Table listing the atomic coordinates of the IISERP-COF31.

Space group: P1; Crystal system: Triclinic.

Lattice parameters: a = 18.2534; b = 31.6061; c = 32.1046 Å; α = 118.47°, β = 90.87°, γ = 89.17°

Atom	x	y	z
C1	0.48424	0.4913	0.32431
C2	0.51578	0.47506	0.29602
N3	0.44927	0.54852	0.30577
C4	0.41724	0.53924	0.35617
C5	0.23697	0.56495	0.31135
C6	0.18728	0.53388	0.30118
C7	0.40327	0.92726	0.22301
C8	0.40964	0.96843	0.18466
C9	0.44071	0.01572	0.21311
N10	0.41953	0.88796	0.32771
C11	0.38361	0.8463	0.30525
C12	0.21982	0.6178	0.382
C13	0.25457	0.60773	0.35154
C14	0.01734	0.44763	0.23552
C15	0.97684	0.41312	0.19822
C16	0.93102	0.39839	0.2255
N17	0.06044	0.50488	0.33433
C18	0.10115	0.50912	0.31032
C19	0.15265	0.54357	0.33092
C20	0.1694	0.58615	0.37185
N21	0.30697	0.64038	0.35916
C22	0.32764	0.69282	0.34992
C23	0.33797	0.61862	0.36331
C24	0.37805	0.63332	0.3172
C25	0.40424	0.60841	0.31572
C26	0.39145	0.56796	0.36033
C27	0.35194	0.55375	0.40709
C28	0.32557	0.57841	0.40828
C29	0.37336	0.72741	0.37813
C30	0.39265	0.77793	0.36724
C31	0.36644	0.795	0.32782
C32	0.32137	0.76048	0.30006
C33	0.30229	0.71081	0.311
C34	0.53948	0.49504	0.23017
C35	0.4787	0.52735	0.28573
N36	0.52476	0.43909	0.33112
C37	0.55973	0.43274	0.30582
C38	0.71834	0.37146	0.40712

C39	0.77223	0.39749	0.40588
C40	0.46618	0.02248	0.27818
C41	0.45686	0.97989	0.30785
C42	0.4274	0.93138	0.28918
N43	0.4962	0.07211	0.30237
C44	0.53102	0.09383	0.3493
C45	0.71744	0.31391	0.32258
C46	0.69139	0.32965	0.36517
C47	0.92362	0.41707	0.28913
C48	0.96802	0.45493	0.32917
C49	0.01492	0.46916	0.30057
N50	0.87315	0.39697	0.30873
C51	0.85118	0.40871	0.35714
C52	0.79676	0.38096	0.36206
C53	0.76854	0.33888	0.32095
N54	0.63842	0.30555	0.36205
C55	0.60969	0.25249	0.36213
C56	0.61614	0.3356	0.34999
C57	0.57187	0.32588	0.38214
C58	0.55231	0.35686	0.37079
C59	0.57682	0.39834	0.32699
C60	0.62036	0.40731	0.29517
C61	0.63973	0.37704	0.30658
C62	0.62553	0.22436	0.39936
C63	0.59949	0.17332	0.39663
C64	0.55667	0.14827	0.35621
C65	0.54057	0.17624	0.31927
C66	0.56642	0.22727	0.32239
C67	0.5039	0.54528	0.22102
C68	0.53384	0.52952	0.19263
C69	0.55921	0.54903	0.12353
O70	0.55408	0.58061	0.08931
O71	0.58635	0.53435	0.09741
C72	0.98244	0.39279	0.12974
C73	0.3843	0.96283	0.11553
O74	0.35777	0.92281	0.09074
O75	0.38981	0.99817	0.08252
O76	0.94555	0.36164	0.09531
O77	0.02417	0.40666	0.10427
C78	0.81756	0.15801	0.82438
C79	0.8491	0.14177	0.79609
N80	0.78259	0.21524	0.80583
C81	0.75056	0.20595	0.85624
C82	0.57029	0.23167	0.81142

C83	0.5206	0.2006	0.80124
C84	0.73659	0.59397	0.72307
C85	0.74296	0.63515	0.68473
C86	0.77403	0.6818	0.71342
N87	0.75285	0.55468	0.82778
C88	0.71693	0.51302	0.80532
C89	0.55314	0.28451	0.88207
C90	0.58789	0.27445	0.85161
C91	0.35066	0.11435	0.73559
C92	0.3101	0.08014	0.69826
C93	0.26428	0.0654	0.72554
N94	0.39376	0.1716	0.8344
C95	0.43447	0.17584	0.81038
C96	0.48597	0.21029	0.83099
C97	0.50272	0.25286	0.87191
N98	0.64029	0.3071	0.85923
C99	0.66096	0.35953	0.84999
C100	0.67129	0.28534	0.86338
C101	0.71136	0.30003	0.81727
C102	0.73756	0.27513	0.81578
C103	0.72477	0.23467	0.86039
C104	0.68526	0.22047	0.90715
C105	0.65889	0.24512	0.90834
C106	0.70668	0.39412	0.8782
C107	0.72597	0.44464	0.86731
C108	0.69976	0.46171	0.82789
C109	0.65469	0.42719	0.80012
C110	0.63561	0.37752	0.81107
C111	0.87279	0.16176	0.73023
C112	0.81202	0.19407	0.78579
N113	0.85808	0.10581	0.83118
C114	0.89305	0.09945	0.80588
C115	0.0516	0.03847	0.90715
C116	0.10549	0.06451	0.90592
C117	0.7995	0.68855	0.77849
C118	0.79018	0.6466	0.80791
C119	0.76072	0.5981	0.78924
N120	0.82952	0.73818	0.80268
C121	0.86434	0.7599	0.84961
C122	0.0507	0.98028	0.82286
C123	0.02465	0.99602	0.86545
C124	0.25688	0.08409	0.78916
C125	0.30128	0.12194	0.82921
C126	0.34824	0.13588	0.80063

N127	0.20641	0.06399	0.80876
C128	0.18444	0.07572	0.85718
C129	0.13002	0.04797	0.86209
C130	0.1018	0.00589	0.82098
N131	0.97173	0.97162	0.86235
C132	0.94301	0.91856	0.86244
C133	0.94946	0.00231	0.85006
C134	0.90519	0.99195	0.88244
C135	0.88563	0.02358	0.87085
C136	0.91014	0.06505	0.82706
C137	0.95368	0.07402	0.79524
C138	0.97305	0.04375	0.80664
C139	0.95885	0.89043	0.89967
C140	0.93281	0.83939	0.89693
C141	0.88999	0.81434	0.85652
C142	0.87389	0.84231	0.81958
C143	0.89974	0.89335	0.82269
C144	0.83722	0.212	0.72108
C145	0.86716	0.19624	0.6927
C146	0.89253	0.21574	0.6236
O147	0.8874	0.24732	0.58937
O148	0.91967	0.20107	0.59748
C149	0.31571	0.0598	0.62978
C150	0.71762	0.62954	0.6156
O151	0.69109	0.58952	0.59081
O152	0.72313	0.66489	0.58258
O153	0.27881	0.02865	0.59534
O154	0.35748	0.07338	0.60434
H155	0.46364	0.47574	0.37713
H156	0.40861	0.5097	0.39696
H157	0.26462	0.55625	0.28709
H158	0.17413	0.49981	0.26812
H159	0.37787	0.89074	0.19816
H160	0.44422	0.04751	0.18181
H161	0.35768	0.84415	0.2594
H162	0.23253	0.65177	0.41511
H163	0.05431	0.45847	0.21063
H164	0.89721	0.36968	0.19548
H165	0.10011	0.48367	0.26651
H166	0.14171	0.59464	0.39657
H167	0.38978	0.66544	0.2806
H168	0.43672	0.62053	0.278
H169	0.34072	0.52214	0.44463
H170	0.29342	0.56504	0.44696

H171	0.39692	0.71635	0.41099
H172	0.43002	0.8047	0.39111
H173	0.29767	0.77116	0.26677
H174	0.26466	0.68563	0.28625
H175	0.56457	0.4833	0.20504
H176	0.58346	0.45572	0.25939
H177	0.69834	0.38514	0.4421
H178	0.79387	0.431	0.44053
H179	0.54296	0.07294	0.38579
H180	0.69688	0.28006	0.28835
H181	0.96462	0.47214	0.38146
H182	0.87344	0.44008	0.39567
H183	0.78858	0.32536	0.2857
H184	0.55116	0.29316	0.41758
H185	0.51641	0.34857	0.39704
H186	0.64114	0.43966	0.25903
H187	0.67579	0.38696	0.27931
H188	0.66066	0.24198	0.43385
H189	0.61417	0.15278	0.42824
H190	0.50545	0.15851	0.28479
H191	0.5505	0.24689	0.29121
H192	0.50026	0.57368	0.18981
H193	0.59552	0.53807	0.05256
H194	0.05642	0.43867	0.12765
H195	0.79696	0.14245	0.87719
H196	0.74193	0.17642	0.89703
H197	0.59794	0.22296	0.78715
H198	0.50745	0.16653	0.76818
H199	0.71119	0.55745	0.69823
H200	0.77795	0.71386	0.68247
H201	0.691	0.51086	0.75946
H202	0.56585	0.31849	0.91518
H203	0.38765	0.12498	0.71093
H204	0.23047	0.03669	0.69552
H205	0.43343	0.15039	0.76657
H206	0.47503	0.26135	0.89663
H207	0.7231	0.33215	0.78066
H208	0.77004	0.28724	0.77806
H209	0.67404	0.18885	0.94469
H210	0.62674	0.23175	0.94702
H211	0.73024	0.38306	0.91105
H212	0.76334	0.47141	0.89118
H213	0.63098	0.43788	0.76684
H214	0.59798	0.35235	0.78631

H215	0.89789	0.15002	0.7051
H216	0.91678	0.12243	0.75945
H217	0.03159	0.05241	0.94156
H218	0.12714	0.09802	0.94056
H219	0.87628	0.73901	0.88609
H220	0.03016	0.94617	0.78921
H221	0.298	0.1394	0.88129
H222	0.2067	0.10709	0.89571
H223	0.12216	-0.00705	0.78531
H224	0.88482	0.95899	0.91751
H225	0.84979	0.0155	0.89709
H226	0.97446	0.10638	0.75909
H227	1.00911	0.05368	0.77938
H228	0.99398	0.90805	0.93415
H229	0.94748	0.81885	0.92855
H230	0.83877	0.82458	0.7851
H231	0.88382	0.91296	0.79152
H232	0.83357	0.24039	0.68988
H233	0.92215	0.20199	0.55228
H234	0.36062	0.06579	0.54972
H235	0.33774	0.91035	0.03941
H236	0.68374	0.58055	0.54158