Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information

Elucidating the role of non-covalent interactions in unexpectedly high and selective CO_2 uptake and catalytic conversion of porphyrin-based ionic organic polymers

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Materials

All reagents and solvents were purchased from commercial suppliers and used without further purification. 5,10,15,20-Tetrakis(4-aminophenyl)porphyrin (**H2-Porph**),[1] 5,10,15,20-tetrakis(4 aminophenyl)porphyrinatozinc(II) (**Zn-Porph**)[2] and 1,1'-bis(2,4-dinitrophenyl)-[4,4'-bipyridine]-1,1'-diium dichloride (**Vio**)[3] were prepared according to the published procedures. While this manuscript was being prepared, the structure of **H2-ICOP** and **Zn-ICOP** has been published by Skorjanc *et al.* via microwave irradiation (**H2-ICOF**) and post-synthetic modification (**Zn-ICOF**) and studied for their bromate removal efficiency.[4]

Synthesis

H2-ICOP: 200 mg (1 eq) **H2-Porph** and 332 mg (2 eq) **Vio** were dissolved in 20 mL DMF: water (4:1, v/v) mixture in a glass bottle with a screw cap. The bottle was kept in the oven for 24 hours at 100 °C. The solids were collected by centrifugation and respectively washed twice with ethanol, thrice with DMSO, twice with water, and once with acetone, then dried in a vacuum oven at 100 °C for 24 h.

H2-ICOP-dx was prepared by the same procedure as described for **H2-ICOP** using 100 mg (1 eq) **H2-Porph** and 170 mg (2 eq) **Vio** in 10 mL 1,4-dioxane: water (4:1, v/v).

Zn-ICOP was prepared by the same procedure as described for **H2-ICOP** using 200 mg (1 eq) **Zn-Porph** and 300 mg (2 eq) **Vio** in 20 mL DMF: water (4:1, v/v).

Zn-ICOP-dx was prepared by the same procedure as described for **H2-ICOP** using 50 mg (1 eq) **Zn-Porph** and 76 mg (2 eq) **Vio** in 5 mL 1,4-dioxane: water (4:1 v/v).

Characterization

Fourier transform infrared (FTIR) spectra were recorded between 4000 and 650 cm^{-1} using a Perkin Elmer Spectrum 100 FT-IR spectrometer with an attenuated total reflection (ATR) accessory featuring a zinc selenide (ZnSe) crystal. Solid-state NMR measurements were carried out with Bruker Ascend 400 MHz spectrometer. The ^{13}C CP/MAS NMR spectra were obtained with a 4-mm double-resonance MAS probe and with a sample spinning rate of 8.0 kHz; a contact time of 2 ms and pulse delay of 3 s were acquired. Diffuse reflectance spectra (DRS) were recorded in the wavelength range of 200–800 nm using an ISR-2600-Plus Shimadzu spectrophotometer. Electron paramagnetic resonance (EPR) signals were recorded using Bruker EMX X-band spectrometer (9.8 GHz). Thermogravimetric analysis (TGA) was carried out on a Mettler Toledo Stare Thermal Analysis System at a heating rate of 10 °C min^{-1} over a temperature range of 25–900 °C under a nitrogen flow (50 mL min^{-1}). Powder X-ray diffraction (PXRD) measurements were carried out on a Bruker Advanced D8 X-ray diffractometer with Cu Kα (λ = 1.5405 Å) radiation source operating at 30 kV and 30 mA. The patterns were recorded over the 2Θ range of 1–50° with step size = 0.02°. The surface morphology and energy dispersive X-ray analysis (EDX) were recorded with an FEI (PHILIPS) XL30 SFEG scanning electron microscope (SEM). Dynamic light scattering (DLS) and zeta potential measurements were performed on a Malvern Zetasizer NanoSeries. Transmission electron microscopy (TEM) images were obtained from Tecnai G2 F20 S-TWIN.

Surface areas and CO2 uptake analyses

Before each analysis, the samples were degassed at 200 ^{o}C for 16 h before the measurements. Surface areas were determined from the adsorption data using Brunauer-Emmett-Teller (BET) method.

Computational Methodology

The geometry optimization was done for both constructed crystal models and molecular fragments (Table S2). Geometry optimization of constructed crystal models was performed with the ABINIT code.[5] The electronic structure calculations were performed in the generalized gradient approximation with the Perdew–Burke–Ernzerhof exchange-correlation energy functional.[6] Orbitals were expanded in plane waves up to a cut-off of 30 Hartrees. The pseudopotential generated in our work was one of those of Troullier–Martins.[7] The nonshift Monkhorst–Pack k-mesh (2x2x6) was used to generate k-points in the irreducible Brillouin zone.[8] To bring the atoms to their equilibrium positions, we performed structural relaxation as implemented in the ABINIT code, which was stopped after the forces on all atoms were less than 0.01 mRy/Å in the relaxed structure.[9] The geometry optimization of molecular fragments containing the non-covalent bonds and molecular electrostatic potential surfaces were calculated by PSI4 software at the DF/aug-cc-pVDZ level. The molecular fragments **H2-ICOP** and **Zn-ICOP** containing two porphyrin cores, chlorine counterion, and positively charged viologen linker were frozen keeping the molecular conformations of optimized crystal models during the geometry optimization (Table S3-S6). The molecular optimizations of constructed models containing the non-covalent bonds were carried out during 50 steps using a module of PSI4 called optking to clarify the mutual orientation of guest molecules and host fragments. It was suggested that the CO_2

uptake capacities can be improved with increasing of pressure. That's way we assumed that the tetrel, pnicogen, sodium and hydrogen bonds in molecular fragments may be formed due to high pressure. Therefore among the relaxed compounds there were chosen the models where the $\mathbf{O_{CO2}\cdots N^{+}}$, $\mathbf{Cl^{-}\cdots C_{CO2}}$, $\mathbf{N\cdots C_{CO2}}$, contacts were less than the sum of their van der Waals radii.[10,11] The typical hydrogen bond distance (1.961 Å) was used for $\mathbf{O_{CO2}\cdots H}$ and sodium bond $\mathbf{O_{CO2}\cdots Zn}$ is equal to 2.6 Å, which is less than that (2.688 Å).[12]

The decomposition of the binding energies of studied compounds was carried out by using the symmetry-adapted perturbation theory (SAPT), which partitions the attractive forces into electrostatic (E_{elst}), exchange-repulsion (E_{exch}), induction (E_{ind}), dispersion (E_{disp}) terms, and the exchange as the repulsive terms.[13–15] All SAPT calculations were done with the Psi4 program using density fitting at the sSAPT0/aug-cc-pVDZ level.[16]

CO_2 conversion

The catalyst (0.16 mol%) and epoxide (1 mL) were placed in the reactor. After sealing and purging with CO_2 to remove air, the reaction pressure was adjusted to 1.0 MPa. Then the reactor was heated to the 80 ^{o}C and stirred for 12 h. After the reaction was completed, the reactor was cooled to ambient temperature, and CO_2 was vented out slowly. The yields were determined by ^{1}H NMR spectra of an aliquot of the reaction mixture. The catalyst was separated from the reaction mixture by centrifugation.

Supporting Figures and Tables

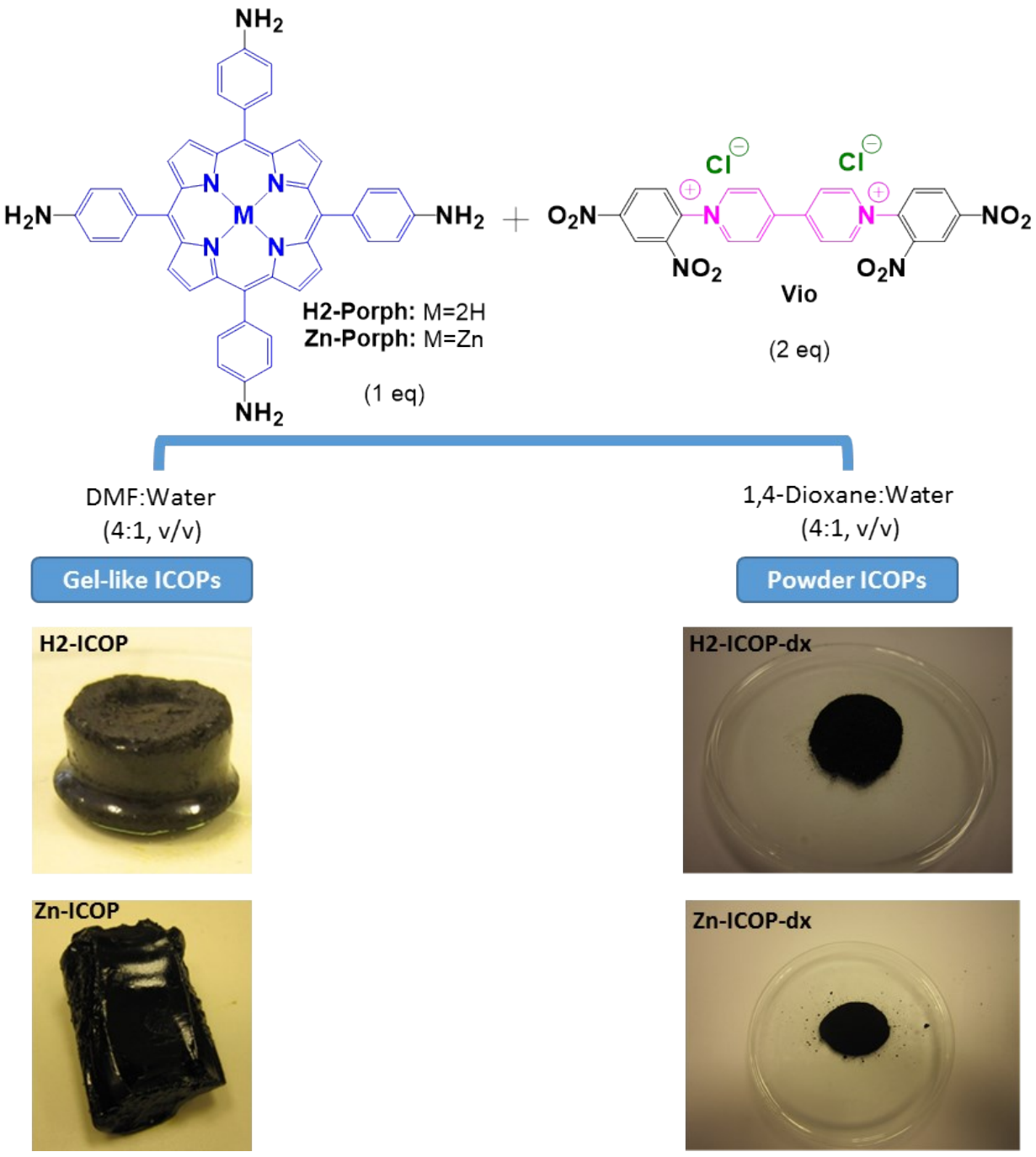


Figure S1. Gel-like or powder materials formed depending on the solvent mixture used.

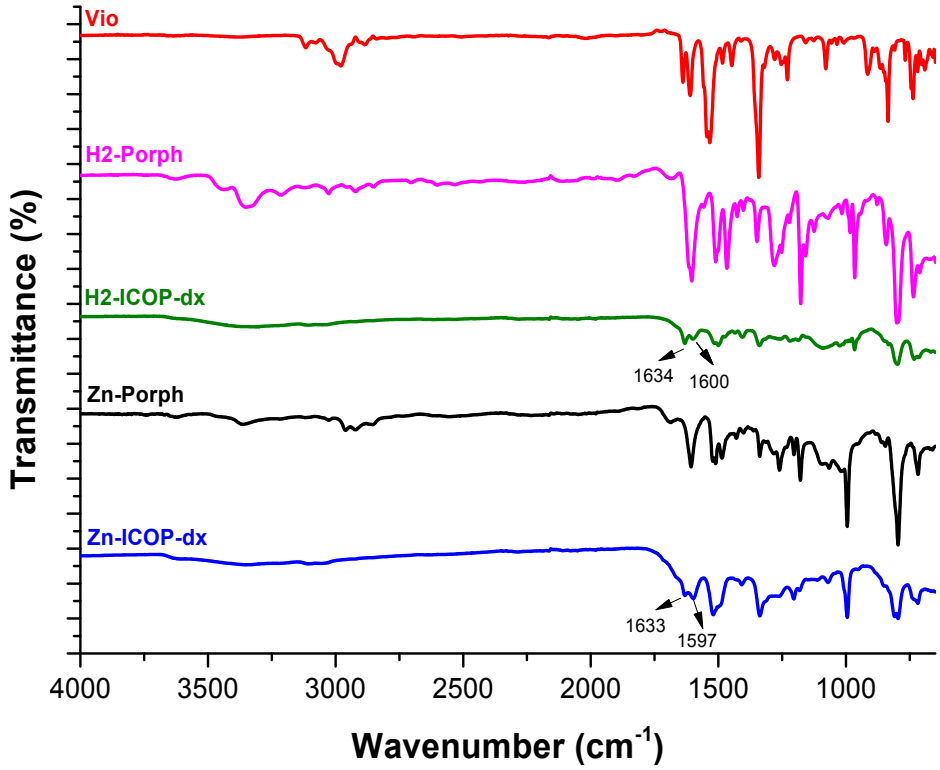


Figure S2. FTIR spectra of **H2-ICOP-dx** and **Zn-ICOP-dx** with the corresponding starting compounds (**H2-Porph**, **Zn-Porph** and **Vio**).

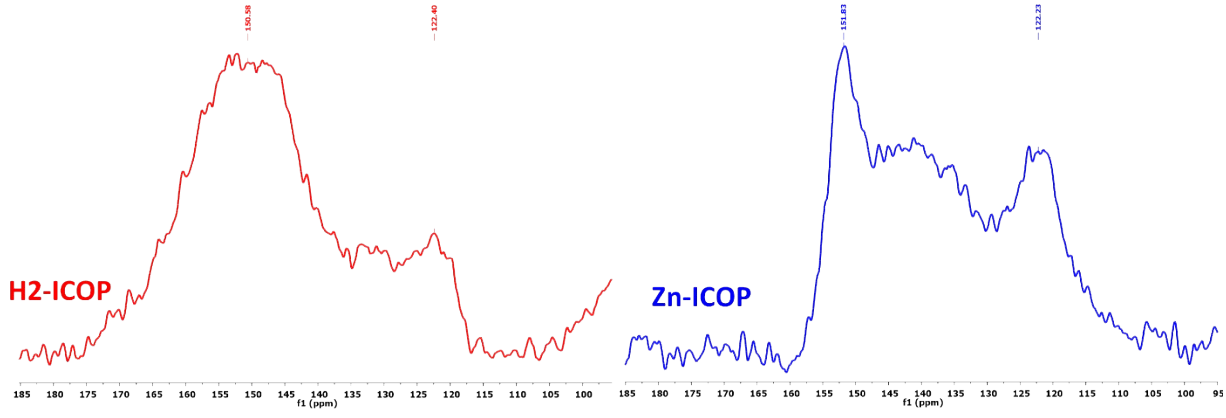


Figure S3. Solid state ^{13}C-NMR of **H2-ICOP** and **Zn-ICOP**.

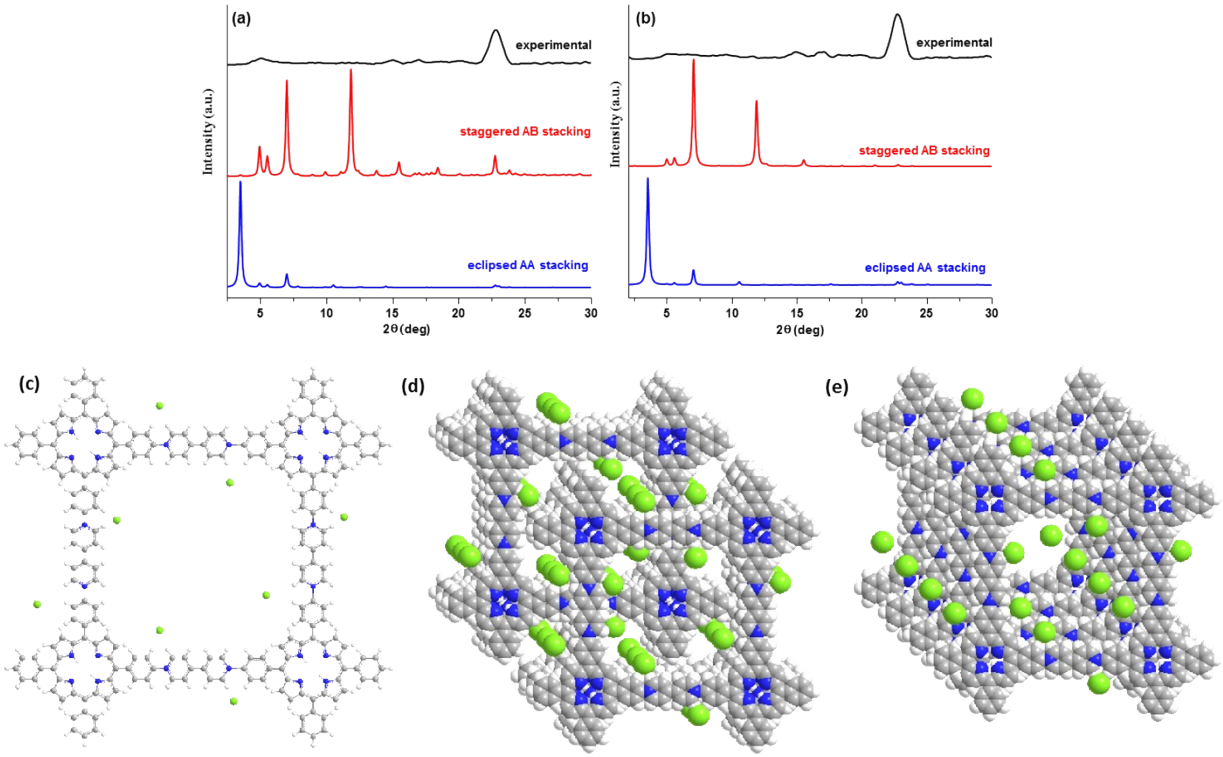


Figure S4. Experimental background subtracted PXRD pattern (black) compared with simulated patterns (red and blue) using two different stacking arrangements for the **H2-ICOP** (**a**) and **Zn-ICOP** (**b**); single 2D layer of **H2-ICOP** (**c**); representations of staggered AB (**d**) and eclipsed AA (**e**) stacking for **H2-ICOP**.

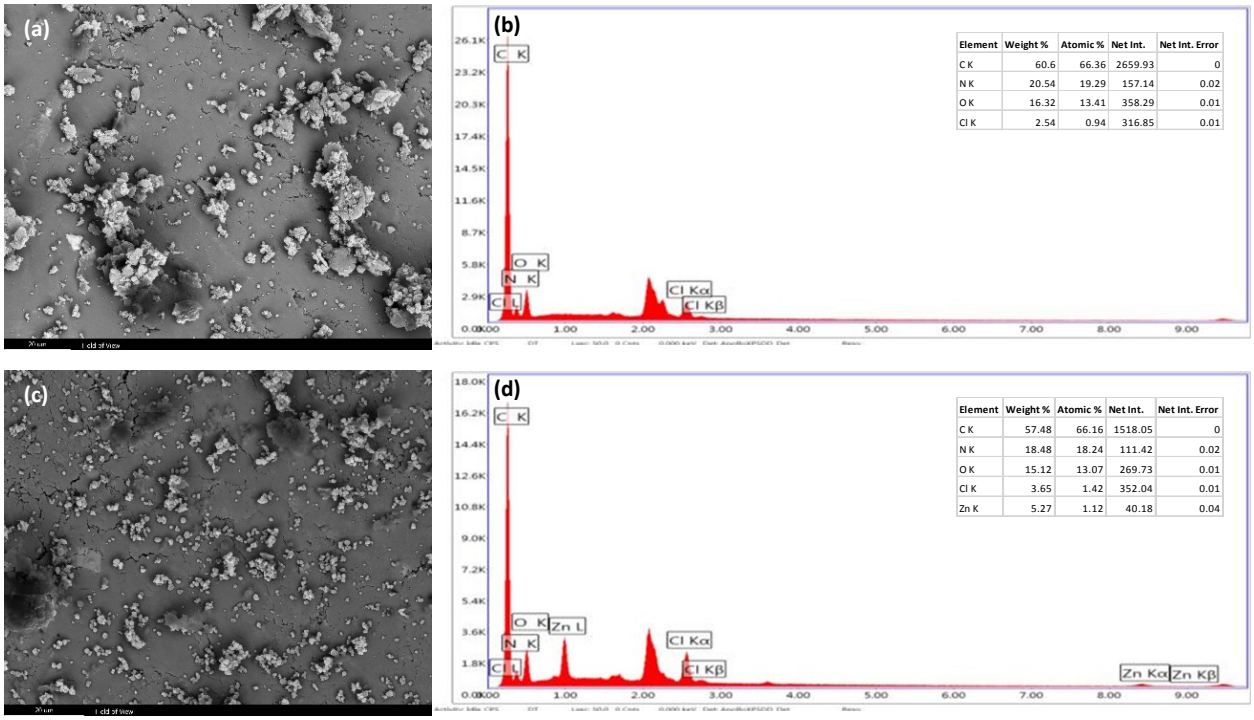


Figure S5. EDS elemental mapping showing an even distribution of constituent elements C, N and Cl for **H2-ICOP** (**b**) and C, N, Cl and Zn for **Zn-ICOP** (**d**).

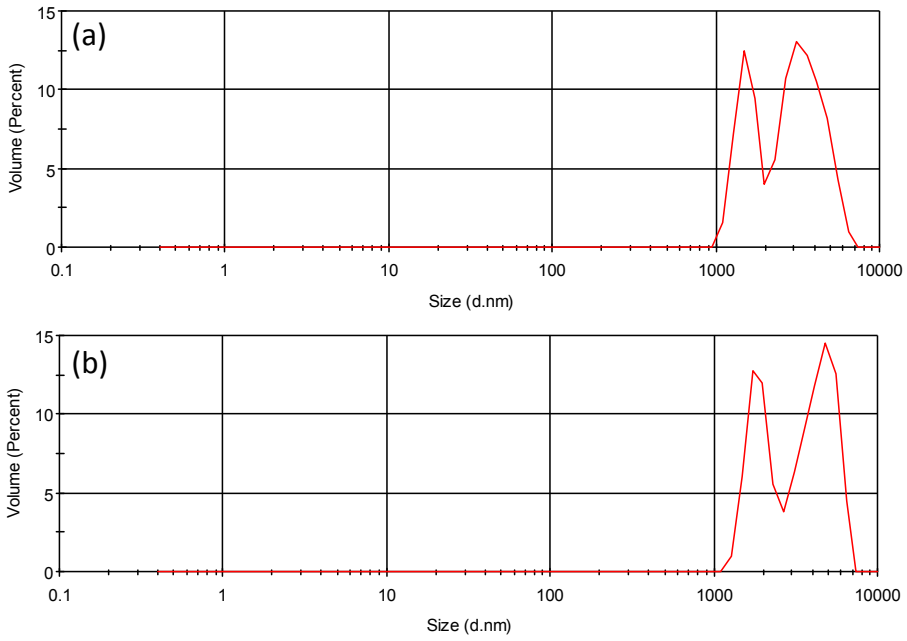
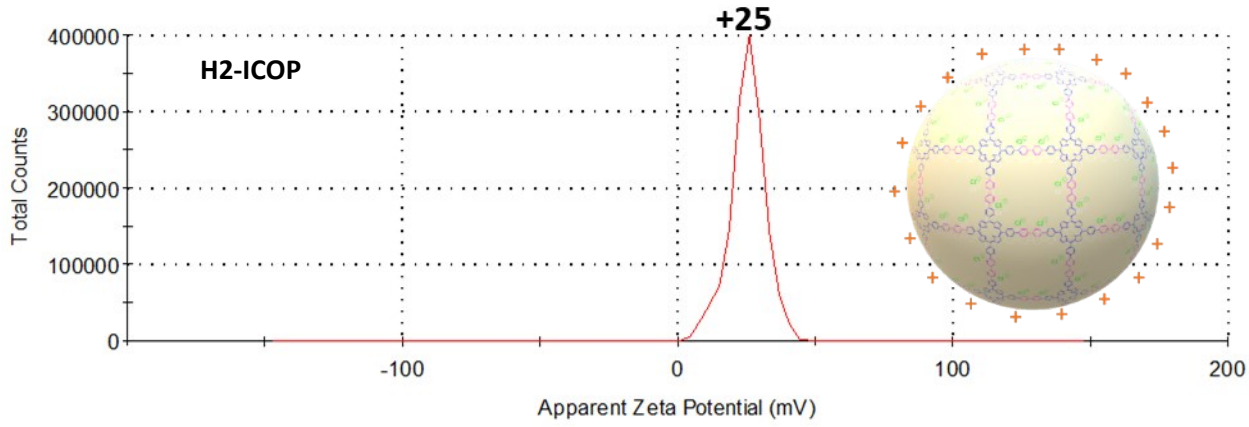


Figure S6. Size distributions of **H2-ICOP**(**a**) and **Zn-ICOP**(**b**) measured by DLS.


+25
H2-ICOP
Total Counts
400000
300000
200000
100000
0
-100
0
100
200
Apparent Zeta Potential (mV)

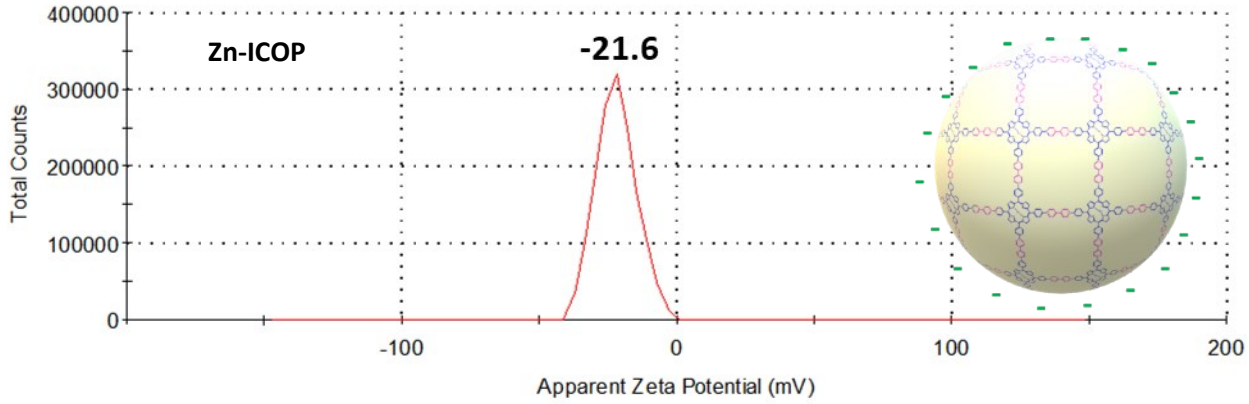

Zn-ICOP
-21.6
Total Counts
400000
300000
200000
100000
0
-100
0
100
200
Apparent Zeta Potential (mV)

Figure S7. Zeta potentials of **H2-ICOP** and **Zn-ICOP** in water.

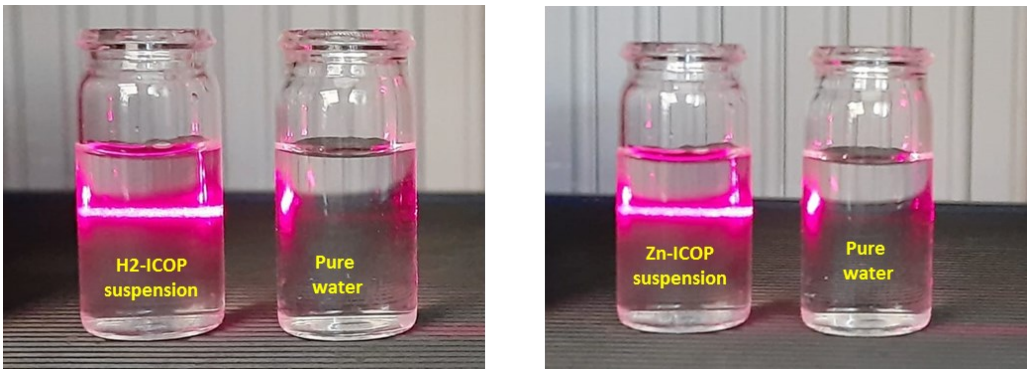


Figure S8. Tyndall effect of suspensions of **H2-ICOP** and **Zn-ICOP** in water.

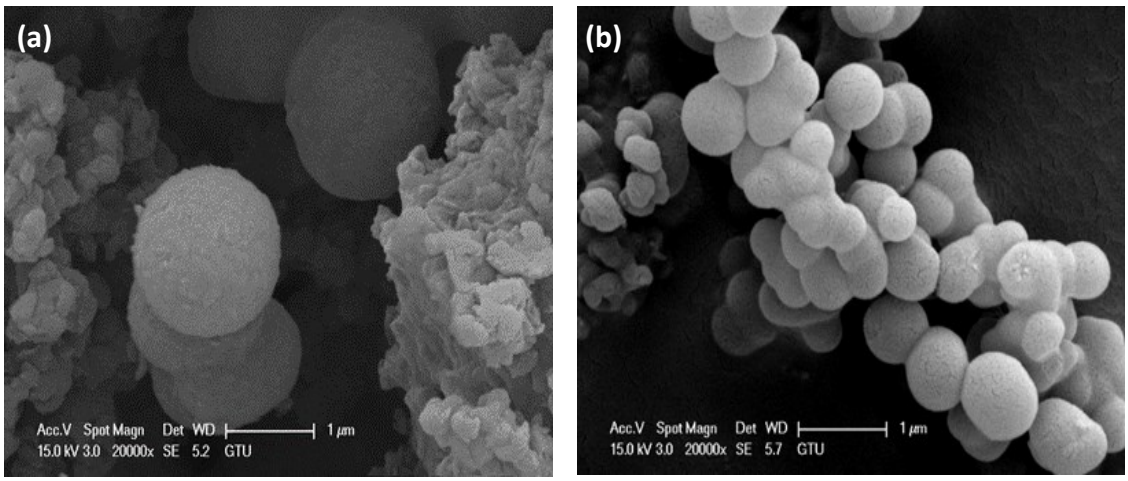


Figure S9. SEM images showing uniform spheres for **H2-ICOP-dx** (**a**) and **Zn-ICOP-dx** (**b**).

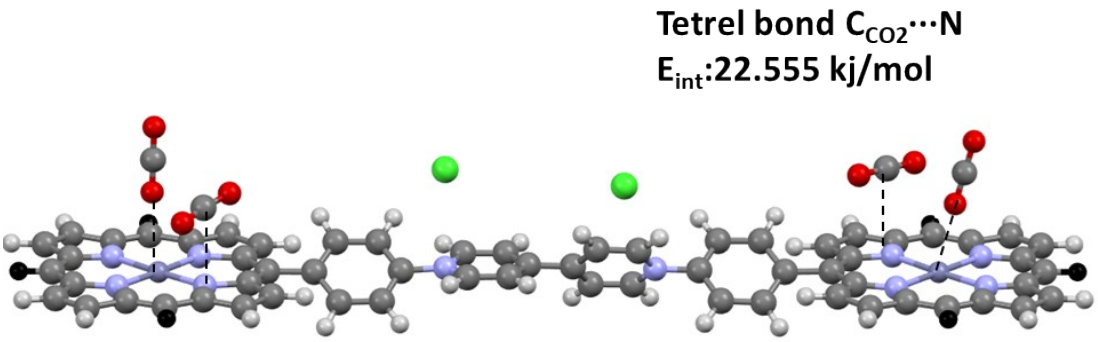


Figure S10. Formation of simultaneous tetrel bonds in **Zn-ICOP**.

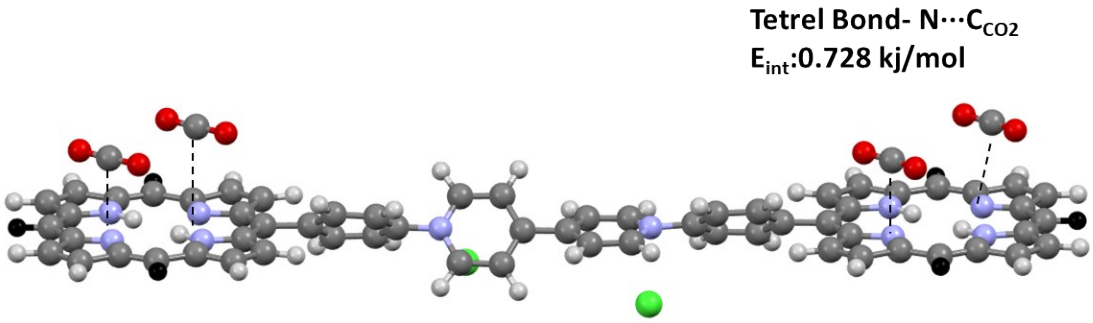


Figure S11. Formation of simultaneous four tetrel bonds in **H2-ICOP**.

Table S1. SAPT results (kJ/mol) for interaction between two CO_2 molecules placed at the same porphyrin fragments in **H2-ICOP** and **Zn-ICOP**. In **H2-ICOP** these molecules form two tetrel bonds, in **Zn-ICOP** molecules form tetrel and spodium bonds respectively.

Compound	Tetrel bond	E_{elst}	E_{exch}	E_{ind}	E_{disp}	E_{int}
H2-ICOP	C_{CO2}···N	1.9	0.1	-0.1	-1.2	**0.7**
Zn-ICOP	C_{CO2}···N	-13.6	63.6	-6.3	-21.1	**22.6**

Table S2. Crystallographic coordinates of **H2-ICOP** and **Zn-ICOP** staggered structures, unit cell parameters: a = b = 35.563, c= 7.8 Å, α = β = γ = 90°, space group P1.

H2-ICOP				**Zn-ICOP**			
C1	0.48031	0.25042	0.38062	C1	0.38115	0.48078	0.25000
C2	0.46756	0.24989	0.41830	C2	0.41834	0.46619	0.25000
C3	0.36392	0.33249	0.40471	C3	0.40482	0.36397	0.33221
C4	0.33618	0.33049	0.37717	C4	0.37711	0.33627	0.33033
C5	0.51926	0.24966	0.38022	H5	0.43105	0.35858	0.40251
C6	0.01934	0.24943	0.11739	H6	0.38072	0.30896	0.39412
C7	0.03106	0.25008	0.07923	C7	0.38115	0.51912	0.25000
C8	0.13365	0.16706	0.09295	C8	0.11645	0.01922	0.25000
C9	0.16152	0.16963	0.12059	C9	0.07925	0.03140	0.25000
C10	0.42862	0.24999	0.42862	C10	0.09277	0.13363	0.16780
C11	0.32797	0.28539	0.27832	C11	0.12049	0.16132	0.16967
C12	0.30178	0.28713	0.25096	H12	0.06654	0.13902	0.09750
C13	0.23937	0.38833	0.20364	H13	0.11688	0.18864	0.10588
C14	0.21209	0.38323	0.17704	N14	0.05690	0.00000	0.25000
C15	0.27963	0.28258	0.32626	N15	0.44070	0.50000	0.25000
C16	0.25205	0.27678	0.30022	C16	0.42867	0.42868	0.25000
C17	0.20648	0.15903	0.23815	H17	0.15262	0.21050	0.46433
C18	0.17978	0.15841	0.21070	H18	0.20266	0.26252	0.48000
C19	0.26385	0.27917	0.26217	H19	0.22115	0.30884	0.28672
C20	0.23600	0.27520	0.23424	H20	0.27430	0.35823	0.28939
C21	0.40470	0.16733	0.36388	C21	0.27873	0.32809	0.28681
C22	0.37715	0.16958	0.33620	C22	0.25070	0.30153	0.28649
C23	0.09294	0.33255	0.13365	C23	0.20400	0.23948	0.38933
C24	0.12044	0.33053	0.16139	C24	0.17717	0.21185	0.38227
C25	0.39906	0.24999	0.39908	H25	0.20957	0.15600	0.07119
C26	0.34299	0.24957	0.34285	H26	0.26193	0.20582	0.07049
C27	0.11738	0.25056	0.01933	H27	0.35659	0.27552	0.28542
C28	0.07923	0.24993	0.03106	C28	0.32647	0.28012	0.28425
C29	0.41822	0.25010	0.46749	C29	0.29979	0.25226	0.27657
C30	0.09856	0.25001	0.09857	C30	0.23828	0.20666	0.15790
C31	0.15438	0.25155	0.15433	C31	0.21046	0.17996	0.15698
C32	0.06903	0.25001	0.06901	C32	0.26244	0.26416	0.27966
H33	0.35862	0.40250	0.43083	N33	0.18189	0.18209	0.27935
H34	0.30914	0.39426	0.38087	C34	0.23394	0.23582	0.27550
H35	0.13898	0.09718	0.06683	N35	0.31418	0.31562	0.25000
H36	0.18855	0.10613	0.11675	H36	0.30878	0.22155	0.26825
H37	0.21054	0.46423	0.15262	H37	0.35727	0.45939	0.25000
H38	0.26251	0.47992	0.20261	H38	0.35338	0.53526	0.25000
H39	0.30888	0.28707	0.22113	CL39	0.39888	0.20774	0.25000
H40	0.35823	0.28941	0.27431	CL40	0.25569	0.10644	0.25000
H41	0.15597	0.07136	0.20960	C41	0.36396	0.40482	0.16780
H42	0.20577	0.07047	0.26193	C42	0.33627	0.37711	0.16967
H43	0.27537	0.28515	0.35657	H43	0.35857	0.43106	0.09750
H44	0.22195	0.26877	0.30867	H44	0.30896	0.38072	0.10588

H45	0.46002	0.25061	0.35750	C45	0.13363	0.09277	0.33220
H46	0.53497	0.24960	0.35384	C46	0.16132	0.12049	0.33033
H47	0.43081	0.09732	0.35862	H47	0.13902	0.06654	0.40251
H48	0.38081	0.10579	0.30908	H48	0.18864	0.11688	0.39412
H49	0.06683	0.40283	0.13898	C49	0.39898	0.39898	0.25000
H50	0.11677	0.39392	0.18858	C50	0.34246	0.34246	0.25000
H51	0.14002	0.25077	0.03997	H51	0.04062	0.14032	0.25000
H52	0.03998	0.24923	0.14004	C52	0.01922	0.11645	0.25000
N53	0.00000	0.24999	0.05637	C53	0.03140	0.07925	0.25000
N54	0.50001	0.25000	0.44118	C54	0.46619	0.41834	0.25000
N55	0.18236	0.27561	0.18239	C55	0.09861	0.09861	0.25000
N56	0.31591	0.25261	0.31454	C56	0.15513	0.15513	0.25000
CL57	0.20785	0.25001	0.39882	H57	0.14032	0.04062	0.25000
CL58	0.10658	0.24997	0.25557	C58	0.06892	0.06892	0.25000
H59	0.50281	0.25001	0.52779	C59	0.61885	0.51922	0.25000
C60	0.38062	0.25042	0.51969	C60	0.58166	0.53381	0.25000
C61	0.41830	0.24989	0.53244	C61	0.59518	0.63603	0.33221
C62	0.40471	0.33249	0.63608	C62	0.62289	0.66373	0.33033
C63	0.37717	0.33049	0.66382	H63	0.56895	0.64142	0.40251
C64	0.38022	0.24966	0.48074	H64	0.61928	0.69104	0.39412
C65	0.11739	0.24943	0.98066	C65	0.61885	0.48088	0.25000
C66	0.07923	0.25008	0.96894	C66	0.88355	0.98078	0.25000
C67	0.09294	0.16706	0.86635	C67	0.92075	0.96860	0.25000
C68	0.12059	0.16963	0.83848	C68	0.90723	0.86637	0.16780
C69	0.42862	0.24999	0.57138	C69	0.87951	0.83868	0.16967
C70	0.27832	0.28539	0.67203	H70	0.93346	0.86098	0.09750
C71	0.25096	0.28713	0.69822	H71	0.88312	0.81136	0.10588
C72	0.20365	0.38833	0.76063	N72	0.94310	0.00000	0.25000
C73	0.17704	0.38323	0.78791	N73	0.55930	0.50000	0.25000
C74	0.32626	0.28258	0.72037	C74	0.57133	0.57132	0.25000
C75	0.30022	0.27678	0.74795	H75	0.84738	0.78950	0.46433
C76	0.23815	0.15903	0.79352	H76	0.79734	0.73748	0.48000
C77	0.21070	0.15841	0.82022	H77	0.77885	0.69116	0.28672
C78	0.26217	0.27917	0.73616	H78	0.72570	0.64177	0.28939
C79	0.23424	0.27520	0.76400	C79	0.72127	0.67191	0.28681
C80	0.36388	0.16733	0.59530	C80	0.74930	0.69847	0.28649
C81	0.33620	0.16958	0.62285	C81	0.79600	0.76052	0.38933
C82	0.13365	0.33255	0.90706	C82	0.82283	0.78815	0.38227
C83	0.16139	0.33053	0.87956	H83	0.79043	0.84400	0.07119
C84	0.39908	0.24999	0.60094	H84	0.73807	0.79418	0.07049
C85	0.34285	0.24957	0.65701	H85	0.64341	0.72448	0.28542
C86	0.01933	0.25056	0.88262	C86	0.67353	0.71988	0.28425
C87	0.03106	0.24993	0.92077	C87	0.70021	0.74774	0.27657
C88	0.46749	0.25010	0.58178	C88	0.76172	0.79334	0.15790
C89	0.09857	0.25001	0.90144	C89	0.78954	0.82004	0.15698
C90	0.15433	0.25155	0.84562	C90	0.73756	0.73584	0.27966
C91	0.06901	0.25001	0.93097	N91	0.81811	0.81791	0.27935
H92	0.43083	0.40250	0.64138	C92	0.76606	0.76418	0.27550

H93	0.38087	0.39426	0.69086	N93	0.68582	0.68438	0.25000
H94	0.06683	0.09718	0.86102	H94	0.69122	0.77845	0.26825
H95	0.11675	0.10613	0.81146	H95	0.64273	0.54061	0.25000
H96	0.15262	0.46423	0.78946	H96	0.64662	0.46474	0.25000
H97	0.20261	0.47992	0.73749	CL97	0.60112	0.79226	0.25000
H98	0.22113	0.28706	0.69112	CL98	0.74431	0.89356	0.25000
H99	0.27431	0.28941	0.64177	C99	0.63604	0.59518	0.16780
H100	0.20960	0.07136	0.84403	C100	0.66373	0.62289	0.16967
H101	0.26193	0.07047	0.79423	H101	0.64143	0.56894	0.09750
H102	0.35657	0.28515	0.72463	H102	0.69104	0.61928	0.10588
H103	0.30867	0.26878	0.77805	C103	0.86637	0.90723	0.33220
H104	0.35750	0.25061	0.53998	C104	0.83868	0.87951	0.33033
H105	0.35384	0.24960	0.46503	H105	0.86098	0.93346	0.40251
H106	0.35862	0.09732	0.56919	H106	0.81136	0.88312	0.39412
H107	0.30908	0.10579	0.61919	C107	0.60102	0.60102	0.25000
H108	0.13898	0.40283	0.93317	C108	0.65754	0.65754	0.25000
H109	0.18858	0.39392	0.88323	H109	0.95938	0.85968	0.25000
H110	0.03997	0.25077	0.85998	C110	0.98078	0.88355	0.25000
H111	0.14004	0.24923	0.96002	C111	0.96860	0.92075	0.25000
N112	0.05637	0.24999	0.00000	C112	0.53381	0.58166	0.25000
N113	0.44118	0.25000	0.50000	C113	0.90139	0.90139	0.25000
N114	0.18239	0.27561	0.81764	C114	0.84487	0.84487	0.25000
N115	0.31454	0.25261	0.68409	H115	0.85968	0.95938	0.25000
CL11	0.39882	0.25001	0.79215	C116	0.93108	0.93108	0.25000
CL11	0.25557	0.24997	0.89342	C117	0.51922	0.38115	0.25000
H118	0.99655	0.24999	0.97460	C118	0.53381	0.41834	0.25000
C119	0.51969	0.25042	0.61938	C119	0.63603	0.40482	0.33221
C120	0.53244	0.24989	0.58170	C120	0.66373	0.37711	0.33033
C121	0.63608	0.33249	0.59529	H121	0.64142	0.43105	0.40251
C122	0.66382	0.33049	0.62283	H122	0.69104	0.38072	0.39412
C123	0.48074	0.24966	0.61978	C123	0.48088	0.38115	0.25000
C124	0.98066	0.24943	0.88261	C124	0.98078	0.11645	0.25000
C125	0.96894	0.25008	0.92077	C125	0.96860	0.07925	0.25000
C126	0.86635	0.16706	0.90705	C126	0.86637	0.09277	0.16780
C127	0.83848	0.16964	0.87941	C127	0.83868	0.12049	0.16967
C128	0.57138	0.24999	0.57138	H128	0.86098	0.06654	0.09750
C129	0.67203	0.28539	0.72168	H129	0.81136	0.11688	0.10588
C130	0.69822	0.28714	0.74904	N130	0.00000	0.05690	0.25000
C131	0.76063	0.38833	0.79636	N131	0.50000	0.44070	0.25000
C132	0.78791	0.38323	0.82296	C132	0.57132	0.42867	0.25000
C133	0.72037	0.28259	0.67374	H133	0.78950	0.15262	0.46433
C134	0.74795	0.27679	0.69978	H134	0.73748	0.20266	0.48000
C135	0.79352	0.15903	0.76185	H135	0.69116	0.22115	0.28672
C136	0.82022	0.15842	0.78930	H136	0.64177	0.27430	0.28939
C137	0.73615	0.27917	0.73783	C137	0.67191	0.27873	0.28681
C138	0.76400	0.27521	0.76576	C138	0.69847	0.25070	0.28649
C139	0.59530	0.16733	0.63612	C139	0.76052	0.20400	0.38933
C140	0.62285	0.16958	0.66380	C140	0.78815	0.17717	0.38227

C141	0.90706	0.33256	0.86635	H141	0.84400	0.20957	0.07119
C142	0.87956	0.33053	0.83861	H142	0.79418	0.26193	0.07049
C143	0.60094	0.24999	0.60092	H143	0.72448	0.35659	0.28542
C144	0.65701	0.24957	0.65715	C144	0.71988	0.32647	0.28425
C145	0.88262	0.25057	0.98067	C145	0.74774	0.29979	0.27657
C146	0.92077	0.24993	0.96894	C146	0.79334	0.23828	0.15790
C147	0.58178	0.25010	0.53251	C147	0.82004	0.21046	0.15698
C148	0.90144	0.25001	0.90143	C148	0.73584	0.26244	0.27966
C149	0.84562	0.25156	0.84567	N149	0.81791	0.18189	0.27935
C150	0.93097	0.25001	0.93099	C150	0.76418	0.23394	0.27550
H151	0.64138	0.40250	0.56917	N151	0.68438	0.31418	0.25000
H152	0.69086	0.39426	0.61913	H152	0.77845	0.30878	0.26825
H153	0.86102	0.09719	0.93317	H153	0.54061	0.35727	0.25000
H154	0.81145	0.10613	0.88325	H154	0.46474	0.35338	0.25000
H155	0.78946	0.46424	0.84738	CL15	0.79226	0.39888	0.25000
H156	0.73749	0.47992	0.79739	CL15	0.89356	0.25569	0.25000
H157	0.69112	0.28707	0.77887	C157	0.59518	0.36396	0.16780
H158	0.64177	0.28941	0.72569	C158	0.62289	0.33627	0.16967
H159	0.84403	0.07136	0.79040	H159	0.56894	0.35857	0.09750
H160	0.79423	0.07047	0.73807	H160	0.61928	0.30896	0.10588
H161	0.72463	0.28515	0.64343	C161	0.90723	0.13363	0.33220
H162	0.77805	0.26878	0.69133	C162	0.87951	0.16132	0.33033
H163	0.53998	0.25061	0.64250	H163	0.93346	0.13902	0.40251
H164	0.46503	0.24960	0.64616	H164	0.88312	0.18864	0.39412
H165	0.56919	0.09733	0.64138	C165	0.60102	0.39898	0.25000
H166	0.61919	0.10580	0.69092	C166	0.65754	0.34246	0.25000
H167	0.93317	0.40283	0.86102	H167	0.85968	0.04062	0.25000
H168	0.88323	0.39392	0.81142	C168	0.88355	0.01922	0.25000
H169	0.85998	0.25077	0.96003	C169	0.92075	0.03140	0.25000
H170	0.96002	0.24924	0.85996	C170	0.58166	0.46619	0.25000
N171	0.00000	0.24999	0.94363	C171	0.90139	0.09861	0.25000
N172	0.49999	0.25000	0.55882	C172	0.84487	0.15513	0.25000
N173	0.81764	0.27562	0.81761	H173	0.95938	0.14032	0.25000
N174	0.68409	0.25261	0.68546	C174	0.93108	0.06892	0.25000
CL17	0.79215	0.25001	0.60118	C175	0.48078	0.61885	0.25000
CL17	0.89342	0.24997	0.74443	C176	0.46619	0.58166	0.25000
H177	0.49719	0.25001	0.47221	C177	0.36397	0.59518	0.33221
C178	0.61938	0.25042	0.48031	C178	0.33627	0.62289	0.33033
C179	0.58170	0.24989	0.46756	H179	0.35858	0.56895	0.40251
C180	0.59529	0.33249	0.36392	H180	0.30896	0.61928	0.39412
C181	0.62283	0.33049	0.33618	C181	0.51912	0.61885	0.25000
C182	0.61978	0.24966	0.51926	C182	0.01922	0.88355	0.25000
C183	0.88261	0.24943	0.01934	C183	0.03140	0.92075	0.25000
C184	0.92077	0.25008	0.03106	C184	0.13363	0.90723	0.16780
C185	0.90706	0.16706	0.13365	C185	0.16132	0.87951	0.16967
C186	0.87941	0.16964	0.16152	H186	0.13902	0.93346	0.09750
C187	0.57138	0.24999	0.42862	H187	0.18864	0.88312	0.10588
C188	0.72168	0.28539	0.32797	N188	0.00000	0.94310	0.25000

C189	0.74904	0.28714	0.30178	N189	0.50000	0.55930	0.25000
C190	0.79635	0.38833	0.23937	C190	0.42868	0.57133	0.25000
C191	0.82296	0.38323	0.21209	H191	0.21050	0.84738	0.46433
C192	0.67374	0.28259	0.27963	H192	0.26252	0.79734	0.48000
C193	0.69978	0.27679	0.25205	H193	0.30884	0.77885	0.28672
C194	0.76185	0.15903	0.20648	H194	0.35823	0.72570	0.28939
C195	0.78930	0.15842	0.17978	C195	0.32809	0.72127	0.28681
C196	0.73783	0.27917	0.26384	C196	0.30153	0.74930	0.28649
C197	0.76576	0.27521	0.23600	C197	0.23948	0.79600	0.38933
C198	0.63612	0.16733	0.40470	C198	0.21185	0.82283	0.38227
C199	0.66380	0.16958	0.37715	H199	0.15600	0.79043	0.07119
C200	0.86635	0.33256	0.09294	H200	0.20582	0.73807	0.07049
C201	0.83861	0.33053	0.12044	H201	0.27552	0.64341	0.28542
C202	0.60092	0.24999	0.39906	C202	0.28012	0.67353	0.28425
C203	0.65715	0.24957	0.34299	C203	0.25226	0.70021	0.27657
C204	0.98067	0.25057	0.11738	C204	0.20666	0.76172	0.15790
C205	0.96894	0.24993	0.07923	C205	0.17996	0.78954	0.15698
C206	0.53251	0.25010	0.41822	C206	0.26416	0.73756	0.27966
C207	0.90143	0.25001	0.09856	N207	0.18209	0.81811	0.27935
C208	0.84567	0.25156	0.15438	C208	0.23582	0.76606	0.27550
C209	0.93099	0.25001	0.06903	N209	0.31562	0.68582	0.25000
H210	0.56917	0.40250	0.35862	H210	0.22155	0.69122	0.26825
H211	0.61913	0.39426	0.30914	H211	0.45939	0.64273	0.25000
H212	0.93317	0.09719	0.13898	H212	0.53526	0.64662	0.25000
H213	0.88325	0.10613	0.18854	CL21	0.20774	0.60112	0.25000
H214	0.84738	0.46424	0.21054	CL21	0.10644	0.74431	0.25000
H215	0.79739	0.47992	0.26251	C215	0.40482	0.63604	0.16780
H216	0.77887	0.28707	0.30888	C216	0.37711	0.66373	0.16967
H217	0.72569	0.28941	0.35823	H217	0.43106	0.64143	0.09750
H218	0.79040	0.07136	0.15597	H218	0.38072	0.69104	0.10588
H219	0.73807	0.07047	0.20577	C219	0.09277	0.86637	0.33220
H220	0.64343	0.28515	0.27537	C220	0.12049	0.83868	0.33033
H221	0.69133	0.26878	0.22195	H221	0.06654	0.86098	0.40251
H222	0.64250	0.25061	0.46002	H222	0.11688	0.81136	0.39412
H223	0.64616	0.24960	0.53497	C223	0.39898	0.60102	0.25000
H224	0.64138	0.09733	0.43081	C224	0.34246	0.65754	0.25000
H225	0.69092	0.10580	0.38081	H225	0.14032	0.95938	0.25000
H226	0.86102	0.40283	0.06683	C226	0.11645	0.98078	0.25000
H227	0.81142	0.39392	0.11677	C227	0.07925	0.96860	0.25000
H228	0.96003	0.25077	0.14002	C228	0.41834	0.53381	0.25000
H229	0.85996	0.24924	0.03998	C229	0.09861	0.90139	0.25000
N230	0.94363	0.25000	0.00000	C230	0.15513	0.84487	0.25000
N231	0.55882	0.25000	0.50000	H231	0.04062	0.85968	0.25000
N232	0.81761	0.27562	0.18236	C232	0.06892	0.93108	0.25000
N233	0.68546	0.25261	0.31591	ZN23	0.00000	0.00000	0.25000
CL23	0.60118	0.25001	0.20785	ZN23	0.50000	0.50000	0.25000
CL23	0.74443	0.24997	0.10658	C1	0.88115	0.48078	0.75000
H236	0.00345	0.24999	0.02540	C2	0.91834	0.46619	0.75000

C237	0.97796	0.75268	0.37691	C3	0.90482	0.36397	0.83221
C238	0.96521	0.75215	0.41459	C4	0.87711	0.33627	0.83033
C239	0.86157	0.83475	0.40100	H5	0.93105	0.35858	0.90251
C240	0.83383	0.83275	0.37346	H6	0.88072	0.30896	0.89412
C241	1.01691	0.75192	0.37651	C7	0.88115	0.51912	0.75000
C242	0.51699	0.75169	0.11368	C8	0.61645	0.01922	0.75000
C243	0.52871	0.75234	0.07552	C9	0.57925	0.03140	0.75000
C244	0.63130	0.66932	0.08924	C10	0.59277	0.13363	0.66780
C245	0.65917	0.67190	0.11688	C11	0.62049	0.16132	0.66967
C246	0.92627	0.75226	0.42491	H12	0.56654	0.13902	0.59750
C247	0.82562	0.78765	0.27461	H13	0.61688	0.18864	0.60588
C248	0.79943	0.78940	0.24725	N14	0.55690	0.00000	0.75000
C249	0.73702	0.89059	0.19993	N15	0.94070	0.50000	0.75000
C250	0.70974	0.88549	0.17333	C16	0.92867	0.42868	0.75000
C251	0.77728	0.78485	0.32255	H17	0.65262	0.21050	0.96433
C252	0.74970	0.77905	0.29651	H18	0.70266	0.26252	0.98000
C253	0.70413	0.66129	0.23444	H19	0.72115	0.30884	0.78672
C254	0.67743	0.66068	0.20699	H20	0.77430	0.35823	0.78939
C255	0.76150	0.78143	0.25846	C21	0.77873	0.32809	0.78681
C256	0.73365	0.77747	0.23053	C22	0.75070	0.30153	0.78649
C257	0.90235	0.66959	0.36017	C23	0.70400	0.23948	0.88933
C258	0.87480	0.67184	0.33249	C24	0.67717	0.21185	0.88227
C259	0.59059	0.83482	0.12994	H25	0.70957	0.15600	0.57119
C260	0.61809	0.83279	0.15768	H26	0.76193	0.20582	0.57049
C261	0.89671	0.75226	0.39537	H27	0.85659	0.27552	0.78542
C262	0.84064	0.75184	0.33914	C28	0.82647	0.28012	0.78425
C263	0.61503	0.75283	0.01562	C29	0.79979	0.25226	0.77657
C264	0.57688	0.75219	0.02735	C30	0.73828	0.20666	0.65790
C265	0.91587	0.75236	0.46378	C31	0.71046	0.17996	0.65698
C266	0.59621	0.75227	0.09486	C32	0.76244	0.26416	0.77966
C267	0.65203	0.75382	0.15062	N33	0.68189	0.18209	0.77935
C268	0.56668	0.75227	0.06530	C34	0.73394	0.23582	0.77550
H269	0.85627	0.90476	0.42712	N35	0.81418	0.31562	0.75000
H270	0.80679	0.89652	0.37716	H36	0.80878	0.22155	0.76825
H271	0.63663	0.59945	0.06312	H37	0.85727	0.45939	0.75000
H272	0.68620	0.60839	0.11304	H38	0.85338	0.53526	0.75000
H273	0.70819	0.96650	0.14891	CL39	0.89888	0.20774	0.75000
H274	0.76016	0.98218	0.19890	CL40	0.75569	0.10644	0.75000
H275	0.80653	0.78933	0.21742	C41	0.86396	0.40482	0.66780
H276	0.85588	0.79167	0.27060	C42	0.83627	0.37711	0.66967
H277	0.65362	0.57362	0.20589	H43	0.85857	0.43106	0.59750
H278	0.70342	0.57273	0.25822	H44	0.80896	0.38072	0.60588
H279	0.77302	0.78742	0.35286	C45	0.63363	0.09277	0.83220
H280	0.71960	0.77104	0.30496	C46	0.66132	0.12049	0.83033
H281	0.95767	0.75287	0.35379	H47	0.63902	0.06654	0.90251
H282	1.03262	0.75186	0.35013	H48	0.68864	0.11688	0.89412
H283	0.92846	0.59959	0.35491	C49	0.89898	0.39898	0.75000
H284	0.87846	0.60806	0.30537	C50	0.84246	0.34246	0.75000

H285	0.56448	0.90509	0.13527	H51	0.54062	0.14032	0.75000
H286	0.61442	0.89618	0.18487	C52	0.51922	0.11645	0.75000
H287	0.63767	0.75303	0.03626	C53	0.53140	0.07925	0.75000
H288	0.53763	0.75150	0.13633	C54	0.96619	0.41834	0.75000
N289	0.49765	0.75226	0.05266	C55	0.59861	0.09861	0.75000
N290	0.99766	0.75226	0.43747	C56	0.65513	0.15513	0.75000
N291	0.68001	0.77788	0.17868	H57	0.64032	0.04062	0.75000
N292	0.81356	0.75487	0.31083	C58	0.56892	0.06892	0.75000
CL29	0.20785	0.75000	0.39882	C59	1.11885	0.51922	0.75000
CL29	0.10658	0.74997	0.25557	C60	1.08166	0.53381	0.75000
H295	1.00046	0.75227	0.52408	C61	1.09518	0.63603	0.83221
C296	0.87827	0.75268	0.51598	C62	1.12289	0.66373	0.83033
C297	0.91595	0.75215	0.52873	H63	1.06895	0.64142	0.90251
C298	0.90236	0.83475	0.63237	H64	1.11928	0.69104	0.89412
C299	0.87482	0.83275	0.66011	C65	1.11885	0.48088	0.75000
C300	0.87787	0.75192	0.47703	C66	1.38355	0.98078	0.75000
C301	0.61504	0.75169	0.97695	C67	1.42075	0.96860	0.75000
C302	0.57688	0.75234	0.96523	C68	1.40723	0.86637	0.66780
C303	0.59059	0.66932	0.86264	C69	1.37951	0.83868	0.66967
C304	0.61824	0.67190	0.83477	H70	1.43346	0.86098	0.59750
C305	0.92627	0.75226	0.56767	H71	1.38312	0.81136	0.60588
C306	0.77597	0.78765	0.66832	N72	1.44310	0.00000	0.75000
C307	0.74861	0.78940	0.69451	N73	1.05930	0.50000	0.75000
C308	0.70130	0.89059	0.75692	C74	1.07133	0.57132	0.75000
C309	0.67469	0.88549	0.78420	H75	1.34738	0.78950	0.96433
C310	0.82391	0.78485	0.71666	H76	1.29734	0.73748	0.98000
C311	0.79787	0.77905	0.74424	H77	1.27885	0.69116	0.78672
C312	0.73580	0.66129	0.78981	H78	1.22570	0.64177	0.78939
C313	0.70835	0.66068	0.81651	C79	1.22127	0.67191	0.78681
C314	0.75982	0.78143	0.73245	C80	1.24930	0.69847	0.78649
C315	0.73189	0.77747	0.76029	C81	1.29600	0.76052	0.88933
C316	0.86153	0.66959	0.59159	C82	1.32283	0.78815	0.88227
C317	0.83385	0.67184	0.61914	H83	1.29043	0.84400	0.57119
C318	0.63130	0.83482	0.90335	H84	1.23807	0.79418	0.57049
C319	0.65904	0.83279	0.87585	H85	1.14341	0.72448	0.78542
C320	0.89673	0.75226	0.59723	C86	1.17353	0.71988	0.78425
C321	0.84050	0.75184	0.65330	C87	1.20021	0.74774	0.77657
C322	0.51698	0.75283	0.87891	C88	1.26172	0.79334	0.65790
C323	0.52871	0.75219	0.91706	C89	1.28954	0.82004	0.65698
C324	0.96514	0.75236	0.57807	C90	1.23756	0.73584	0.77966
C325	0.59622	0.75227	0.89773	N91	1.31811	0.81791	0.77935
C326	0.65198	0.75382	0.84191	C92	1.26606	0.76418	0.77550
C327	0.56666	0.75227	0.92726	N93	1.18582	0.68438	0.75000
H328	0.92848	0.90476	0.63767	H94	1.19122	0.77845	0.76825
H329	0.87852	0.89652	0.68715	H95	1.14273	0.54061	0.75000
H330	0.56448	0.59945	0.85731	H96	1.14662	0.46474	0.75000
H331	0.61440	0.60839	0.80775	CL97	1.10112	0.79226	0.75000
H332	0.65027	0.96650	0.78575	CL98	1.24431	0.89356	0.75000

H333	0.70026	0.98218	0.73378	C99	1.13604	0.59518	0.66780
H334	0.71878	0.78933	0.68741	C100	1.16373	0.62289	0.66967
H335	0.77196	0.79167	0.63806	H101	1.14143	0.56894	0.59750
H336	0.70725	0.57362	0.84032	H102	1.19104	0.61928	0.60588
H337	0.75958	0.57273	0.79052	C103	1.36637	0.90723	0.83220
H338	0.85422	0.78742	0.72092	C104	1.33868	0.87951	0.83033
H339	0.80632	0.77104	0.77434	H105	1.36098	0.93346	0.90251
H340	0.85515	0.75287	0.53627	H106	1.31136	0.88312	0.89412
H341	0.85149	0.75186	0.46132	C107	1.10102	0.60102	0.75000
H342	0.85627	0.59959	0.56548	C108	1.15754	0.65754	0.75000
H343	0.80673	0.60806	0.61548	H109	1.45938	0.85968	0.75000
H344	0.63663	0.90509	0.92946	C110	1.48078	0.88355	0.75000
H345	0.68623	0.89618	0.87952	C111	1.46860	0.92075	0.75000
H346	0.53762	0.75303	0.85627	C112	1.03381	0.58166	0.75000
H347	0.63769	0.75150	0.95631	C113	1.40139	0.90139	0.75000
N348	0.55402	0.75226	-0.00371	C114	1.34487	0.84487	0.75000
N349	0.93883	0.75226	0.49629	H115	1.35968	0.95938	0.75000
N350	0.68004	0.77788	0.81393	C116	1.43108	0.93108	0.75000
N351	0.81219	0.75487	0.68038	C117	1.01922	0.38115	0.75000
CL35	0.39882	0.75000	0.79215	C118	1.03381	0.41834	0.75000
CL35	0.25557	0.74997	0.89342	C119	1.13603	0.40482	0.83221
H354	1.49420	0.75225	0.97089	C120	1.16373	0.37711	0.83033
C355	1.01734	0.75268	0.61567	H121	1.14142	0.43105	0.90251
C356	1.03009	0.75215	0.57799	H122	1.19104	0.38072	0.89412
C357	1.13373	0.83475	0.59158	C123	0.98088	0.38115	0.75000
C358	1.16147	0.83275	0.61912	C124	1.48078	0.11645	0.75000
C359	0.97839	0.75192	0.61607	C125	1.46860	0.07925	0.75000
C360	1.47831	0.75169	0.87890	C126	1.36637	0.09277	0.66780
C361	1.46659	0.75234	0.91706	C127	1.33868	0.12049	0.66967
C362	1.36400	0.66932	0.90334	H128	1.36098	0.06654	0.59750
C363	1.33613	0.67190	0.87570	H129	1.31136	0.11688	0.60588
C364	1.06903	0.75226	0.56767	N130	0.50000	0.05690	0.75000
C365	1.16968	0.78765	0.71797	N131	1.00000	0.44070	0.75000
C366	1.19587	0.78940	0.74533	C132	1.07132	0.42867	0.75000
C367	1.25828	0.89059	0.79265	H133	1.28950	0.15262	0.96433
C368	1.28556	0.88549	0.81925	H134	1.23748	0.20266	0.98000
C369	1.21802	0.78485	0.67003	H135	1.19116	0.22115	0.78672
C370	1.24560	0.77905	0.69607	H136	1.14177	0.27430	0.78939
C371	1.29117	0.66129	0.75814	C137	1.17191	0.27873	0.78681
C372	1.31787	0.66068	0.78559	C138	1.19847	0.25070	0.78649
C373	1.23380	0.78143	0.73412	C139	1.26052	0.20400	0.88933
C374	1.26165	0.77747	0.76205	C140	1.28815	0.17717	0.88227
C375	1.09295	0.66959	0.63241	H141	1.34400	0.20957	0.57119
C376	1.12050	0.67184	0.66009	H142	1.29418	0.26193	0.57049
C377	1.40471	0.83482	0.86264	H143	1.22448	0.35659	0.78542
C378	1.37721	0.83279	0.83490	C144	1.21988	0.32647	0.78425
C379	1.09859	0.75226	0.59721	C145	1.24774	0.29979	0.77657
C380	1.15466	0.75184	0.65344	C146	1.29334	0.23828	0.65790

C381	1.38027	0.75283	0.97696	C147	1.32004	0.21046	0.65698
C382	1.41842	0.75219	0.96523	C148	1.23584	0.26244	0.77966
C383	1.07943	0.75236	0.52880	N149	1.31791	0.18189	0.77935
C384	1.39909	0.75227	0.89772	C150	1.26418	0.23394	0.77550
C385	1.34327	0.75382	0.84196	N151	1.18438	0.31418	0.75000
C386	1.42862	0.75227	0.92728	H152	1.27845	0.30878	0.76825
H387	1.13903	0.90476	0.56546	H153	1.04061	0.35727	0.75000
H388	1.18851	0.89652	0.61542	H154	0.96474	0.35338	0.75000
H389	1.35867	0.59945	0.92946	CL15	1.29226	0.39888	0.75000
H390	1.30910	0.60839	0.87954	CL15	1.39356	0.25569	0.75000
H391	1.28711	0.96650	0.84367	C157	1.09518	0.36396	0.66780
H392	1.23514	0.98218	0.79368	C158	1.12289	0.33627	0.66967
H393	1.18877	0.78933	0.77516	H159	1.06894	0.35857	0.59750
H394	1.13942	0.79167	0.72198	H160	1.11928	0.30896	0.60588
H395	1.34168	0.57362	0.78669	C161	1.40723	0.13363	0.83220
H396	1.29188	0.57273	0.73436	C162	1.37951	0.16132	0.83033
H397	1.22228	0.78742	0.63972	H163	1.43346	0.13902	0.90251
H398	1.27570	0.77104	0.68762	H164	1.38312	0.18864	0.89412
H399	1.03763	0.75287	0.63879	C165	1.10102	0.39898	0.75000
H400	0.96268	0.75186	0.64245	C166	1.15754	0.34246	0.75000
H401	1.06684	0.59959	0.63767	H167	1.35968	0.04062	0.75000
H402	1.11684	0.60806	0.68721	C168	1.38355	0.01922	0.75000
H403	1.43082	0.90509	0.85731	C169	1.42075	0.03140	0.75000
H404	1.38088	0.89618	0.80771	C170	1.08166	0.46619	0.75000
H405	1.35763	0.75303	0.95632	C171	1.40139	0.09861	0.75000
H406	1.45767	0.75150	0.85625	C172	1.34487	0.15513	0.75000
N407	0.49765	0.75226	0.93992	H173	1.45938	0.14032	0.75000
N408	0.99764	0.75226	0.55511	C174	1.43108	0.06892	0.75000
N409	1.31529	0.77788	0.81390	C175	0.98078	0.61885	0.75000
N410	1.18174	0.75487	0.68175	C176	0.96619	0.58166	0.75000
CL41	0.79215	0.75000	0.60118	C177	0.86397	0.59518	0.83221
CL41	0.89342	0.74997	0.74443	C178	0.83627	0.62289	0.83033
H413	0.99484	0.75227	0.46850	H179	0.85858	0.56895	0.90251
C414	1.11703	0.75268	0.47660	H180	0.80896	0.61928	0.89412
C415	1.07935	0.75215	0.46385	C181	1.01912	0.61885	0.75000
C416	1.09294	0.83475	0.36021	C182	0.51922	0.88355	0.75000
C417	1.12048	0.83275	0.33247	C183	0.53140	0.92075	0.75000
C418	1.11743	0.75192	0.51555	C184	0.63363	0.90723	0.66780
C419	1.38026	0.75169	0.01563	C185	0.66132	0.87951	0.66967
C420	1.41842	0.75234	0.02735	H186	0.63902	0.93346	0.59750
C421	1.40471	0.66932	0.12994	H187	0.68864	0.88312	0.60588
C422	1.37706	0.67190	0.15781	N188	0.50000	0.94310	0.75000
C423	1.06903	0.75226	0.42491	N189	1.00000	0.55930	0.75000
C424	1.21933	0.78765	0.32426	C190	0.92868	0.57133	0.75000
C425	1.24669	0.78940	0.29807	H191	0.71050	0.84738	0.96433
C426	1.29400	0.89059	0.23566	H192	0.76252	0.79734	0.98000
C427	1.32061	0.88549	0.20838	H193	0.80884	0.77885	0.78672
C428	1.17139	0.78485	0.27592	H194	0.85823	0.72570	0.78939

C429	1.19743	0.77905	0.24834
C430	1.25950	0.66129	0.20277
C431	1.28695	0.66068	0.17607
C432	1.23548	0.78143	0.26013
C433	1.26341	0.77747	0.23229
C434	1.13377	0.66959	0.40099
C435	1.16145	0.67184	0.37344
C436	1.36400	0.83482	0.08923
C437	1.33626	0.83279	0.11673
C438	1.09857	0.75226	0.39535
C439	1.15480	0.75184	0.33928
C440	1.47832	0.75283	0.11367
C441	1.46659	0.75219	0.07552
C442	1.03016	0.75236	0.41451
C443	1.39908	0.75227	0.09485
C444	1.34332	0.75382	0.15067
C445	1.42864	0.75227	0.06532
H446	1.06682	0.90476	0.35491
H447	1.11678	0.89652	0.30543
H448	1.43082	0.59945	0.13527
H449	1.38090	0.60839	0.18483
H450	1.34503	0.96650	0.20683
H451	1.29504	0.98218	0.25880
H452	1.27652	0.78933	0.30517
H453	1.22334	0.79167	0.35452
H454	1.28805	0.57362	0.15226
H455	1.23572	0.57273	0.20206
H456	1.14108	0.78742	0.27166
H457	1.18898	0.77104	0.21824
H458	1.14015	0.75287	0.45631
H459	1.14381	0.75186	0.53126
H460	1.13903	0.59959	0.42710
H461	1.18857	0.60806	0.37710
H462	1.35867	0.90509	0.06312
H463	1.30907	0.89618	0.11306
H464	1.45768	0.75303	0.13631
H465	1.35761	0.75150	0.03627
N466	1.44128	0.75226	-0.00371
N467	1.05647	0.75226	0.49629
N468	1.31526	0.77788	0.17865
N469	1.18311	0.75487	0.31220
CL47	0.60118	0.75000	0.20785
CL47	0.74443	0.74997	0.10658
H472	0.50110	0.75225	0.02169
END			

C195	0.82809	0.72127	0.78681
C196	0.80153	0.74930	0.78649
C197	0.73948	0.79600	0.88933
C198	0.71185	0.82283	0.88227
H199	0.65600	0.79043	0.57119
H200	0.70582	0.73807	0.57049
H201	0.77552	0.64341	0.78542
C202	0.78012	0.67353	0.78425
C203	0.75226	0.70021	0.77657
C204	0.70666	0.76172	0.65790
C205	0.67996	0.78954	0.65698
C206	0.76416	0.73756	0.77966
N207	0.68209	0.81811	0.77935
C208	0.73582	0.76606	0.77550
N209	0.81562	0.68582	0.75000
H210	0.72155	0.69122	0.76825
H211	0.95939	0.64273	0.75000
H212	1.03526	0.64662	0.75000
CL21	0.70774	0.60112	0.75000
CL21	0.60644	0.74431	0.75000
C215	0.90482	0.63604	0.66780
C216	0.87711	0.66373	0.66967
H217	0.93106	0.64143	0.59750
H218	0.88072	0.69104	0.60588
C219	0.59277	0.86637	0.83220
C220	0.62049	0.83868	0.83033
H221	0.56654	0.86098	0.90251
H222	0.61688	0.81136	0.89412
C223	0.89898	0.60102	0.75000
C224	0.84246	0.65754	0.75000
H225	0.64032	0.95938	0.75000
C226	0.61645	0.98078	0.75000
C227	0.57925	0.96860	0.75000
C228	0.91834	0.53381	0.75000
C229	0.59861	0.90139	0.75000
C230	0.65513	0.84487	0.75000
H231	0.54062	0.85968	0.75000
C232	0.56892	0.93108	0.75000
ZN23	0.50000	0.00000	0.75000
ZN23	1.00000	0.50000	0.75000

Table S3. Cartesian coordinates (Å) of **H2-ICOP** for **N···C_{CO2}** (I) and **Cl^-···C_{CO2}** (II) tetrel bonds.

I				II			
H	35.582	1.962	34.561	H	35.500	1.952	34.719
C	34.957	1.951	31.402	C	34.935	1.948	31.441
C	34.495	1.962	32.786	C	34.517	1.953	32.801
C	31.404	1.952	34.926	C	31.442	1.957	34.936
C	32.817	1.997	34.570	C	32.801	1.952	34.517
C	33.218	1.986	33.197	C	33.164	1.952	33.165
H	30.582	1.948	34.233	H	30.636	1.958	34.200
H	34.270	1.948	30.579	H	34.200	1.946	30.635
C	39.862	1.951	34.958	C	39.805	1.948	34.935
C	38.445	1.950	34.581	C	38.446	1.953	34.517
C	36.290	1.952	31.413	C	36.312	1.957	31.442
C	36.740	1.952	32.806	C	36.730	1.952	32.801
C	38.021	1.951	33.210	C	38.082	1.952	33.164
H	36.984	1.955	30.596	H	37.047	1.958	30.636
H	40.675	1.948	34.255	H	40.612	1.946	34.200
N	35.608	1.953	33.568	N	35.624	1.952	33.615
C	17.051	1.937	49.230	C	17.110	1.955	49.183
C	16.672	1.957	50.562	C	16.656	1.951	50.525
C	18.443	1.911	49.199	C	18.498	1.949	49.168
C	15.325	1.955	51.059	C	15.269	1.952	50.893
C	14.897	1.951	52.343	C	14.899	1.953	52.277
H	16.405	1.949	48.371	H	16.388	1.957	48.359
H	19.016	1.878	48.303	H	19.057	1.949	48.229
N	17.810	1.962	51.307	N	17.812	1.952	51.340
H	17.832	1.963	54.549	H	17.912	1.952	54.425
C	13.538	1.953	54.130	C	13.559	1.955	54.137
C	14.966	1.952	54.503	C	14.901	1.951	54.591
C	13.501	1.951	52.791	C	13.545	1.949	52.749
C	15.412	1.952	55.879	C	15.269	1.952	55.978
C	16.697	1.951	56.314	C	16.654	1.953	56.349
H	12.711	1.956	54.820	H	12.736	1.957	54.860
H	12.630	1.951	52.154	H	12.605	1.949	52.190
N	15.737	1.949	53.452	N	15.717	1.952	53.436
C	18.514	1.955	57.691	C	18.513	1.955	57.688
C	18.964	1.963	56.297	C	18.968	1.951	56.346
C	17.176	1.951	57.706	C	17.126	1.949	57.703
C	20.247	1.977	55.861	C	20.355	1.952	55.978
C	20.674	1.979	54.485	C	20.725	1.953	54.593
H	19.184	1.956	58.533	H	19.236	1.957	58.512
H	16.539	1.949	58.573	H	16.566	1.949	58.642
N	17.829	1.950	55.543	N	17.811	1.952	55.531
H	17.801	1.963	52.300	H	17.711	1.952	52.445
C	22.099	2.022	52.761	C	22.065	1.955	52.734

C 20.707 1.994 52.297	C 20.722 1.951 52.280
C 21.204 2.613 48.674	C 21.206 2.596 48.588
C 22.146 2.596 47.669	C 22.188 2.581 47.600
C 22.094 1.982 54.094	C 22.079 1.949 54.122
C 31.379 1.903 36.256	C 31.441 1.948 36.313
C 32.762 1.966 36.730	C 32.801 1.953 36.730
C 32.268 1.249 40.330	C 32.313 1.304 40.384
C 31.333 1.321 41.342	C 31.328 1.325 41.378
C 20.316 1.962 50.978	C 20.355 1.952 50.893
C 25.653 2.188 47.291	C 25.709 2.228 47.308
C 26.639 2.229 46.366	C 26.684 2.242 46.374
C 28.372 3.019 44.105	C 28.369 3.032 44.151
C 29.307 2.963 43.119	C 29.317 2.993 43.179
C 24.009 2.166 45.630	C 24.001 2.207 45.585
C 24.954 2.159 44.634	C 24.929 2.161 44.602
C 27.173 1.241 42.979	C 27.140 1.242 42.979
C 28.144 1.243 42.027	C 28.118 1.237 42.028
C 26.265 2.178 45.024	C 26.284 2.180 45.023
C 27.301 2.146 44.010	C 27.279 2.149 44.031
C 22.592 1.249 50.025	C 22.661 1.307 50.041
C 23.590 1.298 49.071	C 23.647 1.324 49.059
C 30.904 2.656 38.971	C 30.862 2.597 38.935
C 29.900 2.643 39.920	C 29.874 2.581 39.914
C 21.379 1.943 49.889	C 21.407 1.952 49.840
C 23.352 1.983 47.899	C 23.410 1.949 47.842
C 34.971 2.006 39.796	C 34.936 1.957 39.805
C 34.526 1.969 38.486	C 34.517 1.952 38.446
C 18.921 1.942 50.510	C 18.970 1.953 50.522
C 32.098 1.948 39.124	C 32.112 1.952 39.135
C 30.170 2.015 41.109	C 30.126 1.964 41.123
C 33.143 1.959 38.035	C 33.165 1.952 38.082
H 20.335 3.197 48.464	H 20.276 3.143 48.399
H 21.986 3.148 46.763	H 22.056 3.079 46.636
H 33.142 0.665 40.523	H 33.243 0.759 40.575
H 31.492 0.831 42.293	H 31.464 0.829 42.340
H 30.165 3.608 43.084	H 30.187 3.625 43.124
H 28.434 3.739 44.902	H 28.406 3.747 44.976
H 27.674 2.275 46.652	H 27.746 2.242 46.627
H 25.844 2.248 48.343	H 25.851 2.260 48.385
H 28.141 0.589 41.177	H 28.157 0.557 41.180
H 26.336 0.571 42.919	H 26.293 0.550 42.954
H 22.965 2.160 45.409	H 22.921 2.227 45.433
H 24.661 2.182 43.599	H 24.627 2.099 43.530
H 22.961 2.063 52.137	H 22.888 1.957 52.011
H 22.960 1.964 54.736	H 23.019 1.949 54.681
H 22.800 0.669 50.898	H 22.848 0.760 50.970

H 24.530 0.795 49.240	H 24.613 0.826 49.189
H 30.719 3.231 38.090	H 30.673 3.145 38.004
H 28.943 3.124 39.770	H 28.906 3.076 39.783
H 34.358 2.064 40.659	H 34.200 1.958 40.612
H 30.528 1.831 36.886	H 30.635 1.946 37.048
N 33.603 1.995 35.612	N 33.615 1.952 35.624
N 19.886 1.968 53.434	N 19.907 1.952 53.436
N 29.184 2.062 42.140	N 29.126 2.152 42.120
N 24.370 2.083 46.907	N 24.419 1.972 46.877
C 36.362 1.968 39.790	Cl 23.426 5.010 46.013
C 36.744 1.942 38.470	Cl 26.663 4.050 40.890
C 39.874 1.954 36.296	C 36.313 1.948 39.805
C 38.484 1.952 36.716	C 36.730 1.953 38.446
C 38.085 1.946 37.994	C 39.805 1.957 36.312
H 40.693 1.957 36.991	C 38.446 1.952 36.730
H 37.016 1.959 40.640	C 38.082 1.952 38.082
N 35.633 1.938 37.696	H 40.612 1.958 37.047
N 37.650 1.950 35.605	H 37.048 1.946 40.612
H 35.659 1.952 36.702	N 35.624 1.952 37.632
H 14.639 1.952 56.630	N 37.632 1.952 35.624
H 38.785 1.952 32.456	H 35.746 1.952 36.528
H 14.583 1.954 50.275	H 14.461 1.952 56.782
H 21.010 1.958 56.623	H 38.889 1.952 32.359
H 32.444 1.961 32.453	H 14.465 1.952 50.085
H 38.827 1.951 38.773	H 21.158 1.952 56.786
Cl 23.469 5.006 45.973	H 32.358 1.952 32.360
Cl 26.706 3.981 40.896	H 38.890 1.952 38.888
C 20.264 -0.967 53.741	C 22.315 8.151 45.411
O 20.368 -0.989 54.871	O 21.440 8.048 46.156
O 20.383 -0.985 52.605	O 23.191 8.253 44.666
C 33.344 -0.998 35.236	C 24.913 6.415 39.204
O 33.150 -0.997 36.360	O 24.037 6.311 39.950
O 33.543 -1.034 34.113	O 25.788 6.517 38.459

Table S4. Cartesian coordinates (Å) of **H2-ICOP** for $\mathbf{O_{CO2}}\cdots\mathbf{N^+}$ (I) pnicogen bonds and $\mathbf{O_{CO2}}\cdots\mathbf{H}$ (II) hydrogen bonds.

I	II
H 35.337 2.240 34.364	H 35.337 2.240 34.364
C 34.640 2.232 31.246	C 34.640 2.232 31.246
C 34.229 2.239 32.576	C 34.229 2.239 32.576
C 31.097 2.161 34.744	C 31.097 2.161 34.744
C 32.495 2.244 34.370	C 32.495 2.244 34.370
C 32.900 2.248 33.085	C 32.900 2.248 33.085
H 30.254 2.156 34.070	H 30.254 2.156 34.070
H 33.999 2.230 30.381	H 33.999 2.230 30.381
C 39.594 2.230 34.770	C 39.594 2.229 34.770
C 38.200 2.225 34.360	C 38.200 2.225 34.360

C 36.033 2.227 31.250	C 36.032 2.227 31.250
C 36.445 2.229 32.578	C 36.445 2.229 32.578
C 37.777 2.228 33.077	C 37.777 2.228 33.077
H 36.678 2.227 30.389	H 36.678 2.227 30.389
H 40.449 2.231 34.113	H 40.449 2.232 34.113
N 35.334 2.233 33.344	N 35.334 2.233 33.344
C 16.728 2.168 49.123	C 16.728 2.168 49.123
C 16.385 2.239 50.438	C 16.385 2.239 50.438
C 18.139 2.101 49.071	C 18.139 2.101 49.071
C 15.038 2.246 50.956	C 15.038 2.246 50.956
C 14.620 2.234 52.223	C 14.620 2.234 52.223
H 16.063 2.178 48.273	H 16.063 2.178 48.273
H 18.699 2.021 48.163	H 18.699 2.021 48.163
N 17.526 2.242 51.172	N 17.526 2.242 51.172
H 17.483 2.221 54.362	H 17.483 2.221 54.362
C 13.248 2.228 53.993	C 13.248 2.228 53.993
C 14.668 2.230 54.365	C 14.668 2.231 54.365
C 13.232 2.230 52.654	C 13.232 2.230 52.654
C 15.106 2.229 55.751	C 15.106 2.229 55.751
C 16.383 2.227 56.155	C 16.383 2.227 56.155
H 12.410 2.229 54.674	H 12.410 2.229 54.674
H 12.382 2.229 51.989	H 12.382 2.229 51.989
N 15.467 2.232 53.352	N 15.467 2.232 53.352
C 18.195 2.227 57.534	C 18.195 2.227 57.534
C 18.647 2.219 56.127	C 18.647 2.219 56.127
C 16.867 2.230 57.545	C 16.867 2.230 57.545
C 19.912 2.202 55.685	C 19.912 2.202 55.685
C 20.320 2.207 54.291	C 20.320 2.208 54.291
H 18.867 2.230 58.376	H 18.867 2.230 58.376
H 16.198 2.232 58.387	H 16.198 2.232 58.387
N 17.508 2.224 55.378	N 17.508 2.224 55.378
H 17.579 2.257 52.186	H 17.579 2.257 52.186
C 21.788 2.360 52.625	C 21.788 2.360 52.625
C 20.403 2.249 52.124	C 20.403 2.249 52.124
C 20.878 2.967 48.620	C 20.878 2.967 48.620
C 21.820 2.968 47.616	C 21.820 2.968 47.616
C 21.740 2.287 53.955	C 21.740 2.288 53.955
C 31.064 2.076 36.081	C 31.064 2.076 36.081
C 32.470 2.185 36.533	C 32.470 2.185 36.533
C 31.959 1.460 40.117	C 31.959 1.460 40.117
C 31.037 1.550 41.138	C 31.037 1.550 41.138
C 20.008 2.201 50.839	C 20.008 2.201 50.839
C 25.302 2.614 47.146	C 25.302 2.614 47.146
C 26.281 2.391 46.254	C 26.281 2.391 46.254
C 28.066 3.342 43.902	C 28.066 3.342 43.902
C 29.010 3.255 42.923	C 29.011 3.255 42.923

C 23.675 2.470 45.511	C 23.675 2.470 45.511
C 24.620 2.490 44.526	C 24.620 2.490 44.526
C 26.863 1.566 42.813	C 26.863 1.566 42.813
C 27.834 1.549 41.846	C 27.834 1.549 41.846
C 25.950 2.466 44.894	C 25.950 2.466 44.894
C 26.959 2.505 43.833	C 26.959 2.505 43.833
C 22.197 1.439 49.884	C 22.197 1.439 49.884
C 23.201 1.518 48.941	C 23.201 1.518 48.941
C 30.686 3.019 38.820	C 30.686 3.019 38.820
C 29.680 3.010 39.766	C 29.680 3.010 39.766
C 21.033 2.202 49.770	C 21.033 2.202 49.770
C 22.998 2.283 47.808	C 22.998 2.283 47.808
C 34.717 2.365 39.707	C 34.717 2.365 39.707
C 34.196 2.261 38.334	C 34.196 2.261 38.334
C 18.607 2.170 50.357	C 18.607 2.170 50.357
C 31.831 2.237 38.961	C 31.831 2.237 38.962
C 29.904 2.298 40.923	C 29.904 2.298 40.923
C 32.890 2.222 37.923	C 32.891 2.222 37.923
H 20.019 3.598 48.482	H 20.019 3.598 48.483
H 21.669 3.586 46.748	H 21.669 3.586 46.748
H 32.801 0.805 40.246	H 32.801 0.805 40.246
H 31.192 1.020 42.065	H 31.192 1.020 42.065
H 29.868 3.899 42.869	H 29.868 3.899 42.869
H 28.157 4.086 44.670	H 28.157 4.086 44.670
H 27.302 2.678 46.573	H 27.302 2.679 46.573
H 25.517 2.495 48.206	H 25.517 2.495 48.206
H 27.809 0.897 40.992	H 27.809 0.897 40.992
H 26.039 0.877 42.731	H 26.039 0.877 42.731
H 22.625 2.396 45.277	H 22.625 2.396 45.277
H 24.323 2.526 43.488	H 24.323 2.526 43.488
H 22.680 2.490 52.048	H 22.680 2.490 52.048
H 22.556 2.307 54.656	H 22.555 2.307 54.656
H 22.351 0.798 50.734	H 22.351 0.798 50.734
H 24.109 0.958 49.103	H 24.109 0.958 49.103
H 30.552 3.644 37.954	H 30.552 3.643 37.954
H 28.745 3.545 39.636	H 28.745 3.545 39.636
H 34.137 2.481 40.594	H 34.137 2.481 40.594
H 30.172 1.958 36.659	H 30.172 1.958 36.659
N 33.280 2.255 35.513	N 33.280 2.255 35.513
N 19.546 2.191 53.257	N 19.546 2.192 53.257
N 28.908 2.337 41.956	N 28.908 2.337 41.956
N 24.027 2.386 46.804	N 24.027 2.386 46.803
C 36.049 2.293 39.675	C 36.049 2.293 39.675
C 36.472 2.218 38.289	C 36.472 2.218 38.289
C 39.593 2.226 36.118	C 39.593 2.226 36.118
C 38.188 2.218 36.504	C 38.188 2.218 36.504

C 37.747 2.211 37.867	C 37.747 2.211 37.867
H 40.443 2.231 36.785	H 40.443 2.231 36.785
H 36.717 2.305 40.520	H 36.718 2.305 40.520
N 35.312 2.207 37.558	N 35.313 2.207 37.558
N 37.387 2.219 35.476	N 37.386 2.219 35.476
H 35.277 2.193 36.543	H 35.277 2.193 36.543
H 14.341 2.230 56.501	H 14.341 2.230 56.501
H 38.533 2.229 32.306	H 38.532 2.229 32.306
H 14.288 2.241 50.184	H 14.288 2.241 50.184
H 20.699 2.216 56.413	H 20.699 2.216 56.413
H 32.127 2.243 32.332	H 32.127 2.243 32.332
H 38.515 2.220 38.624	H 38.515 2.220 38.624
C 29.287 0.306 44.807	C 33.795 0.089 35.098
O 28.858 0.669 45.808	O 34.741 0.690 35.343
O 29.719 -0.051 43.804	O 32.848 -0.516 34.859
C 24.168 -0.935 45.675	C 18.999 0.307 53.387
O 24.360 -1.127 44.561	O 20.017 -0.199 53.533
O 23.980 -0.729 46.788	O 17.986 0.825 53.234
Cl 23.476 5.320 45.789	Cl 23.476 5.320 45.789
Cl 26.454 4.129 40.659	Cl 26.454 4.129 40.659

Table S5. Cartesian coordinates (Å) of **Zn-ICOP** for **N···C_{CO2}** (I) and **Cl^-···C_{CO2}** (II) tetrel bonds.

I	II
Zn 17.819 1.956 53.425	Zn 17.813 1.954 53.436
Zn 35.621 1.946 35.632	Zn 35.623 1.950 35.623
C 34.957 1.951 31.402	C 34.943 1.949 31.433
C 34.495 1.962 32.786	C 34.509 1.951 32.789
C 31.404 1.952 34.926	C 31.413 1.947 34.931
C 32.817 1.997 34.570	C 32.802 1.958 34.541
C 33.218 1.986 33.197	C 33.185 1.954 33.201
H 30.582 1.948 34.233	H 30.609 1.954 34.218
H 34.270 1.948 30.579	H 34.234 1.947 30.620

C 39.862 1.951 34.958	C 39.841 1.950 34.948
C 38.445 1.950 34.581	C 38.452 1.952 34.550
C 36.290 1.952 31.413	C 36.303 1.955 31.441
C 36.740 1.952 32.806	C 36.733 1.953 32.804
C 38.021 1.951 33.210	C 38.058 1.952 33.207
H 36.984 1.955 30.596	H 37.015 1.958 30.629
H 40.675 1.948 34.255	H 40.640 1.947 34.227
N 35.608 1.953 33.568	N 35.608 1.952 33.592
C 17.051 1.937 49.230	C 17.091 1.949 49.199
C 16.672 1.957 50.562	C 16.662 1.955 50.558
C 18.443 1.911 49.199	C 18.447 1.931 49.176
C 15.325 1.955 51.059	C 15.321 1.953 50.986
C 14.897 1.951 52.343	C 14.905 1.952 52.343
H 16.405 1.949 48.371	H 16.409 1.954 48.363
H 19.016 1.878 48.303	H 19.027 1.916 48.272
N 17.810 1.962 51.307	N 17.802 1.956 51.330
C 13.538 1.953 54.130	C 13.538 1.954 54.133
C 14.966 1.952 54.503	C 14.934 1.952 54.535
C 13.501 1.951 52.791	C 13.512 1.951 52.787
C 15.412 1.952 55.879	C 15.343 1.952 55.898
C 16.697 1.951 56.314	C 16.684 1.952 56.332
H 12.711 1.956 54.820	H 12.721 1.957 54.836
H 12.630 1.951 52.154	H 12.623 1.950 52.174
N 15.737 1.949 53.452	N 15.723 1.952 53.431
C 18.514 1.955 57.691	C 18.517 1.954 57.679
C 18.964 1.963 56.297	C 18.958 1.953 56.321
C 17.176 1.951 57.706	C 17.155 1.951 57.696
C 20.247 1.977 55.861	C 20.297 1.951 55.892
C 20.674 1.979 54.485	C 20.711 1.948 54.533
H 19.184 1.956 58.533	H 19.206 1.957 58.512
H 16.539 1.949 58.573	H 16.552 1.949 58.597
N 17.829 1.950 55.543	N 17.824 1.952 55.541
C 22.099 2.022 52.761	C 22.084 1.977 52.764
C 20.707 1.994 52.297	C 20.697 1.955 52.333
C 21.204 2.613 48.674	C 21.212 2.598 48.625
C 22.146 2.596 47.669	C 22.166 2.579 47.631
C 22.094 1.982 54.094	C 22.103 1.956 54.103
C 31.379 1.903 36.256	C 31.407 1.920 36.267
C 32.762 1.966 36.730	C 32.793 1.946 36.697
C 32.268 1.249 40.330	C 32.280 1.276 40.363
C 31.333 1.321 41.342	C 31.328 1.325 41.364
C 20.316 1.962 50.978	C 20.306 1.950 50.947
C 25.653 2.188 47.291	C 25.674 2.198 47.292
C 26.639 2.229 46.366	C 26.659 2.233 46.363
C 28.372 3.019 44.105	C 28.367 3.025 44.126
C 29.307 2.963 43.119	C 29.305 2.973 43.139

C 24.009 2.166 45.630	C 24.011 2.177 45.613
C 24.954 2.159 44.634	C 24.952 2.158 44.615
C 27.173 1.241 42.979	C 27.157 1.242 42.982
C 28.144 1.243 42.027	C 28.131 1.247 42.033
C 26.265 2.178 45.024	C 26.261 2.180 45.024
C 27.301 2.146 44.010	C 27.296 2.148 44.013
C 22.592 1.249 50.025	C 22.625 1.280 50.025
C 23.590 1.298 49.071	C 23.619 1.310 49.064
C 30.904 2.656 38.971	C 30.885 2.623 38.958
C 29.900 2.643 39.920	C 29.888 2.615 39.913
C 21.379 1.943 49.889	C 21.390 1.946 49.860
C 23.352 1.983 47.899	C 23.374 1.964 47.875
C 34.971 2.006 39.796	C 34.974 1.981 39.803
C 34.526 1.969 38.486	C 34.518 1.958 38.445
C 18.921 1.942 50.510	C 18.943 1.948 50.533
C 32.098 1.948 39.124	C 32.106 1.948 39.136
C 30.170 2.015 41.109	C 30.154 2.001 41.113
C 33.143 1.959 38.035	C 33.171 1.951 38.058
H 20.335 3.197 48.464	H 20.322 3.165 48.423
H 21.986 3.148 46.763	H 22.022 3.107 46.702
H 33.142 0.665 40.523	H 33.177 0.718 40.556
H 31.492 0.831 42.293	H 31.478 0.833 42.320
H 30.165 3.608 43.084	H 30.174 3.616 43.105
H 28.434 3.739 44.902	H 28.419 3.737 44.939
H 27.674 2.275 46.652	H 27.708 2.261 46.635
H 25.844 2.248 48.343	H 25.846 2.254 48.356
H 28.141 0.589 41.177	H 28.149 0.580 41.184
H 26.336 0.571 42.919	H 26.318 0.564 42.939
H 22.965 2.160 45.409	H 22.956 2.191 45.422
H 24.661 2.182 43.599	H 24.651 2.141 43.574
H 22.961 2.063 52.137	H 22.907 2.005 52.090
H 22.960 1.964 54.736	H 22.997 1.954 54.707
H 22.800 0.669 50.898	H 22.829 0.727 50.921
H 24.530 0.795 49.240	H 24.572 0.815 49.215
H 30.719 3.231 38.090	H 30.692 3.179 38.062
H 28.943 3.124 39.770	H 28.924 3.092 39.774
H 34.358 2.064 40.659	H 34.292 2.011 40.621
H 30.528 1.831 36.886	H 30.600 1.892 36.956
N 33.603 1.995 35.612	N 33.613 1.960 35.625
N 19.886 1.968 53.434	N 19.901 1.945 53.435
N 29.184 2.062 42.140	N 29.158 2.087 42.140
N 24.370 2.083 46.907	N 24.394 2.053 46.890
C 36.362 1.968 39.790	C 36.326 1.957 39.804
C 36.744 1.942 38.470	C 36.750 1.947 38.450
C 39.874 1.954 36.296	C 39.844 1.955 36.296
C 38.484 1.952 36.716	C 38.457 1.953 36.697

C 38.085 1.946 37.994	C 38.069 1.950 38.041
H 40.693 1.957 36.991	H 40.642 1.958 37.018
H 37.016 1.959 40.640	H 37.026 1.951 40.623
N 35.633 1.938 37.696	N 35.637 1.947 37.653
N 37.650 1.950 35.605	N 37.638 1.952 35.626
H 14.639 1.952 56.630	H 14.560 1.952 56.683
H 38.785 1.952 32.456	H 38.824 1.952 32.428
H 14.583 1.954 50.275	H 14.553 1.953 50.188
H 21.010 1.958 56.623	H 21.069 1.952 56.685
H 32.444 1.961 32.453	H 32.416 1.953 32.426
H 38.827 1.951 38.773	H 38.833 1.952 38.820
Cl 23.469 5.006 45.973	Cl 23.447 5.006 45.997
Cl 26.706 3.981 40.896	Cl 26.681 4.018 40.895
C 20.264 -0.967 53.741	C 22.318 8.143 45.410
O 20.368 -0.989 54.871	O 21.448 8.052 46.147
O 20.383 -0.985 52.605	O 23.180 8.262 44.674
C 33.344 -0.998 35.236	C 24.912 6.408 39.204
O 33.150 -0.997 36.360	O 24.046 6.315 39.939
O 33.543 -1.034 34.113	O 25.779 6.521 38.467

Table S6. Cartesian coordinates (Å) of **Zn-ICOP** for $\mathbf{O_{CO2}\cdots N^{+}}$ pnicogen (I) and $\mathbf{O_{CO2}\cdots Zn}$ spodium bonds (II).

I	II
Zn 17.517 2.233 53.275	Zn 17.809 1.938 53.433
Zn 35.323 2.220 35.451	Zn 35.639 1.981 35.617
C 34.640 2.232 31.246	C 34.971 1.965 31.380
C 34.229 2.239 32.576	C 34.559 1.976 32.768
C 31.097 2.161 34.744	C 31.417 1.893 34.907
C 32.495 2.244 34.370	C 32.812 1.961 34.519
C 32.900 2.248 33.085	C 33.224 1.968 33.199
H 30.254 2.156 34.070	H 30.595 1.859 34.214
H 33.999 2.230 30.381	H 34.290 1.981 30.547
C 39.594 2.230 34.770	C 39.870 1.913 34.928
C 38.200 2.225 34.360	C 38.498 1.958 34.522
C 36.033 2.227 31.250	C 36.319 1.970 31.379
C 36.445 2.229 32.578	C 36.750 1.982 32.760
C 37.777 2.228 33.077	C 38.059 1.982 33.176
H 36.678 2.227 30.389	H 36.991 1.982 30.539
H 40.449 2.231 34.113	H 40.711 1.953 34.257
N 35.334 2.233 33.344	N 35.637 1.998 33.565
C 16.728 2.168 49.123	C 17.077 1.891 49.223
C 16.385 2.239 50.438	C 16.694 2.009 50.610
C 18.139 2.101 49.071	C 18.418 1.838 49.181
C 15.038 2.246 50.956	C 15.377 2.031 51.041
C 14.620 2.234 52.223	C 14.940 2.038 52.382

H 16.063 2.178 48.273	H 16.382 1.865 48.403
H 18.699 2.021 48.163	H 19.004 1.723 48.292
N 17.526 2.242 51.172	N 17.824 2.027 51.375
C 13.248 2.228 53.993	C 13.562 1.971 54.152
C 14.668 2.230 54.365	C 14.940 2.012 54.569
C 13.232 2.230 52.654	C 13.557 1.978 52.798
C 15.106 2.229 55.751	C 15.374 1.989 55.893
C 16.383 2.227 56.155	C 16.713 1.963 56.314
H 12.410 2.229 54.674	H 12.723 1.928 54.824
H 12.382 2.229 51.989	H 12.702 1.940 52.144
N 15.467 2.232 53.352	N 15.741 2.047 53.464
C 18.195 2.227 57.534	C 18.505 1.978 57.670
C 18.647 2.219 56.127	C 18.906 1.947 56.295
C 16.867 2.230 57.545	C 17.146 1.982 57.684
C 19.912 2.202 55.685	C 20.241 1.956 55.846
C 20.320 2.207 54.291	C 20.660 1.956 54.526
H 18.867 2.230 58.376	H 19.184 1.970 58.505
H 16.198 2.232 58.387	H 16.502 1.974 58.546
N 17.508 2.224 55.378	N 17.808 1.844 55.507
C 21.788 2.360 52.625	C 22.063 2.062 52.782
C 20.403 2.249 52.124	C 20.680 1.960 52.325
C 20.878 2.967 48.620	C 21.182 2.709 48.747
C 21.820 2.968 47.616	C 22.132 2.715 47.745
C 21.740 2.287 53.955	C 22.045 2.019 54.126
C 31.064 2.076 36.081	C 31.390 1.850 36.244
C 32.470 2.185 36.533	C 32.776 1.982 36.715
C 31.959 1.460 40.117	C 32.249 1.168 40.265
C 31.037 1.550 41.138	C 31.309 1.232 41.277
C 20.008 2.201 50.839	C 20.262 1.942 50.966
C 25.302 2.614 47.146	C 25.615 2.193 47.334
C 26.281 2.391 46.254	C 26.614 2.238 46.417
C 28.066 3.342 43.902	C 28.420 2.985 44.115
C 29.010 3.255 42.923	C 29.340 2.926 43.113
C 23.675 2.470 45.511	C 23.986 2.171 45.661
C 24.620 2.490 44.526	C 24.949 2.199 44.673
C 26.863 1.566 42.813	C 27.141 1.293 42.951
C 27.834 1.549 41.846	C 28.121 1.268 41.988
C 25.950 2.466 44.894	C 26.265 2.200 45.057
C 26.959 2.505 43.833	C 27.305 2.155 44.023
C 22.197 1.439 49.884	C 22.486 1.157 50.015
C 23.201 1.518 48.941	C 23.490 1.219 49.066
C 30.686 3.019 38.820	C 30.973 2.744 38.979
C 29.680 3.010 39.766	C 29.962 2.728 39.923
C 21.033 2.202 49.770	C 21.319 1.927 49.898
C 22.998 2.283 47.808	C 23.295 1.993 47.934
C 34.717 2.365 39.707	C 35.004 2.056 39.849

C 34.196 2.261 38.334	C 34.549 2.027 38.475
C 18.607 2.170 50.357	C 18.905 1.944 50.559
C 31.831 2.237 38.961	C 32.121 1.954 39.111
C 29.904 2.298 40.923	C 30.180 1.999 41.072
C 32.890 2.222 37.923	C 33.177 1.976 38.048
H 20.019 3.598 48.482	H 20.329 3.353 48.625
H 21.669 3.586 46.748	H 22.012 3.350 46.882
H 32.801 0.805 40.246	H 33.100 0.524 40.396
H 31.192 1.020 42.065	H 31.446 0.694 42.206
H 29.868 3.899 42.869	H 30.215 3.549 43.084
H 28.157 4.086 44.670	H 28.581 3.636 44.965
H 27.302 2.678 46.573	H 27.643 2.286 46.740
H 25.517 2.495 48.206	H 25.789 2.244 48.395
H 27.809 0.897 40.992	H 28.099 0.634 41.109
H 26.039 0.877 42.731	H 26.231 0.729 42.819
H 22.625 2.396 45.277	H 22.941 2.127 45.430
H 24.323 2.526 43.488	H 24.652 2.261 43.638
H 22.680 2.490 52.048	H 22.927 2.178 52.162
H 22.556 2.307 54.656	H 22.888 2.041 54.793
H 22.351 0.798 50.734	H 22.629 0.510 50.864
H 24.109 0.958 49.103	H 24.405 0.662 49.210
H 30.552 3.644 37.954	H 30.858 3.390 38.127
H 28.745 3.545 39.636	H 29.039 3.280 39.803
H 34.137 2.481 40.594	H 34.389 2.087 40.721
H 30.172 1.958 36.659	H 30.525 1.713 36.858
N 33.280 2.255 35.513	N 33.593 1.982 35.624
N 19.546 2.191 53.257	N 19.872 1.936 53.409
N 28.908 2.337 41.956	N 29.190 2.045 42.109
N 24.027 2.386 46.804	N 24.329 2.073 46.943
C 36.049 2.293 39.675	C 36.355 2.165 39.820
C 36.472 2.218 38.289	C 36.745 2.075 38.446
C 39.593 2.226 36.118	C 39.867 1.855 36.288
C 38.188 2.218 36.504	C 38.494 1.904 36.692
C 37.747 2.211 37.867	C 38.056 1.960 38.008
H 40.443 2.231 36.785	H 40.705 1.862 36.962
H 36.717 2.305 40.520	H 37.040 2.119 40.649
N 35.312 2.207 37.558	N 35.619 2.050 37.667
N 37.387 2.219 35.476	N 37.696 1.938 35.599
H 14.341 2.230 56.501	H 14.613 1.968 56.671
H 38.533 2.229 32.306	H 38.827 1.986 32.411
H 14.288 2.241 50.184	H 14.612 1.982 50.271
H 20.699 2.216 56.413	H 21.018 1.962 56.605
H 32.127 2.243 32.332	H 32.456 1.979 32.436
H 38.515 2.220 38.624	H 38.808 1.994 38.786
Cl 23.476 5.320 45.789	Cl 23.557 5.015 45.868
Cl 26.454 4.129 40.659	Cl 26.759 3.815 40.834

C 29.287 0.306 44.807	C 17.123 -1.653 53.071
O 28.858 0.669 45.808	O 17.364 -0.540 53.142
O 29.719 -0.051 43.804	O 16.889 -2.766 53.003
C 24.168 -0.935 45.675	C 35.680 -1.692 36.020
O 24.360 -1.127 44.561	O 35.708 -2.812 36.228
O 23.980 -0.729 46.788	O 35.651 -0.572 35.807

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