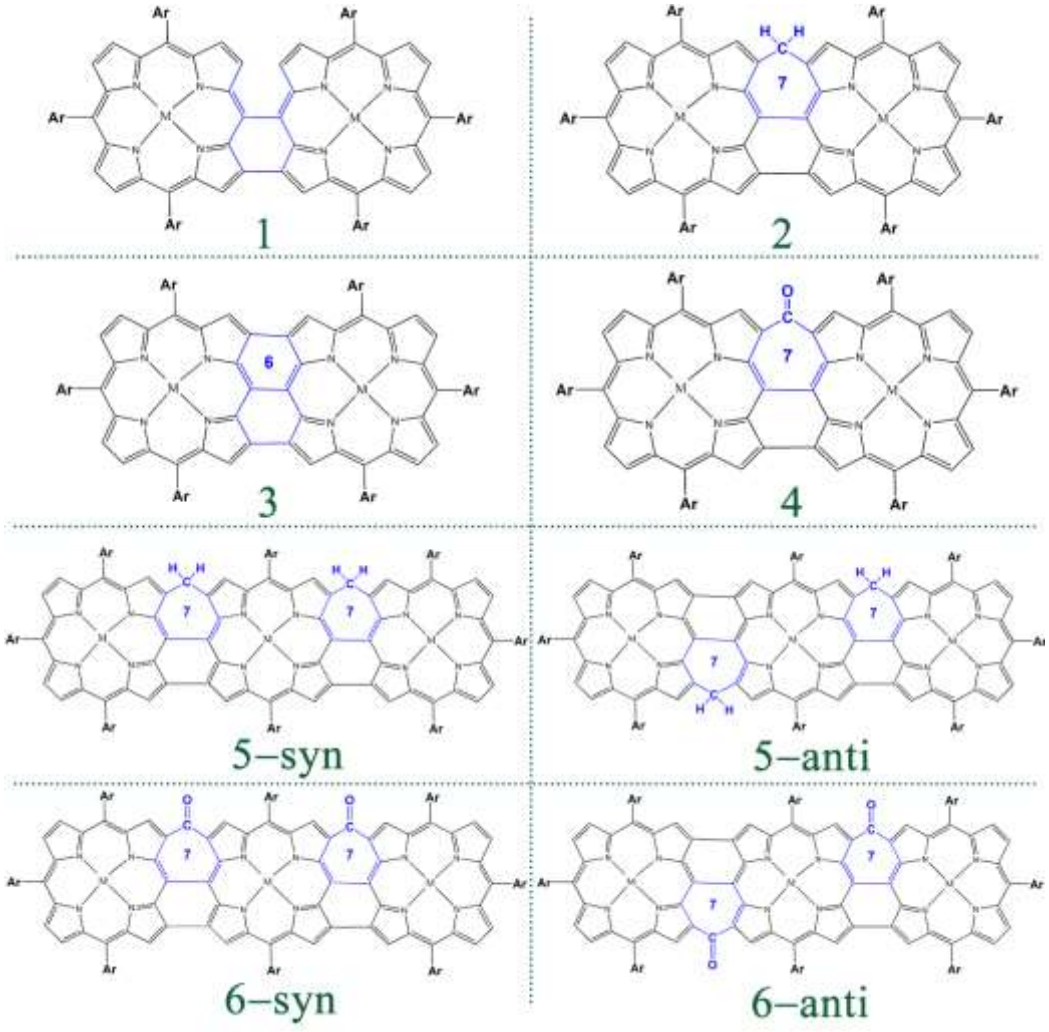

Figure S1. The Geometric structures of the porphyrin derivatives.

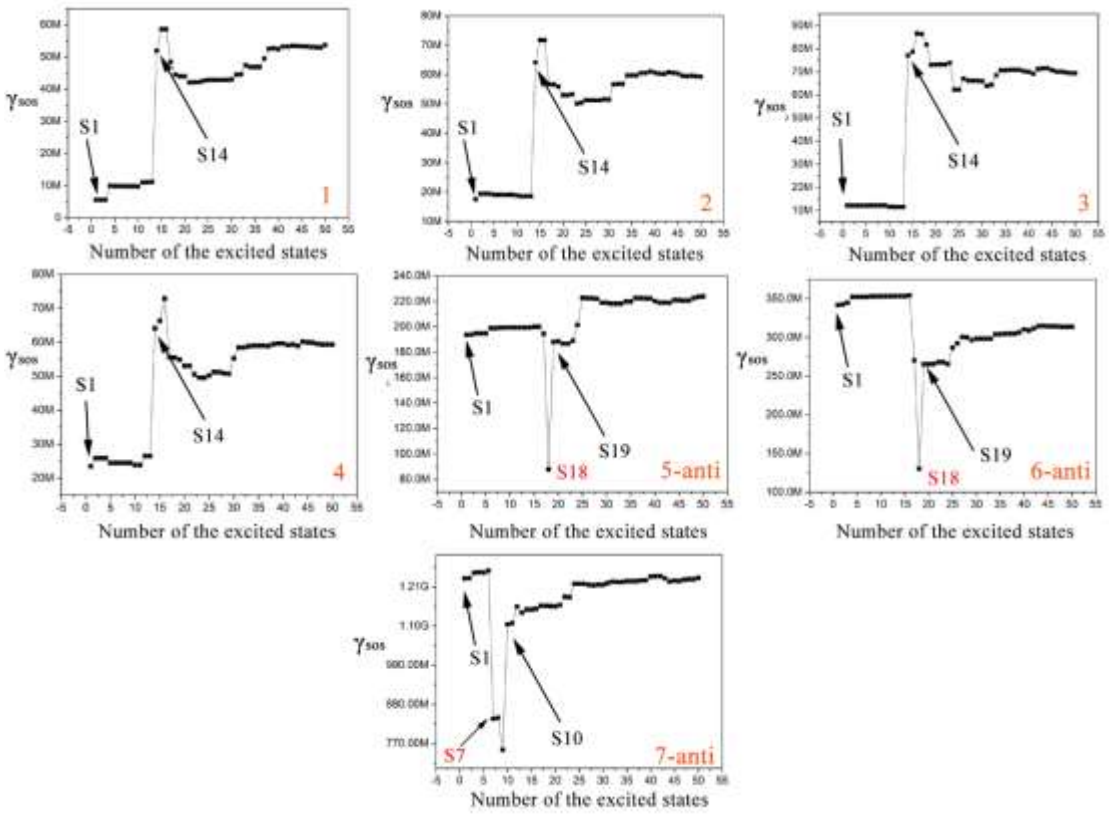

Figure S2. Convergent behavior of γ_{tot} values of all studied complexes dependent on the first 50 states.

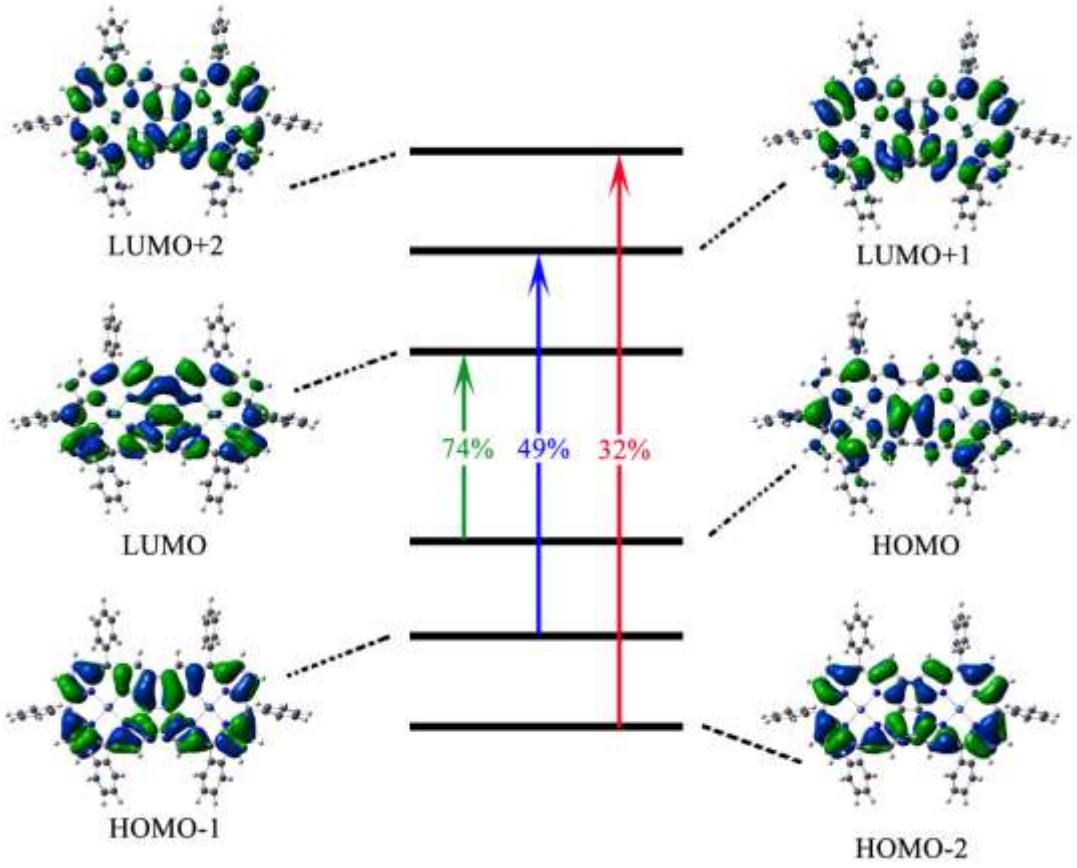

Figure S3. Molecular orbitals involved in the crucial intense electronic transitions in the absorption spectra of complex **1**.

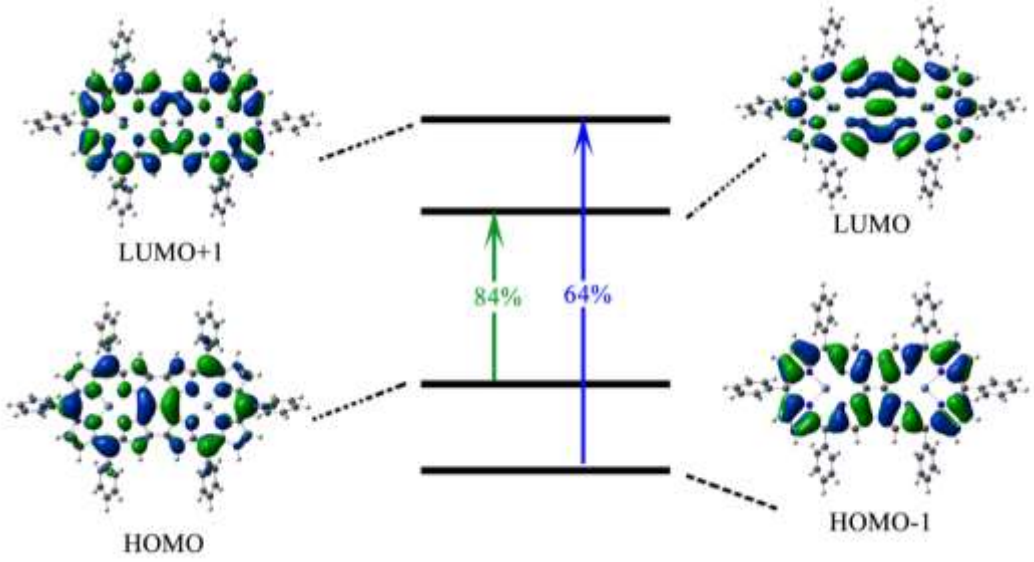

Figure S4. Molecular orbitals involved in the crucial intense electronic transitions in the absorption spectra of complex **3**.

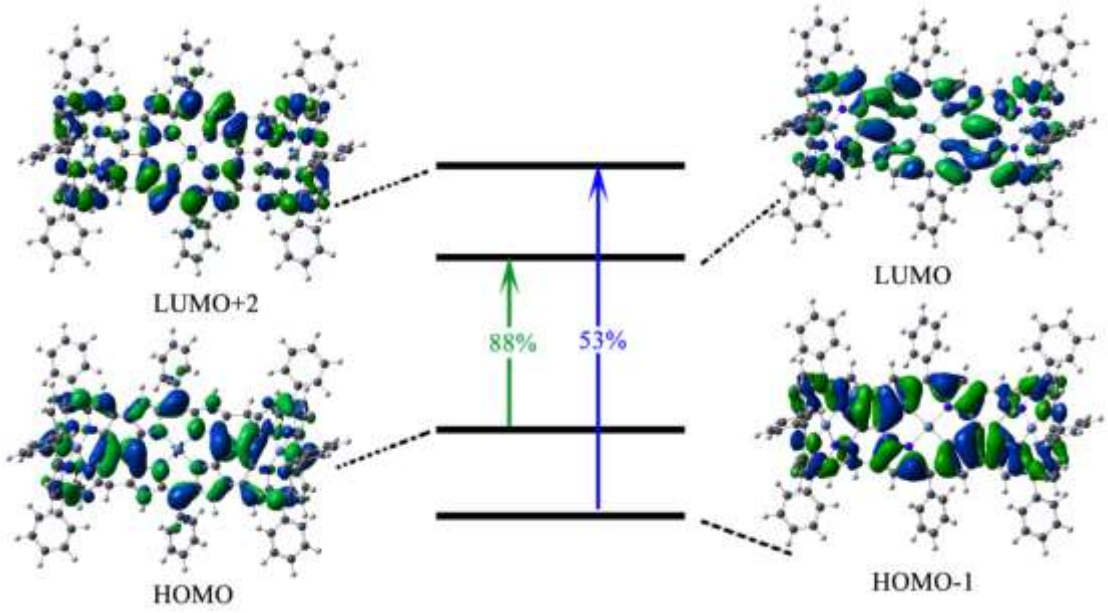

Figure S5. Molecular orbitals involved in the crucial intense electronic transitions in the absorption spectra of complex **5-anti**.

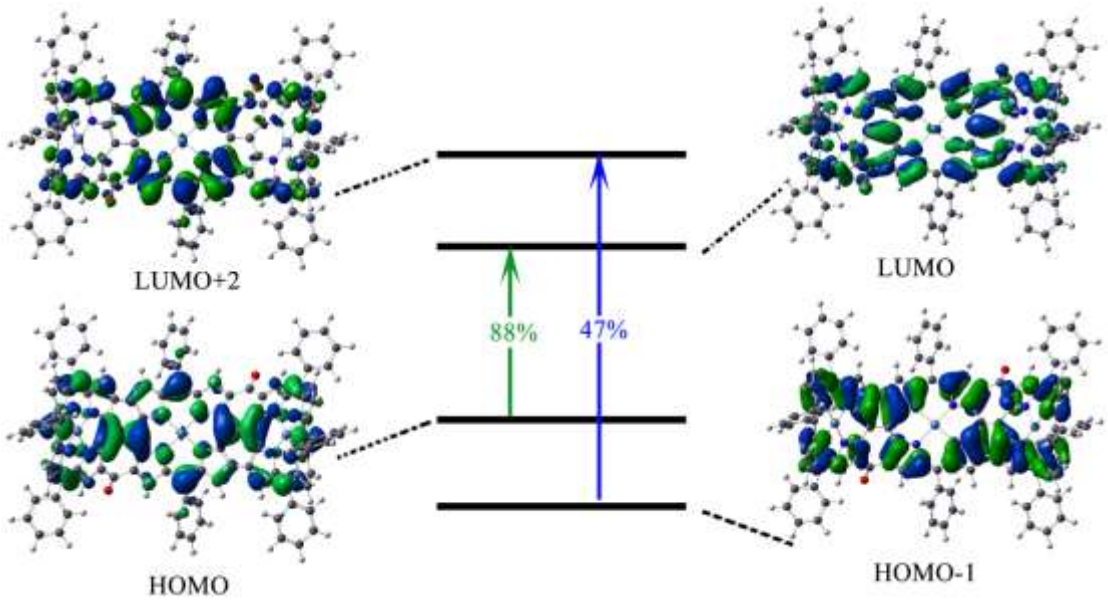

Figure S6. Molecular orbitals involved in the crucial intense electronic transitions in the absorption spectra of complex **6-anti**.

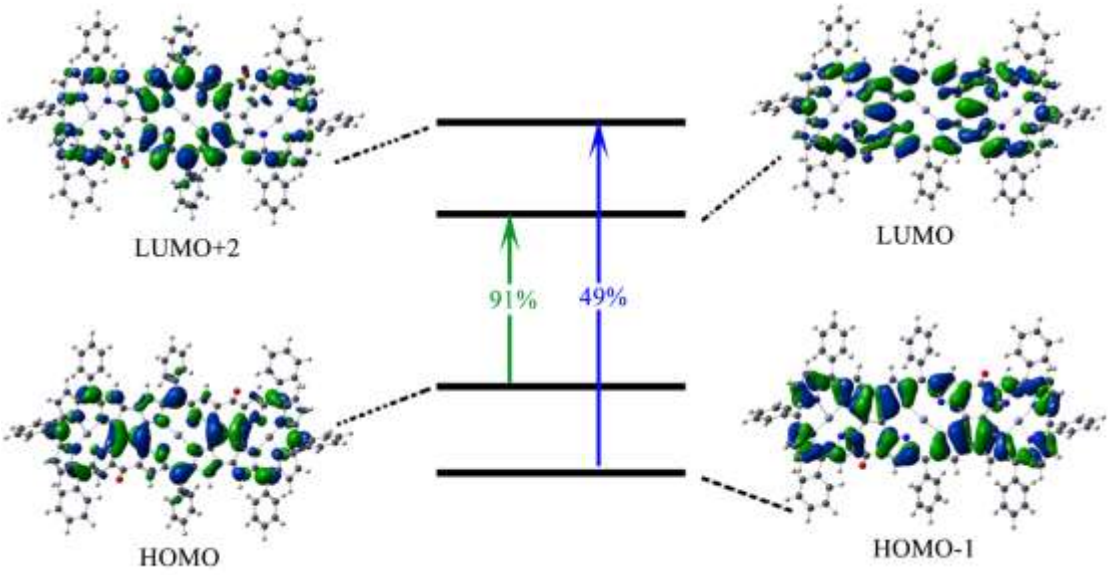

Figure S7. Molecular orbitals involved in the crucial intense electronic transitions in the absorption spectra of complex **7-anti**.

III Cartesian Coordinates of Optimized Structures

1

symmetry c1

C	-1.41923100	1.16160400	0.11146600
C	-0.71733800	2.41912300	0.03558800
C	-1.67371400	3.39764100	0.14143700
H	-1.53658900	4.46904400	0.13852700
C	-2.94166600	2.73069200	0.22988600
C	-4.18000900	3.37778400	0.16152700
C	-5.36086000	2.66873400	-0.08384500
C	-6.62780100	3.27655200	-0.39790700
H	-6.83073000	4.33680800	-0.36916600
C	-7.47475100	2.27036100	-0.74627700
C	-6.75135800	1.03667900	-0.57902600
C	-7.34058300	-0.23135000	-0.68376600
C	-6.72487800	-1.36744600	-0.15511200
C	-7.36199100	-2.65114500	-0.00153900
C	-6.52712500	-3.41920700	0.74864100
H	-6.67150500	-4.43860000	1.07547800
C	-5.34387700	-2.63522700	0.99631900
C	-4.19608800	-3.13266100	1.63179800
C	-2.96343300	-2.49097700	1.51403900
C	-1.70461700	-3.03796300	1.95237300

H	-1.59040000	-3.91934800	2.56579500
C	-0.72699800	-2.24862900	1.43263800
H	0.34130000	-2.34576900	1.55527900
C	-1.38412600	-1.17347300	0.73072100
C	-0.72556300	-0.05329900	0.18622800
C	-4.21090500	4.86905600	0.25318300
C	-3.87870500	5.50369100	1.46101400
H	-3.61457700	4.89693900	2.32268700
C	-3.89455400	6.89542800	1.56339600
C	-4.23714000	7.67671200	0.45795400
H	-4.24861500	8.76047000	0.53701100
C	-4.54811200	5.66572300	-0.85301500
H	-4.78835200	5.18763400	-1.79839400
C	-4.29475300	-4.43507900	2.35691500
C	-5.10883800	-4.54286200	3.49661400
H	-5.64887300	-3.66712900	3.84565300
C	-5.21922400	-5.75216500	4.18397700
C	-4.52255600	-6.87801200	3.74004100
H	-4.60909400	-7.82032500	4.27433000
C	-3.71666800	-6.78675800	2.60326500
C	-3.60403500	-5.57653100	1.91747000
H	-2.98698000	-5.51293100	1.02582900

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C	1.67611500	3.38549000	-0.18870400
H	1.53657500	4.45421400	-0.25610200
C	2.94467300	2.71440300	-0.21882600
C	4.18838100	3.34990700	-0.16279900
C	5.36489700	2.63090900	0.08047700
C	6.61310100	3.23855500	0.46280100
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C	6.50680700	-3.44353100	-0.81197500
H	6.64598400	-4.45887500	-1.15330200
C	5.31531200	-2.66085600	-1.02074000
C	4.14952300	-3.15717000	-1.62351000
C	2.92055300	-2.51660800	-1.46900100
C	1.65106100	-3.06522200	-1.87311700
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C	0.68688000	-2.27150000	-1.33643000

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C	0.71564600	-0.06074100	-0.11910300
C	4.26640300	4.83955700	-0.25645500
C	3.72482400	5.66600300	0.74133000
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C	4.90644600	5.44082300	-1.35205900
H	5.32992700	4.81067100	-2.12924900
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C	3.55665900	-5.60273200	-1.89272800
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C	5.09407000	-5.76932800	-4.21335900
C	5.00268900	-4.56132300	-3.52089800
H	5.52723000	-3.68308500	-3.88688200
N	-2.76626600	1.35801400	0.23623800

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N	-5.47055000	-1.39087200	0.42518100
N	-2.74818700	-1.31073900	0.82039900
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Ni	-4.11466900	-0.01356100	0.31577900
Ni	4.10474100	-0.04042600	-0.30409800
C	-4.56164400	7.05755000	-0.75097100
H	3.39294000	7.67898100	1.42565000
H	5.48712700	7.27752300	-2.31135700
H	-3.64117000	7.36840600	2.50853400
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H	3.12805000	-7.68772500	-2.20814500
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C	8.90743000	-0.14599900	2.60933300
C	9.82435200	-0.71226500	0.44924800
C	10.17994900	-0.23976500	3.17455700

H	8.05311300	0.10862400	3.23044400
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H	9.68863900	-0.88197800	-0.61512600
C	11.27883400	-0.57031000	2.37891900
H	10.31143900	-0.05642900	4.23770100
H	11.94825500	-1.05262000	0.38543300
H	12.27002900	-0.64243900	2.81850400
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H	-8.50991800	2.34325600	-1.04609600
H	8.33696300	-2.94506500	0.29663100
H	-8.33066900	-2.91450100	-0.39959600

2

symmetry c1

C	1.74034753	1.24448384	-5.69082165
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C	2.48705953	3.26945684	-6.34309165
H	2.59894153	4.24532884	-6.79329865
C	3.46647653	2.61044284	-5.52776065
C	4.59486753	3.22986984	-4.99167465
C	5.44688053	2.56149784	-4.09937865
C	6.39647953	3.21221084	-3.23549965
H	6.56323753	4.27864084	-3.19203565
C	6.98159753	2.23798384	-2.48600865
H	7.72961353	2.35048284	-1.71527065
C	6.43806753	0.98209484	-2.93636265
C	6.94229053	-0.27643216	-2.59826365
C	6.49532753	-1.43631916	-3.24607165
C	7.21524453	-2.68321416	-3.25094965
H	8.13701153	-2.86576716	-2.71813465
C	6.54381853	-3.52598616	-4.08220065
H	6.80285853	-4.53860016	-4.35345665
C	5.37027053	-2.82219416	-4.53146765
C	4.29974153	-3.40865416	-5.21521965

C	3.09887553	-2.71616616	-5.41311665
C	1.84373353	-3.35879816	-5.66942165
H	1.70752253	-4.42021316	-5.81602565
C	0.88362453	-2.38361916	-5.58900565
C	1.57304953	-1.13545416	-5.38969165
C	0.91353253	0.09918184	-5.54888565
C	4.87100053	4.66584884	-5.29191565
C	3.95625253	5.67612084	-4.95005865
H	3.02905453	5.40564584	-4.45338065
C	4.23641953	7.01526484	-5.22470265
C	5.43529853	7.36936984	-5.84714765
H	5.65253453	8.41231084	-6.06172165
C	6.35489053	6.37549284	-6.18889965
C	6.07708053	5.03695384	-5.91008365
H	6.79258353	4.26530784	-6.18005865
C	8.05210953	-0.39834616	-1.60714965
C	9.30863453	0.18831284	-1.83211665
H	9.48031153	0.73870884	-2.75261465
C	10.33576053	0.05508784	-0.89692065
C	10.12590053	-0.66710916	0.27977535
H	10.92577953	-0.76914816	1.00826235
C	8.88365453	-1.26094116	0.51240035

C	7.85766553	-1.13091416	-0.42426865
H	6.89068853	-1.59056816	-0.24011665
C	4.37200253	-4.83705816	-5.64249465
C	4.26079853	-5.16585216	-7.00388965
H	4.13741453	-4.36901616	-7.73189165
C	4.31856753	-6.49502116	-7.42435165
C	4.47988053	-7.52038316	-6.49031865
H	4.52322253	-8.55581916	-6.81734165
C	4.58010753	-7.20799416	-5.13283165
C	4.52635953	-5.87859216	-4.71234165
H	4.58834853	-5.64060516	-3.65448865
C	-1.40244847	1.24444184	-5.69087665
C	-1.07226647	2.44146984	-6.42576365
C	-2.14930247	3.26930084	-6.34335765
H	-2.26124547	4.24511184	-6.79367965
C	-3.12873147	2.61025484	-5.52806065
C	-4.25723547	3.22959184	-4.99211465
C	-5.10915947	2.56126584	-4.09968765
C	-6.05881447	3.21201984	-3.23589365
H	-6.22576447	4.27842884	-3.19266565
C	-6.64366147	2.23787584	-2.48608865
H	-7.39159447	2.35043784	-1.71528065

C	-6.09998847	0.98196484	-2.93621565
C	-6.60398047	-0.27658616	-2.59781065
C	-6.15700547	-1.43650016	-3.24558065
C	-6.87686947	-2.68342816	-3.25032765
H	-7.79852047	-2.86602716	-2.71732865
C	-6.20559747	-3.52615416	-4.08175365
H	-6.46468647	-4.53875616	-4.35300365
C	-5.03214947	-2.82232516	-4.53122265
C	-3.96171047	-3.40874316	-5.21515465
C	-2.76087447	-2.71622016	-5.41315665
C	-1.50571847	-3.35883116	-5.66947265
H	-1.36948947	-4.42024616	-5.81606365
C	-0.54562747	-2.38363616	-5.58902565
C	-1.23507547	-1.13548316	-5.38972565
C	-0.57558847	0.09916684	-5.54890765
C	-4.53362747	4.66545984	-5.29262765
C	-5.73973647	5.03620184	-5.91094865
H	-6.45505647	4.26436184	-6.18085665
C	-6.01782147	6.37463384	-6.19002665
C	-5.09847347	7.36876784	-5.84839065
H	-5.31591247	8.41162584	-6.06316965
C	-3.89956647	7.01502984	-5.22577865

C	-3.61913347	5.67600484	-4.95086465
H	-2.69193047	5.40582784	-4.45403965
C	-7.71357147	-0.39853516	-1.60645265
C	-8.97023747	0.18790784	-1.83119465
H	-9.14222047	0.73816184	-2.75171865
C	-9.99713347	0.05462884	-0.89575065
C	-9.78690147	-0.66741016	0.28097335
H	-10.58659747	-0.76949416	1.00965535
C	-8.54451547	-1.26104116	0.51337335
C	-7.51876047	-1.13096316	-0.42354065
H	-6.55167447	-1.59045516	-0.23956065
C	-4.03398347	-4.83711416	-5.64250665
C	-3.92281947	-5.16581016	-7.00393165
H	-3.79947247	-4.36891816	-7.73187965
C	-3.98058547	-6.49494716	-7.42449465
C	-4.14185047	-7.52038316	-6.49053465
H	-4.18519047	-8.55579416	-6.81763465
C	-4.24202447	-7.20809616	-5.13302065
C	-4.18828047	-5.87872616	-4.71242965
H	-4.25020647	-5.64082916	-3.65455365
C	0.16895253	2.64483584	-7.22918665
H	0.16898753	1.94260184	-8.07899065

H	0.16895653	3.65093984	-7.66186865
N	3.02857153	1.33434084	-5.20938265
N	5.45754453	1.20540184	-3.88459165
N	5.38089053	-1.52807616	-4.04849965
N	2.91901253	-1.35723016	-5.23380165
N	-2.69070447	1.33422384	-5.20953265
N	-5.11958147	1.20521684	-3.88456165
N	-5.04271647	-1.52821716	-4.04820965
N	-2.58103747	-1.35728516	-5.23387065
Ni	4.19610853	-0.08779316	-4.58245565
Ni	-3.85811847	-0.08791616	-4.58242865
H	4.69304553	-8.00046716	-4.39764965
H	4.23893853	-6.72854816	-8.48278665
H	-3.90099047	-6.72839016	-8.48295165
H	-4.35491347	-8.00062416	-4.39789165
H	-8.37120547	-1.82476616	1.42625235
H	-10.96446247	0.51029584	-1.09055065
H	-3.18285447	7.78286784	-4.94637765
H	-6.95268147	6.63995084	-6.67669365
H	3.51951653	7.78289384	-4.94521765
H	7.28972553	6.64110784	-6.67545265
H	11.30297753	0.51092284	-1.09188365

H	8.71063053	-1.82478416	1.42526035

3

symmetry c2

C	1.42236100	1.21409400	-0.12070300
C	0.71410300	2.45749500	-0.29068800
C	1.67450000	3.42128800	-0.44050100
H	1.53988200	4.47889300	-0.61207700
C	2.94738400	2.76467500	-0.30590200
C	4.17185000	3.42889700	-0.28656400
C	5.36776000	2.76391800	0.00572400
C	6.59787000	3.45306600	0.29446900
H	6.72898900	4.52415500	0.25212700
C	7.50206800	2.50936900	0.66488600
H	8.52582500	2.65181300	0.97703200
C	6.84311800	1.23460400	0.55576400
C	7.48421000	0.01063300	0.75186800
C	6.85378000	-1.20827400	0.49434400
C	7.54622100	-2.46976400	0.47412900
H	8.59180500	-2.60355900	0.70870700
C	6.64374500	-3.40843100	0.08704700
H	6.79605900	-4.46983700	-0.04112900

C	5.38870800	-2.72961400	-0.10150900
C	4.19175900	-3.39702400	-0.38064400
C	2.96134000	-2.74430500	-0.34905300
C	1.69142800	-3.40898900	-0.46856400
H	1.56216100	-4.46580300	-0.64923100
C	0.72651200	-2.45300800	-0.29826100
C	1.42865100	-1.20633900	-0.12727300
C	0.73577300	0.00194500	-0.06593200
C	4.21172100	4.90713300	-0.51137500
C	3.66260300	5.80019200	0.42258800
H	3.20460500	5.40790000	1.32628200
C	3.71157000	7.17802000	0.20479600
C	4.31053200	7.68567400	-0.95002300
H	4.34800000	8.75839700	-1.11964200
C	4.86310800	6.80733400	-1.88443600
C	4.81609500	5.42971600	-1.66571000
H	5.24396300	4.74745600	-2.39505100
C	8.91529000	-0.00441400	1.18932000
C	9.25749500	-0.46420300	2.47072600
H	8.47086700	-0.79885400	3.14136300
C	10.58936500	-0.48730900	2.88761800
C	11.60142400	-0.05477600	2.02827100

H	12.63851800	-0.07357100	2.35229900
C	11.27369900	0.40030300	0.74933700
C	9.94162100	0.42524000	0.33320900
H	9.68965200	0.77232800	-0.66502200
C	4.23639800	-4.86756400	-0.65312400
C	4.78065500	-5.34792800	-1.85450200
H	5.16027000	-4.63924000	-2.58539200
C	4.83012300	-6.71793100	-2.11678400
C	4.33895100	-7.63008900	-1.18047700
H	4.37797400	-8.69677700	-1.38434600
C	3.79902700	-7.16412400	0.02009300
C	3.74853600	-5.79398200	0.28201500
H	3.33598800	-5.43382500	1.22038900
C	-1.42865100	1.20633800	-0.12727500
C	-0.72651200	2.45300600	-0.29827000
C	-1.69142800	3.40898600	-0.46857500
H	-1.56216200	4.46579900	-0.64925000
C	-2.96134000	2.74430400	-0.34905500
C	-4.19176000	3.39702200	-0.38064600
C	-5.38870800	2.72961400	-0.10150700
C	-6.64374400	3.40843100	0.08704900
H	-6.79605900	4.46983600	-0.04112900

C	-7.54621900	2.46976500	0.47413600
H	-8.59180300	2.60356100	0.70871600
C	-6.85377800	1.20827500	0.49435500
C	-7.48420800	-0.01063100	0.75188400
C	-6.84311600	-1.23460300	0.55578100
C	-7.50206600	-2.50936800	0.66490800
H	-8.52582200	-2.65181100	0.97705900
C	-6.59786900	-3.45306500	0.29449000
H	-6.72898800	-4.52415400	0.25215000
C	-5.36776000	-2.76391800	0.00573800
C	-4.17185100	-3.42889700	-0.28654900
C	-2.94738400	-2.76467600	-0.30588800
C	-1.67450000	-3.42129000	-0.44048800
H	-1.53988200	-4.47889500	-0.61206100
C	-0.71410300	-2.45749700	-0.29067700
C	-1.42236100	-1.21409500	-0.12069500
C	-0.73577300	-0.00194600	-0.06593100
C	-4.23639900	4.86756200	-0.65313100
C	-4.78065900	5.34792200	-1.85450900
H	-5.16027600	4.63923100	-2.58539600
C	-4.83012800	6.71792300	-2.11679600
C	-4.33895400	7.63008400	-1.18049300

H	-4.37797900	8.69677200	-1.38436600
C	-3.79902700	7.16412500	0.02007700
C	-3.74853600	5.79398300	0.28200400
H	-3.33598600	5.43382900	1.22037900
C	-8.91528500	0.00441700	1.18934300
C	-9.94162000	-0.42524500	0.33324100
H	-9.68965600	-0.77234200	-0.66498900
C	-11.27369700	-0.40030700	0.74937400
C	-11.60141600	0.05478400	2.02830700
H	-12.63850900	0.07358000	2.35233900
C	-10.58935300	0.48732500	2.88764400
C	-9.25748600	0.46421700	2.47074600
H	-8.47085500	0.79887500	3.14137600
C	-4.21172400	-4.90713400	-0.51135800
C	-4.81610300	-5.42971700	-1.66569100
H	-5.24397200	-4.74745700	-2.39503100
C	-4.86311800	-6.80733500	-1.88441500
C	-4.31054000	-7.68567600	-0.95000400
H	-4.34800900	-8.75839800	-1.11962200
C	-3.71157200	-7.17802100	0.20481200
C	-3.66260400	-5.80019300	0.42260300
H	-3.20460200	-5.40790000	1.32629600

N	2.77889500	1.39982500	-0.12671500
N	5.52584500	1.40287700	0.17126500
N	5.52951700	-1.37748300	0.14083800
N	2.78614100	-1.38321500	-0.14983100
N	-2.78614100	1.38321400	-0.14982900
N	-5.52951600	1.37748300	0.14084500
N	-5.52584500	-1.40287600	0.17127700
N	-2.77889400	-1.39982600	-0.12670600
Ni	4.15707200	0.01058200	0.00802100
Ni	-4.15707100	-0.01058200	0.00802900
H	3.28582100	7.85461200	0.94114600
H	5.32959600	7.19344800	-2.78691600
H	12.05562800	0.73242600	0.07144700
H	10.83501000	-0.84142100	3.88533400
H	5.25018300	-7.07155900	-3.05468300
H	3.42059600	-7.86727700	0.75740800
H	-5.32961000	-7.19345000	-2.78689400
H	-3.28582200	-7.85461200	0.94116200
H	-10.83499400	0.84144600	3.88535800
H	-12.05562800	-0.73243700	0.07149100
H	-3.42059600	7.86728000	0.75738900
H	-5.25019100	7.07154800	-3.05469500

4

symmetry c1

C	1.59137723	1.59321038	-4.95972910
C	1.25991523	2.86002038	-5.56958810
C	2.40048423	3.61846338	-5.57905810
H	2.48947823	4.61231938	-5.98868710
C	3.40137323	2.87817238	-4.89316110
C	4.59488523	3.43422838	-4.41804110
C	5.44937623	2.72161838	-3.56786810
C	6.45358123	3.31622138	-2.72495810
H	6.68151523	4.37138538	-2.68516910
C	6.99203423	2.30954038	-1.98308610
H	7.75703423	2.37871638	-1.22402410
C	6.37068623	1.08616938	-2.42471410
C	6.80573423	-0.20318362	-2.09387610
C	6.32252523	-1.32349262	-2.78088710
C	6.96780823	-2.61286362	-2.78928910
H	7.83662023	-2.87168562	-2.20184210
C	6.30264423	-3.38362762	-3.69198810
H	6.50190423	-4.40752462	-3.97341910
C	5.20976023	-2.58922362	-4.19315310
C	4.15793923	-3.09526562	-4.96437610

C	2.96750323	-2.38027362	-5.12547210
C	1.71991223	-2.97304462	-5.50769010
H	1.58540323	-3.99743262	-5.82165810
C	0.75986623	-2.02001562	-5.29503410
C	1.43953623	-0.80778962	-4.91593710
C	0.76690023	0.43356338	-4.90642210
C	4.93523023	4.85422738	-4.72793810
C	4.11275523	5.91756638	-4.31986310
H	3.20559223	5.70521838	-3.76190510
C	4.45973323	7.23775338	-4.60874910
C	5.63368123	7.51862138	-5.31063810
H	5.90116823	8.54694238	-5.53821310
C	6.46308023	6.47103038	-5.71631910
C	6.11968923	5.15109938	-5.42297210
H	6.76377123	4.33715438	-5.74377610
C	7.88428923	-0.39695162	-1.07999310
C	7.61794423	-1.12491062	0.09147390
H	6.62089523	-1.52625462	0.24993490
C	8.61264123	-1.32446462	1.04949890
C	9.89349523	-0.80544562	0.85013190
H	10.66868523	-0.96155462	1.59547490
C	10.17388723	-0.08821762	-0.31483210

C	9.17870323	0.11399238	-1.27195510
H	9.40542623	0.65856738	-2.18400310
C	4.27016823	-4.48645462	-5.50498110
C	5.06451523	-4.73282262	-6.63506010
H	5.57963923	-3.90376562	-7.11248810
C	5.19063623	-6.02470862	-7.14869710
C	4.52738023	-7.09053762	-6.53759810
H	4.62573523	-8.09634662	-6.93700510
C	3.73915223	-6.85789362	-5.40860410
C	3.61253323	-5.56601062	-4.89494710
H	3.00784923	-5.38882462	-4.00971510
C	-1.57239177	1.55912538	-4.98225810
C	-1.26064177	2.82393838	-5.60764010
C	-2.42319877	3.54593138	-5.66676910
H	-2.52955477	4.52837638	-6.09902510
C	-3.42095077	2.79069338	-4.99363010
C	-4.65083477	3.31893138	-4.58265110
C	-5.49961177	2.61729238	-3.71939210
C	-6.58209677	3.20185138	-2.97072410
H	-6.89067377	4.23505938	-3.03452710
C	-7.08875677	2.21827238	-2.17773310
H	-7.91146977	2.27964238	-1.48038010

C	-6.35314577	1.01622538	-2.48070810
C	-6.73251377	-0.26602562	-2.06230310
C	-6.21035477	-1.40798562	-2.67785610
C	-6.74996577	-2.73831862	-2.54652010
H	-7.55238777	-3.01859462	-1.88033410
C	-6.07621377	-3.52807362	-3.42588210
H	-6.20768077	-4.58409462	-3.61188710
C	-5.06499977	-2.70332562	-4.03781310
C	-4.01665477	-3.20449762	-4.81944810
C	-2.85863177	-2.45521662	-5.04723110
C	-1.60499377	-3.01853962	-5.45486110
H	-1.44831577	-4.04298362	-5.75760710
C	-0.66650677	-2.03738962	-5.27829510
C	-1.36921477	-0.83819062	-4.89873810
C	-0.72390677	0.41833938	-4.90605310
C	-5.03829677	4.70600038	-4.97850510
C	-6.19074577	4.91345138	-5.75446010
H	-6.77618477	4.05578038	-6.07384510
C	-6.57752977	6.20135738	-6.12636710
C	-5.82410577	7.30496638	-5.72101810
H	-6.12533277	8.30816438	-6.01020710
C	-4.68266577	7.11266838	-4.94020110

C	-4.29266877	5.82464238	-4.57170910
H	-3.41117177	5.68089538	-3.95379410
C	-7.80232477	-0.39374162	-1.02709210
C	-9.08187877	-0.87632862	-1.34621510
H	-9.30294677	-1.15983462	-2.37137610
C	-10.06964377	-0.97770362	-0.36542410
C	-9.79586277	-0.59651062	0.94978190
H	-10.56535477	-0.67591062	1.71293190
C	-8.52923877	-0.10885262	1.27770190
C	-7.54170077	-0.00576462	0.29698390
H	-6.55567277	0.37110638	0.55437490
C	-4.09365777	-4.62334862	-5.28780310
C	-4.96631777	-4.96596662	-6.33210110
H	-5.56505977	-4.18890762	-6.79930210
C	-5.06285177	-6.28589162	-6.77583510
C	-4.29253777	-7.28530762	-6.17815110
H	-4.36828277	-8.31307662	-6.52281510
C	-3.42695877	-6.95769862	-5.13244310
C	-3.32901077	-5.63757862	-4.68967410
H	-2.66467677	-5.38737062	-3.86721210
C	-0.00031777	3.38146838	-6.10354810
N	2.92148423	1.60851338	-4.59430510

N	5.39177523	1.36592238	-3.35506010
N	5.25103123	-1.32681862	-3.64579010
N	2.78260123	-1.05337262	-4.77895310
N	-2.91049377	1.54597338	-4.64639810
N	-5.36458877	1.28752138	-3.39924710
N	-5.16695477	-1.41050762	-3.58087410
N	-2.70235277	-1.11604362	-4.73258410
O	-0.00265977	4.36181438	-6.85024310
Ni	4.08521023	0.14684038	-4.08241410
Ni	-4.03404377	0.07481038	-4.07815310
H	3.81284823	8.04705338	-4.28101210
H	7.37767523	6.67987638	-6.26489410
H	11.17112023	0.30947038	-0.48381710
H	8.38502823	-1.88399462	1.95293990
H	5.80646223	-6.19677662	-8.02743910
H	3.22568323	-7.68323362	-4.92232710
H	-5.73951777	-6.53186062	-7.58988610
H	-2.83083777	-7.73103162	-4.65509110
H	-8.30712077	0.19059038	2.29852190
H	-11.05587777	-1.34868862	-0.63172610
H	-4.09487777	7.96611238	-4.61311310
H	-7.46651377	6.34128738	-6.73559310

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symmetry c2

C	-5.39905787	-1.16450320	-8.11106361
C	-5.48477887	-2.31371720	-8.98211861
C	-6.45884987	-3.12011420	-8.47997561
H	-6.80714787	-4.05755220	-8.88899861
C	-6.94663887	-2.50245420	-7.28093761
C	-7.76241587	-3.13576320	-6.34498861
C	-8.09476787	-2.52748020	-5.12463561
C	-8.60807187	-3.22862220	-3.97760461
H	-8.81240287	-4.28872420	-3.94081561
C	-8.73076187	-2.31302420	-2.97743461
H	-9.06582087	-2.47565720	-1.96377961
C	-8.35520687	-1.03742620	-3.53076661
C	-8.55535287	0.19635980	-2.90554461
C	-8.37104287	1.39988480	-3.59883661
C	-8.88129287	2.67324980	-3.15950261
H	-9.40061787	2.84163780	-2.22738561
C	-8.61075287	3.57076580	-4.14595561
H	-8.84241087	4.62562280	-4.17284161
C	-7.88547287	2.86090180	-5.16738661
C	-7.22132787	3.48269780	-6.22932461

C	-6.28433787	2.79545680	-7.00554361
C	-5.28666987	3.43019880	-7.81470761
H	-5.20633687	4.49351180	-7.98513061
C	-4.43708687	2.43916080	-8.23370861
C	-4.99997387	1.19033480	-7.78263561
C	-4.54547787	-0.04364020	-8.29327361
C	-9.07382187	0.25140480	-1.50620661
C	-10.34184987	-0.25179620	-1.17132161
H	-10.96292687	-0.68643120	-1.94925761
C	-10.81300787	-0.18205120	0.14040739
C	-10.02532487	0.39195780	1.14050339
H	-10.39224487	0.44494680	2.16200839
C	-8.76512587	0.90069080	0.81952939
C	-8.29520087	0.83424780	-0.49265061
H	-7.31322087	1.22769580	-0.73998061
C	-7.42972887	4.94914080	-6.44601061
C	-8.60091687	5.40503980	-7.06975661
H	-9.34200487	4.68226480	-7.40004561
C	-8.81527187	6.76972780	-7.27119561
C	-7.86253087	7.69938880	-6.84989461
H	-8.02918887	8.76173780	-7.00669461
C	-6.69550587	7.25712280	-6.22335361

C	-6.48141087	5.89257880	-6.02098561
H	-5.57762087	5.55087080	-5.52403761
C	-1.02570087	-2.60200220	-10.22745561
C	-2.28816587	-3.20502420	-10.54439761
H	-2.42400387	-4.15320420	-11.04459861
C	-3.26076387	-2.36361120	-10.09226161
C	-2.59700887	-1.21471720	-9.53033361
C	-3.22865887	-0.06520420	-8.97814361
C	-2.52910687	1.15167880	-9.10165361
C	-3.17958487	2.41987580	-8.91267361
C	-2.33292487	3.37826980	-9.41677761
H	-2.48189087	4.44741680	-9.45723061
C	-1.14153087	2.69452880	-9.82049161
C	0.21126413	-3.24974720	-10.27687061
C	0.29909913	-4.66915120	-10.72341861
C	1.15157813	-5.01821220	-11.78533161
H	1.72627113	-4.24017020	-12.27949661
C	1.25320213	-6.34155420	-12.21455961
C	0.51228513	-7.34322320	-11.58366761
H	0.59325613	-8.37465120	-11.91615361
C	-0.32950587	-7.01230920	-10.51963561
C	-0.43590787	-5.68808320	-10.09329361

H	-1.07830287	-5.43756120	-9.25442561
Ni	-7.02835287	0.12257380	-5.93532961
Ni	0.12120313	0.03556880	-9.62282661
N	-6.34504687	-1.26391520	-7.11467461
N	-7.91731287	-1.19825420	-4.83186661
N	-7.77370987	1.52779580	-4.83263361
N	-6.09985987	1.42288480	-6.99716361
N	-1.23641587	-1.34324520	-9.68464961
N	-1.26630387	1.33940180	-9.60223061
C	-8.23173287	-4.53220520	-6.58845461
C	-7.32590687	-5.59530620	-6.74059661
H	-6.26006587	-5.39699020	-6.67544761
C	-7.78249087	-6.89646220	-6.95490961
C	-9.15249987	-7.15857420	-7.02179761
H	-9.50749887	-8.17180820	-7.18996161
C	-10.06365887	-6.11160220	-6.86734861
C	-9.60744587	-4.81136720	-6.64838661
H	-10.31785987	-3.99783120	-6.53142561
C	5.64144713	1.23556980	-8.11094361
C	5.72717713	2.38482480	-8.98194361
C	6.70124113	3.19119880	-8.47975061
H	7.04954313	4.12865780	-8.88872461

C	7.18901813	2.57348180	-7.28073761
C	8.00478513	3.20674580	-6.34474961
C	8.33712313	2.59840580	-5.12442161
C	8.85041213	3.29949380	-3.97735161
H	9.05474313	4.35959480	-3.94050861
C	8.97309113	2.38384980	-2.97722261
H	9.30813813	2.54643480	-1.96355561
C	8.59754213	1.10827680	-3.53061861
C	8.79767913	-0.12553820	-2.90545261
C	8.61337713	-1.32903020	-3.59880261
C	9.12362113	-2.60241620	-3.15952261
H	9.64293413	-2.77084820	-2.22740661
C	8.85309513	-3.49988520	-4.14602161
H	9.08475413	-4.55474120	-4.17295361
C	8.12782813	-2.78997420	-5.16742761
C	7.46369713	-3.41171920	-6.22940361
C	6.52671513	-2.72444220	-7.00560161
C	5.52905813	-3.35914620	-7.81480861
H	5.44872813	-4.42245020	-7.98528461
C	4.67947913	-2.36808820	-8.23377161
C	5.24235913	-1.11928320	-7.78263161
C	4.78786913	0.11471580	-8.29321661

C	9.31613013	-0.18064920	-1.50610961
C	10.58415313	0.32253580	-1.17118361
H	11.20524113	0.75720780	-1.94909161
C	11.05529313	0.25272980	0.14054839
C	10.26759713	-0.32132720	1.14060639
H	10.63450313	-0.37436420	2.16211339
C	9.00740313	-0.83004620	0.81959139
C	8.53749513	-0.76354020	-0.49259161
H	7.55551813	-1.15697720	-0.73995361
C	7.67210313	-4.87815120	-6.44615861
C	8.84330613	-5.33401820	-7.06990161
H	9.58439913	-4.61122520	-7.40013861
C	9.05766613	-6.69869520	-7.27140561
C	8.10491813	-7.62837820	-6.85017061
H	8.27158113	-8.69072020	-7.00701961
C	6.93787913	-7.18614520	-6.22363161
C	6.72377813	-5.82161220	-6.02120061
H	5.81997713	-5.47993020	-5.52425461
C	1.26811313	2.67316780	-10.22732061
C	2.53058313	3.27620380	-10.54422061
H	2.66642613	4.22440680	-11.04437761
C	3.50317613	2.43477080	-10.09211161

C	2.83941413	1.28585080	-9.53024361
C	3.47105913	0.13631080	-8.97810161
C	2.77150813	-1.08056620	-9.10167861
C	3.42198413	-2.34877120	-8.91275061
C	2.57532913	-3.30714220	-9.41690661
H	2.72429613	-4.37628820	-9.45740761
C	1.38394013	-2.62338220	-9.82060261
C	0.03115013	3.32091380	-10.27671961
C	-0.05668187	4.74033880	-10.72320561
C	-0.90914887	5.08944580	-11.78511161
H	-1.48383587	4.31142580	-12.27931861
C	-1.01076987	6.41280680	-12.21428161
C	-0.26986087	7.41444880	-11.58333661
H	-0.35082887	8.44589180	-11.91577761
C	0.57191813	7.08348780	-10.51930961
C	0.67831713	5.75924380	-10.09302661
H	1.32070213	5.50868380	-9.25416161
N	6.58742413	1.33493480	-7.11453961
N	8.15966413	1.26916580	-4.83171661
N	8.01605913	-1.45688320	-4.83261361
N	6.34223613	-1.35187020	-6.99715761
N	1.47882313	1.41438580	-9.68457061

N	1.50871113	-1.26826520	-9.60227761
C	8.47410413	4.60319980	-6.58814461
C	7.56828013	5.66630680	-6.74025061
H	6.50243813	5.46798780	-6.67512361
C	8.02486613	6.96747280	-6.95449761
C	9.39487513	7.22958880	-7.02135661
H	9.74987613	8.24283080	-7.18946961
C	10.30603313	6.18260980	-6.86694361
C	9.84981813	4.88236480	-6.64804661
H	10.56023013	4.06882380	-6.53111461
Ni	7.27071613	-0.05160920	-5.93525161
H	-9.72652987	7.10523880	-7.75929261
H	-5.95176787	7.97433080	-5.88613061
H	-8.14458187	1.34844180	1.59126639
H	-11.79941087	-0.57110620	0.37899339
H	-1.66815987	6.66047980	-13.04348961
H	1.14208913	7.85840680	-10.01363261
H	7.30865913	7.77784680	-7.06238461
H	11.37412213	6.37671380	-6.91888661
H	12.04169313	0.64177380	0.37916539
H	8.38684813	-1.27783320	1.59129839
H	9.96893613	-7.03418020	-7.75949961

H	6.19413513	-7.90337120	-5.88646061
H	1.91060213	-6.58919020	-13.04377161
H	-0.89968287	-7.78725020	-10.01399961
H	-11.13174687	-6.30570220	-6.91931361
H	-7.06628287	-7.70683020	-7.06282461
C	4.97997713	2.56807580	-10.26185861
H	5.32686013	1.81916180	-10.99283661
H	5.21832913	3.54775980	-10.68955661
C	-4.73756387	-2.49690620	-10.26203361
H	-4.97590987	-3.47657020	-10.68978161
H	-5.08443787	-1.74795820	-10.99297961

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symmetry c1

C	-5.61841490	-1.41379555	-8.77788141
C	-5.67985390	-2.62028055	-9.57267241
C	-6.77128090	-3.33007755	-9.14599841
H	-7.10405490	-4.27142655	-9.55395541
C	-7.31665990	-2.63448855	-8.03311241
C	-8.23062590	-3.19748955	-7.13561841
C	-8.55698790	-2.56781955	-5.92742241
C	-9.13944490	-3.22993655	-4.78963441
H	-9.43163690	-4.26951255	-4.76157441

C	-9.18782290	-2.31410455	-3.78314441
H	-9.53914790	-2.45515955	-2.77181241
C	-8.70544590	-1.06983055	-4.32685341
C	-8.81029490	0.17705745	-3.69817241
C	-8.57836690	1.36227745	-4.40635641
C	-9.02012090	2.66488445	-3.97584641
H	-9.48923090	2.87438945	-3.02559641
C	-8.77091690	3.52615945	-4.99952341
H	-8.97222490	4.58649845	-5.04594941
C	-8.12011290	2.76508245	-6.03539841
C	-7.50426090	3.33122245	-7.15853541
C	-6.59589490	2.60303945	-7.93173341
C	-5.63250290	3.19589845	-8.81078741
H	-5.58015590	4.24370245	-9.06569341
C	-4.76461990	2.19669445	-9.16332141
C	-5.28040290	0.97015045	-8.60658841
C	-4.77494890	-0.28864655	-9.00694441
C	-9.29314690	0.26924245	-2.28826541
C	-10.58756390	-0.13784055	-1.92519241
H	-11.25712490	-0.52443555	-2.68817241
C	-11.02295390	-0.03267655	-0.60354641
C	-10.17249290	0.48090045	0.37782859

H	-10.51166590	0.56127545	1.40703959
C	-8.88540090	0.89426845	0.02826659
C	-8.45073890	0.79297745	-1.29387841
H	-7.44771990	1.11203245	-1.56313741
C	-7.72820790	4.78377345	-7.43829941
C	-8.95519890	5.20965545	-7.96995741
H	-9.72422790	4.47321745	-8.18656841
C	-9.18889790	6.56164545	-8.22670641
C	-8.20110990	7.50925045	-7.95135841
H	-8.38312790	8.56182945	-8.15073941
C	-6.97926590	7.09774045	-7.41497441
C	-6.74477590	5.74576245	-7.15867441
H	-5.79807390	5.42983645	-6.72927241
C	-1.20548490	-2.75817455	-11.06448841
C	-2.43612990	-3.43515455	-11.28100741
H	-2.58178390	-4.38676755	-11.76761741
C	-3.42014290	-2.68155455	-10.69180941
C	-2.79958190	-1.47564155	-10.19878841
C	-3.45820690	-0.31792955	-9.68836041
C	-2.80954190	0.91602745	-9.92592441
C	-3.51363090	2.16842945	-9.84816041
C	-2.71131990	3.11886445	-10.42929741

H	-2.90692090	4.17347545	-10.55653041
C	-1.48486690	2.45933045	-10.76361841
C	0.06234110	-3.33827555	-11.22170741
C	0.20026610	-4.71544755	-11.77495241
C	1.00354310	-4.92784855	-12.90881041
H	1.49573810	-4.07934455	-13.37534141
C	1.15736310	-6.20647255	-13.44442841
C	0.52147810	-7.29779355	-12.84892141
H	0.64210010	-8.29428155	-13.26509641
C	-0.26757090	-7.10246055	-11.71348141
C	-0.42773790	-5.82320355	-11.18052341
H	-1.02794390	-5.68004155	-10.28709941
C	-4.80725390	-3.14619355	-10.62781041
Ni	-7.32745490	-0.00021955	-6.73898141
Ni	-0.13219790	-0.11740455	-10.43525341
N	-6.65175490	-1.42486255	-7.86611641
N	-8.27668790	-1.25838955	-5.62405241
N	-8.02868690	1.44273945	-5.66671341
N	-6.37932790	1.23844045	-7.83235641
N	-1.45141990	-1.52529055	-10.47396241
N	-1.55641890	1.12217745	-10.43605941
O	-5.19365190	-4.06111355	-11.35736741

C	-8.80210590	-4.55163155	-7.39701141
C	-7.98777090	-5.69258755	-7.48932341
H	-6.91343990	-5.59138355	-7.36693141
C	-8.54735490	-6.95012055	-7.71783341
C	-9.92957890	-7.08918955	-7.85844741
H	-10.36423090	-8.06842655	-8.03988241
C	-10.75049190	-5.96369955	-7.76204741
C	-10.19234990	-4.70679555	-7.52797541
H	-10.83217190	-3.83173755	-7.45664741
C	5.35403110	1.17883845	-8.77780041
C	5.41549010	2.38536045	-9.57253541
C	6.50694910	3.09510445	-9.14584941
H	6.83973610	4.03646645	-9.55376341
C	7.05234610	2.39943145	-8.03302541
C	7.96637210	2.96234745	-7.13553641
C	8.29270810	2.33263445	-5.92735741
C	8.87523110	2.99469245	-4.78956841
H	9.16753210	4.03423845	-4.76151141
C	8.92350310	2.07886045	-3.78307441
H	9.27483510	2.21988045	-2.77173941
C	8.44100210	0.83463245	-4.32678241
C	8.54571510	-0.41226455	-3.69809641

C	8.31373310	-1.59746355	-4.40629741
C	8.75537610	-2.90010555	-3.97577341
H	9.22440410	-3.10965455	-3.02549341
C	8.50619810	-3.76134955	-4.99948541
H	8.70744810	-4.82169855	-5.04591341
C	7.85551310	-3.00021655	-6.03539641
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7-anti

symmetry c1

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Zn	0.30125475	-0.30686041	-7.68870773
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