

Electronic Supplementary Information

Theoretical design and characterization of new terpolymer donors based on PTB7Ir for high-efficiency triplet-material-based organic photovoltaics

Shuangbao Li,^{*a} Yang Chen,^a Zhen Li,^a Jianpo Zhang,^a Jie Chen,^a Yun Geng^b and Zhongmin Su^{*b, c, d}

a.School of Chemical and Pharmaceutical Engineering, Jilin Institute of Chemical Technology, Jilin, 132022, P. R. China.

b.Institute of Functional Material Chemistry, Faculty of Chemistry, Northeast Normal University, Changchun, 130024, P. R. China.

c.School of Chemistry and Environmental Engineering, Changchun University of Science and Technology, Changchun, 130022, P. R. China.

d.Jilin Provincial Science and Technology Innovation Center of Optical Materials and Chemistry, Changchun, 130022, P. R. China

*Corresponding author: Dr. Shuangbao Li; Prof. Zhongmin Su

School of Chemical and Pharmaceutical Engineering,

Jilin Institute of Chemical Technology,

Jilin, 132022, P. R. China

E-mail Address: lishb997@nenu.edu.cn

zmsu@nenu.edu.cn

CONTENTS

Section S1. A comparative analysis of intermolecular charge transfer properties	(Page S1)
Fig. S1. Optimized interface geometries of Configuration-1 (a), and Configuration-2 (b), respectively.	(Page S1)
Fig. S2. CDD maps of $^1\text{CT}_1$ of Configuration-1 (a), $^1\text{CT}_1$ of Configuration-2 (b), $^3\text{CT}_1$ of Configuration-1 (c) and $^3\text{CT}_1$ of Configuration-2 (d), where the violet and turquoise colors refer to the increase and decrease in electron density, respectively.	(Page S1)
Table S1. Calculated energy level values of E_{Coul} , E_{CT1} and $-\Delta G_{\text{CRT}}$ for Configuration-1 and Configuration-2 , respectively.	(Page S2)
Section S2. List of Figures	
Fig. S3. Schematic illustration of twist angles between donor and acceptor moieties of 2 and 6-11 . The green dotted boxes represent the highlights.	(Page S2)
Fig. S4. Hole-electron pairs of NTOs in S_1 and T_1 states of 1-3 and 5-11 .	(Page S3)
Section S3. List of Tables	
Table S2. The HOMO energy levels (E_{HOMO}) of PTB7Ir and 1-11 molecules calculated at the B3LYP/6-31G(d) (LANL2DZ for Ir atom) level.	(Page S4)
Table S3. Calculated vertical excitation energies (E_g), oscillator strengths (f) and excitation characters of S_1 states for PTB7Ir and 1-11 at the B3LYP/6-31G(d) (LANL2DZ for Ir atom) level in o-dichlorobenzene solvent.	(Page S4)
Section S4. Coordinates of molecules	
Table S4. The coordinate of PTB7Ir.	(Page S4)
Table S5. The coordinate of 1 .	(Page S7)
Table S6. The coordinate of 2 .	(Page S10)
Table S7. The coordinate of 3 .	(Page S13)
Table S8. The coordinate of 4 .	(Page S15)
Table S9. The coordinate of 5 .	(Page S18)
Table S10. The coordinate of 6 .	(Page S21)
Table S11. The coordinate of 7 .	(Page S23)
Table S12. The coordinate of 8 .	(Page S26)
Table S13. The coordinate of 9 .	(Page S29)
Table S14. The coordinate of 10 .	(Page S31)
Table S15. The coordinate of 11 .	(Page S34)
Table S16. The coordinate of PTB7Ir/PC ₇₁ BM.	(Page S37)
Table S17. The coordinate of PTB7Ir/PC ₇₁ BM calculated by PBE0-D2 functional.	(Page S40)
Table S18. The coordinate of 1 /PC ₇₁ BM.	(Page S44)
Table S19. The coordinate of 2 /PC ₇₁ BM.	(Page S48)
Table S20. The coordinate of 3 /PC ₇₁ BM.	(Page S52)
Table S21. The coordinate of 4 /PC ₇₁ BM.	(Page S56)
Table S22. The coordinate of 5 /PC ₇₁ BM.	(Page S60)
Table S23. The coordinate of 6 /PC ₇₁ BM.	(Page S64)
Table S24. The coordinate of 7 /PC ₇₁ BM.	(Page S67)
Table S25. The coordinate of 8 /PC ₇₁ BM.	(Page S71)
Table S26. The coordinate of 9 /PC ₇₁ BM.	(Page S75)
Table S27. The coordinate of 10 /PC ₇₁ BM.	(Page S78)
Table S28. The coordinate of 11 /PC ₇₁ BM.	(Page S82)

Section S1. A comparative analysis of intermolecular charge transfer properties

To save the computational cost, we demonstrated a comparative analysis of intermolecular charge transfer properties of PTB7Ir/PC₇₁BM based on the ground-state geometries calculated by PBE0 (**Configuration-1**) and PBE0-D2 (**Configuration-2**) functionals, respectively. Note that PBE0-D2 is a functional considering dispersion correction, which presents the high computational cost. The optimized interface geometries are shown in Fig. S1, and coordinates of molecules are listed in Table S15 and Table S16 in Section S4, respectively. Seen from Fig. S1, **Configuration-1** is almost similar to **Configuration-2**.

The CDD maps of ¹CT₁ and ³CT₁ states of **Configuration-1** and **Configuration-2** are shown in Fig. S2, respectively. The results indicate that the two interface configurations exhibit similar intermolecular charge transfer behaviors. The calculated energy level values of CT₁, E_{Coul} and $-\Delta G_{\text{CRT}}$ for **Configuration-1** and **Configuration-2** are summarized in Table S1, respectively. According to Table S1, the difference between E_{Coul} values of **Configuration-1** and **Configuration-2** is only 0.02 eV, indicating that Coulomb interaction between donor and acceptor would be slightly overestimated without dispersion correction. Additionally, the differences of E_{CT1} and $-\Delta G_{\text{CRT}}$ values between **Configuration-1** and **Configuration-2** are both only 0.06 eV, which is a value of acceptable error. Therefore, to save the computational cost, ground-state geometries of D/PC₇₁BM complexes can be performed by PBE0 functional instead of PBE0-D2 functional with dispersion correction.

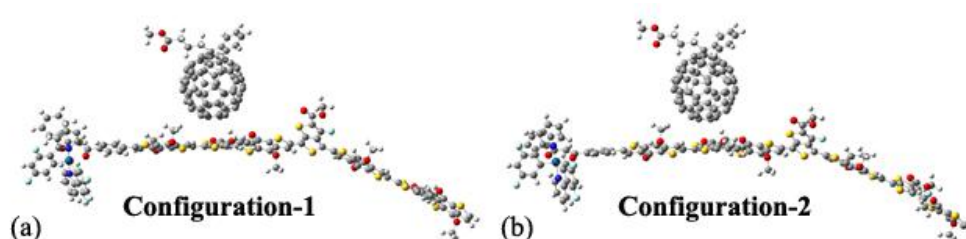


Fig. S1. Optimized interface geometries of **Configuration-1** (a), and **Configuration-2** (b), respectively.

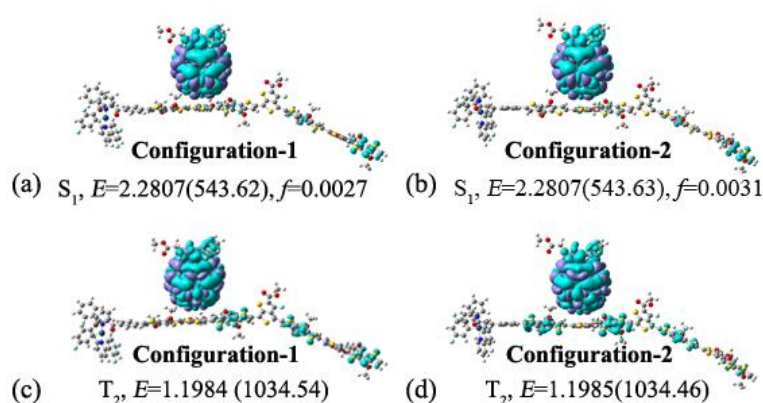


Fig. S2. CDD maps of ¹CT₁ of **Configuration-1** (a), ¹CT₁ of **Configuration-2** (b), ³CT₁ of **Configuration-1** (c) and ³CT₁ of **Configuration-2** (d), where the violet and turquoise colors refer to the increase and decrease in electron density, respectively.

Table S1. Calculated energy level values of E_{Coul} , E_{CT1} and $-\Delta G_{\text{CRT}}$ for **Configuration-1** and **Configuration-2**, respectively.

	PTB7Ir	
	Configuration-1	Configuration-2
$E_{\text{Coul}}/\text{eV}$	-0.19	-0.17
E_{CT1}/eV	1.22	1.16
$-\Delta G_{\text{CRT}}/\text{eV}$	-0.06	-0.12

Section S2. List of Figures

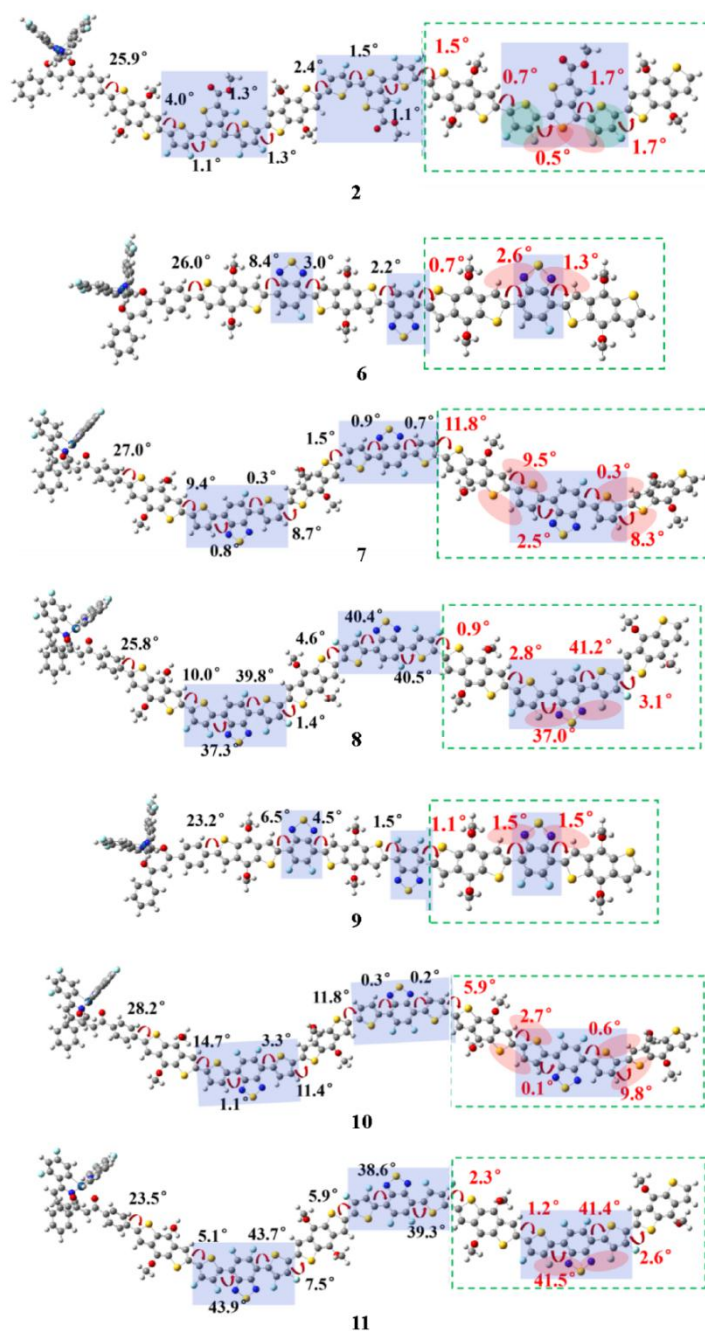


Fig. S3. Schematic illustration of twist angles between donor and acceptor moieties of **2** and **6-11**. The green dotted boxes represent the highlights.

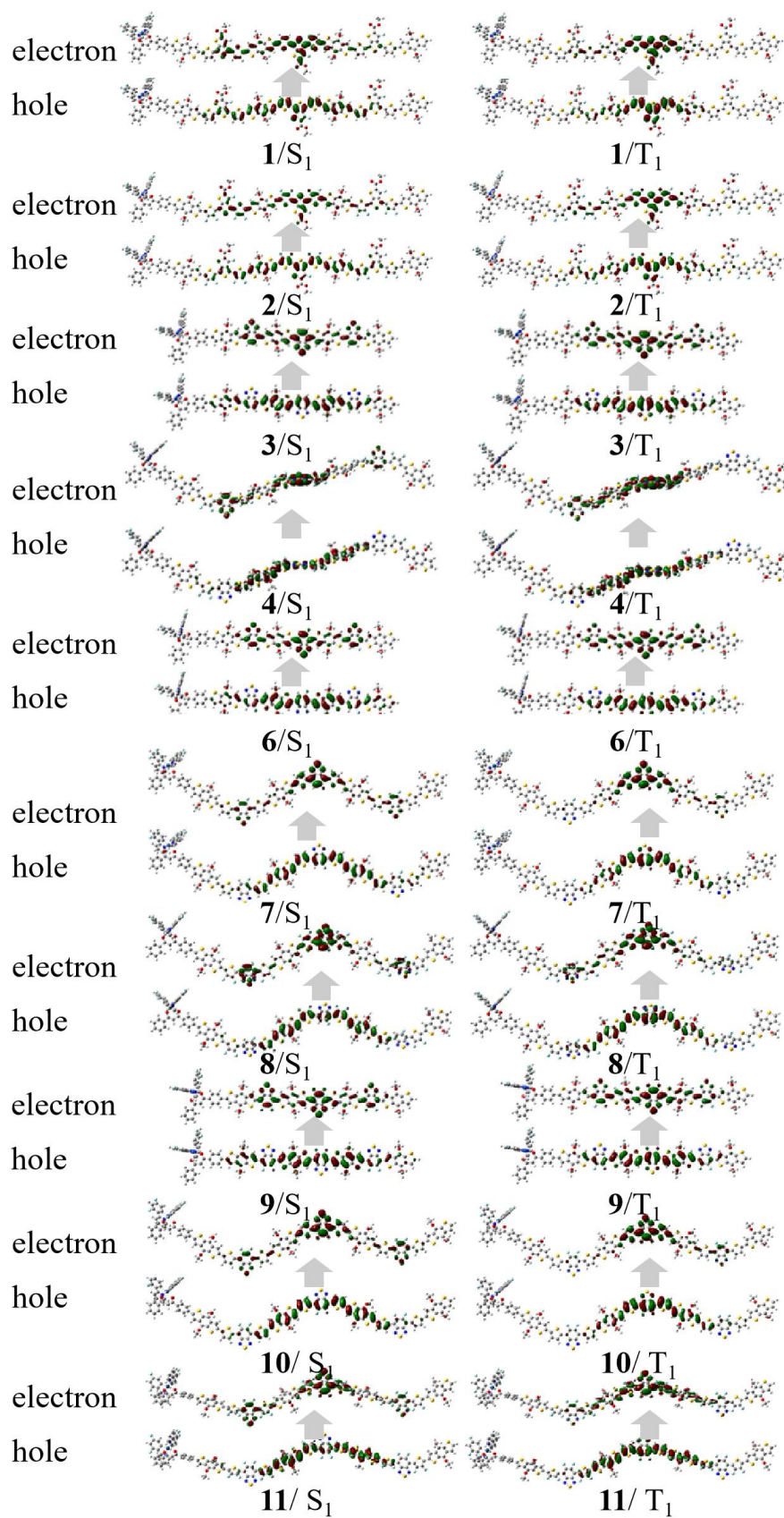


Fig. S4. Hole-electron pairs of NTOs in S_1 and T_1 states of **1-3** and **5-11**.

Section S3. List of Tables

Table S2. The HOMO energy levels (E_{HOMO}) of PTB7Ir and **1-11** molecules calculated at the B3LYP/6-31G(d) (LANL2DZ for Ir atom) level.

	PTB7Ir	1	2	3	4	5	6	7	8	9	10	11
$E_{\text{HOMO}}/\text{eV}$	-4.98	-4.85	-4.95	-5.11	-4.94	-5.18	-5.14	-4.97	-5.21	-5.17	-5.00	-5.25

Table S3. Calculated vertical excitation energies (E_g), oscillator strengths (f) and excitation characters of S_1 states for PTB7Ir and **1-11** at the B3LYP/6-31G(d) (LANL2DZ for Ir atom) level in o-dichlorobenzene solvent.

Molecule	$E_g/\text{eV}(\text{nm})$	f	Composition ^a
PTB7Ir	1.87(665)	3.035	H→L(93%)
1	1.76(706)	5.463	H→L(85%)
2	1.70(727)	5.627	H→L(86%)
3	1.77(702)	3.237	H→L(92%)
4	1.69 (734)	4.050	H→L(83%), H-1→L+1(11%)
5	1.96(634)	3.055	H→L(79%), H-1→L+1(13%)
6	1.75(708)	3.058	H→L(89%)
7	1.70 (731)	3.965	H→L(82%)
8	1.92(646)	3.133	H→L(78%), H-1→L+1(13%)
9	1.77(702)	2.888	H→L(91%)
10	1.72 (719)	3.984	H→L(83%), H-1→L+1(11%)
11	1.95(634)	3.112	H→L(77%), H-1→L+1(13%)

^aH denotes HOMO and L denotes LUMO.

Section S4. Coordinates of molecules

Table S4. The coordinate of PTB7Ir (213 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	-2.5489018019	-1.035875715	-0.3316402376	C	-7.2781978073	-7.4537451879	-1.3638635094
C	-2.6276032364	1.4323028579	0.1689184701	C	-6.1643021479	-8.3305446658	-1.4648961928
C	-3.2118892128	0.1718410922	-0.0537874291	C	-7.6055626164	-10.2119495984	-1.7738872562
C	-3.3511298952	-2.2862207927	-0.4951996391	C	-8.7183545344	-9.3332915744	-1.682050597
C	-2.7519602058	-3.381213984	-1.1297060468	C	-8.5781595974	-7.9658734525	-1.4908398793
C	-3.4464055218	-4.5650639445	-1.319939465	C	-6.8703970563	-6.1033169928	-1.1396731611
C	-4.7666368039	-4.7073814731	-0.8675566986	H	-7.5735381005	-5.2835606454	-1.0478420645
C	-5.3555881687	-3.6207108182	-0.2023636798	C	-8.0111176333	-11.5637148021	-1.9732520381
C	-4.6633924574	-2.4328490817	-0.0259874408	S	-10.2244559571	-10.1962971348	-1.8182869958
H	-4.2903533189	0.1295892171	0.0009100662	H	-7.307040887	-12.3824154517	-2.0750731427
H	-1.7273507223	-3.2823480817	-1.4728014966	S	-4.6639630127	-7.4709821564	-1.269224452
H	-2.9648798633	-5.3871822593	-1.8435232879	C	-6.3044383369	-9.6953170662	-1.6761667203
H	-6.3567319935	-3.7221540269	0.2065530918	C	-5.5151581045	-5.945065681	-1.0748295547
H	-5.1434769864	-1.6279677692	0.5218453336	C	-9.3707001889	-11.7200954802	-2.0310100659
C	-3.520064993	2.608444848	0.4070860464	O	-5.2172467225	-10.5192225992	-1.7506649848
C	-4.8472605351	2.6579852387	-0.0361481301	O	-9.6702596581	-7.151072881	-1.3904205001

C	-2.9940085024	3.7174095643	1.0811295855	C	-4.6919273783	-10.6567789895	-3.0654779838
C	-5.6324455119	3.7802073311	0.2051372023	H	-3.8359373521	-11.3296923673	-2.9856076122
H	-5.2645115324	1.8308508246	-0.6026383058	H	-5.4371539098	-11.0896570082	-3.7447409321
C	-3.7821995355	4.8337564431	1.3323203374	H	-4.3597574291	-9.6899764245	-3.4633470672
H	-1.9561718706	3.6865284482	1.3970994119	C	-10.1018459826	-6.6167234828	-2.6364503339
C	-5.1055734332	4.8679304214	0.8973164722	H	-10.9757799167	-5.9993018839	-2.4198645729
H	-6.6574339513	3.8075287219	-0.1547853582	H	-9.3186359588	-5.9983193551	-3.0928995964
H	-3.3617691488	5.6824541205	1.86518195	H	-10.3840306247	-7.4146460059	-3.3341925277
H	-5.7215302839	5.7425293754	1.0889492928	C	-10.1071449679	-12.9423536292	-2.2208122057
O	-1.2978357229	-1.1889611607	-0.5066031476	C	-15.3850274807	-37.6627228282	-8.8555551645
O	-1.3839157082	1.6902540235	0.2321798564	C	-14.2971880068	-36.1335175438	-7.4514031918
Ir	0.2189629445	0.3159862995	-0.2218625753	C	-14.818986915	-37.4601887779	-7.5567172961
C	1.553383842	1.7768603518	-0.0808639852	C	-14.6787227293	-38.2018248369	-6.3866418211
C	2.3149289999	2.1199593375	1.0396830216	S	-13.8815401763	-37.2304138398	-5.1933772988
C	1.6891117751	2.5581952092	-1.2635873651	S	-14.4854608325	-35.2154422356	-8.9218585497
C	3.1666631156	3.2111680785	0.9861860123	F	-15.9520566025	-38.8064128812	-9.2073056699
H	2.2563877662	1.5509937531	1.9615807128	C	-15.28213409	-36.582995729	-9.6815101164
C	2.5636621599	3.649359009	-1.255162975	O	-16.3227601061	-37.4840415776	-11.5688976976
C	3.3119610567	3.9998367552	-0.1482677594	C	-16.7624457207	-37.3474226398	-12.9186491812
H	3.9829914133	4.8496356589	-0.1707513366	H	-17.2218480278	-38.3023896532	-13.1731808852
C	0.8913459999	2.1203066924	-2.3995271997	H	-17.4887391608	-36.534994718	-13.0061811556
C	0.8498429164	2.6896606696	-3.6788093538	H	-15.9167810752	-37.1386262568	-13.5792895981
C	0.0511004085	2.1259958743	-4.6606196242	C	-15.7214195441	-36.399085118	-11.0681051596
H	1.4472260215	3.5656241842	-3.8877018959	O	-15.5487934153	-35.3668316632	-11.6814147824
C	-0.6313267299	0.4712153302	-3.0881023045	C	-15.6118097651	-41.3867950475	-4.6924526069
C	-0.7042033723	0.9925665686	-4.3678227031	C	-15.5301176651	-41.9994177044	-5.9714717306
H	0.0210296321	2.5684451703	-5.6523255155	C	-16.0515984308	-44.1367205173	-5.0384647252
H	-1.1858065163	-0.4104474117	-2.785708939	C	-16.1382144	-43.5229183817	-3.7594260461
H	-1.3378752239	0.5188299078	-5.1095288815	C	-15.9373794001	-42.1617550616	-3.5693306053
C	1.2681925273	-1.4172377477	1.861602949	C	-15.3390064585	-39.989614122	-4.7599890945
C	-0.2967340559	0.1093850844	2.7176149247	H	-15.3554544916	-39.3402116096	-3.8914921561
C	1.4133408698	-1.9800395304	3.1361924038	C	-16.2866417491	-45.5502878403	-4.9644473328
C	-0.18657491	-0.4078656518	3.9962752906	S	-16.5023691994	-44.6923798862	-2.519253994
H	-0.9496753648	0.9414243073	2.4780385431	H	-16.2442794094	-46.2081993612	-5.8245349961
C	0.6849533209	-1.4752977993	4.2014171427	S	-15.1194712181	-40.8485934531	-7.2094694856
H	2.0977390268	-2.804615574	3.2758573741	C	-15.7574250879	-43.3555455694	-6.1643741936
H	-0.7711382215	0.0180711777	4.8043316006	C	-15.0638999009	-39.546598888	-6.0281497169
H	0.799356347	-1.9124390182	5.1893123586	C	-16.5405997407	-45.9682395005	-3.6998165744
C	1.968259775	-1.796774707	0.642916334	H	-16.7413218798	-46.9804938421	-3.3717673627
C	2.9205527947	-2.8151444469	0.5350639022	O	-15.656310175	-43.9142200517	-7.4076567874
C	1.6418234923	-1.0349981916	-0.5150350779	O	-16.0142528084	-41.6001731157	-2.3267422829
C	3.56748265	-3.1120563399	-0.648816009	C	-16.8896287299	-43.9603478653	-8.1142922485
C	2.299710427	-1.3235465702	-1.7137472879	H	-16.6720233064	-44.4128939552	-9.0837701604
C	3.2358643251	-2.3439241413	-1.757758204	H	-17.6281428606	-44.5723229633	-7.5811241278

H	4.3023870895	-3.905730743	-0.7029805102	H	-17.2978105911	-42.95332353	-8.265366361
H	2.0968834417	-0.7659340217	-2.6219965837	C	-17.315407673	-41.1358621655	-1.9872970612
N	0.4029640643	-0.3797011389	1.6850195543	H	-17.2406889098	-40.7208494656	-0.9803028786
N	0.1361398404	1.0173502713	-2.1350739324	H	-17.6497773048	-40.3551581038	-2.6821577678
F	3.8546632509	-2.611152023	-2.9149954927	H	-18.0426277782	-41.9571009435	-1.9907794509
F	3.2461071143	-3.5580216055	1.6099176483	C	-7.2749648719	-28.0451075404	-1.3070786625
F	2.708504154	4.4133119711	-2.3547577524	C	-8.2564283375	-25.9394742436	-1.6188901658
F	3.886118286	3.5305418545	2.0696260406	C	-8.386122098	-27.3406997222	-1.8696925263
C	-13.1662936088	-14.6396864617	-3.0737328328	C	-9.2655079377	-25.168493676	-2.1648322748
C	-11.419315349	-13.1523063503	-2.5979164617	C	-9.5103638614	-27.6641889715	-2.6251975144
C	-11.7893660934	-14.5291475348	-2.7007318851	S	-10.3998601502	-26.215655707	-2.9632108171
C	-10.7502138592	-15.4038582659	-2.3927605397	S	-6.8192380457	-25.5473679364	-0.7131823228
S	-9.3350123216	-14.482850134	-1.9994343934	F	-7.1475469383	-29.3592335835	-1.4109748127
S	-12.7309372986	-12.0697626857	-2.984138504	C	-6.3785103798	-27.2454265732	-0.6626408204
F	-13.7649658085	-15.8119121457	-3.2210980521	O	-4.8744290968	-28.8921320182	0.0328819996
C	-13.7897793424	-13.4418628266	-3.2622375638	C	-3.6755952864	-29.2602675527	0.7120902908
O	-15.9098117422	-14.2376243978	-3.8354448098	H	-3.6069622001	-30.3436211719	0.6150442841
C	-17.2595490073	-13.9857340459	-4.2205350606	H	-2.809444198	-28.7765505894	0.2527660209
H	-17.7204608857	-14.9677658079	-4.3254407482	H	-3.7258641284	-28.9701600103	1.7649311603
H	-17.7744586656	-13.398145228	-3.4558041411	C	-5.1376962708	-27.5806171908	0.0432299909
H	-17.2938628008	-13.4410472073	-5.167825316	O	-4.437627165	-26.7452486439	0.575350873
C	-15.1696793102	-13.1381530708	-3.6533552573	C	-11.2545545053	-30.4056446735	-4.4449371339
O	-15.5801834748	-12.0053108163	-3.7935498662	C	-10.7497714079	-31.2834750767	-3.4476172751
C	-9.853501016	-18.9744113617	-1.8249969984	C	-11.8638245578	-33.1450196599	-4.4502959887
C	-10.840455908	-19.2954858226	-2.7960655494	C	-12.363119197	-32.2666882356	-5.4506487745
C	-10.3338193008	-21.6244658577	-2.6160565842	C	-12.0634843988	-30.9123784986	-5.4747888588
C	-9.3524025578	-21.3020408619	-1.6391880647	C	-10.8255292121	-29.0651037998	-4.2326780465
C	-9.1072445746	-20.0014695962	-1.2246485358	H	-11.0980620306	-28.2454280614	-4.8883421211
C	-9.7763797913	-17.57141285	-1.5971157977	C	-12.3149867639	-34.4825712255	-4.644873082
H	-9.0859089273	-17.1237372873	-0.8906047316	S	-13.3871152202	-33.1062372193	-6.5811848551
C	-10.3738996994	-23.0222782014	-2.8864366456	H	-12.0380223423	-35.3008151001	-3.9891007777
S	-8.5262112349	-22.7256351421	-1.0720891137	S	-9.7718529971	-30.4371383454	-2.2846111349
H	-11.0248296522	-23.4597121965	-3.6356504232	C	-11.0270000337	-32.6433319315	-3.4411191351
S	-11.6379003702	-17.8705137752	-3.394760557	C	-10.0262285442	-28.9143274457	-3.1273586906
C	-11.1021024373	-20.5997122624	-3.1910487415	C	-13.1232405856	-34.6294174436	-5.7414066822
C	-10.6616746439	-16.8436694193	-2.3519533757	O	-10.5371282547	-33.4604078028	-2.4623994783
C	-9.4774177976	-23.7463068107	-2.1433823118	O	-12.5689376836	-30.0878707895	-6.4381190753
O	-12.0462934235	-20.872868042	-4.1395179238	C	-9.2796711485	-34.0455640645	-2.7818597219
O	-8.1450673631	-19.7244571496	-0.2969692247	H	-9.0017996431	-34.6625030778	-1.9251706288
C	-13.3320517002	-21.1600307554	-3.6017121607	H	-9.3529720028	-34.6737626032	-3.6784847588
H	-13.9863411117	-21.3499464053	-4.4547413213	H	-8.5140329489	-33.2765081074	-2.9414477162
H	-13.3020706365	-22.0476577527	-2.9573243094	C	-11.7663019892	-30.0141275148	-7.6117203826
H	-13.7194899924	-20.3099747608	-3.0268544019	H	-12.2851447372	-29.3402962631	-8.2959955729
C	-8.6253248674	-19.7068499746	1.0427933834	H	-10.7713486349	-29.6120561489	-7.3831111665

H	-7.7639258646	-19.4814357698	1.6742067516	H	-11.6591057509	-30.9990720362	-8.0820227603
H	-9.3920826482	-18.9336144321	1.1770699198	C	-13.74768539	-35.8347998629	-6.2197435388
H	-9.0411623148	-20.6811419308	1.3272825513				

Table S5. The coordinate of **1** (255 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	-3.1996265369	-0.3229511621	0.5416669811	C	-6.9732002654	-13.5151638058	-3.2337129619
C	-4.0158150995	1.9329019173	1.3150277255	C	-8.2213074179	-14.1044719156	-3.2424102602
C	-4.1973273582	0.6029789806	0.8931275021	S	-5.7652023433	-14.6525146452	-3.7491764482
C	-3.601658422	-1.7108269214	0.1617805433	C	-8.2069675982	-15.4487317622	-3.65796862
C	-2.6990620748	-2.4889695522	-0.5731182017	H	-9.1228211536	-13.5758121713	-2.9508539859
C	-3.0198850081	-3.7798881682	-0.9615018389	C	-6.9432875677	-15.9125472299	-3.9729655578
C	-4.2519950979	-4.353067544	-0.6128659562	H	-9.0979613113	-16.0634258803	-3.7326243887
C	-5.1424023326	-3.5839375107	0.1527866073	C	-6.589683208	-19.6805118319	-5.1071488707
C	-4.8259093539	-2.2870919374	0.5256054017	C	-7.0655151588	-21.0114210196	-5.3742721506
H	-5.2189111188	0.2546510704	0.8367184043	C	-8.3820166409	-21.3903031324	-5.5752624407
H	-1.7384898309	-2.0580404892	-0.8357993299	S	-6.0310391013	-22.409640207	-5.3950906261
H	-2.311212261	-4.3482218517	-1.5587727335	C	-8.5497477099	-22.7749244986	-5.7492940417
H	-6.079419263	-4.0215689747	0.484614413	H	-9.1967182957	-20.6753964739	-5.6234932958
H	-5.5272949633	-1.7367908018	1.1451845525	C	-7.3643970811	-23.4807511215	-5.6863766808
C	-5.2220682206	2.7709261856	1.5967777809	H	-9.5078769526	-23.2452593954	-5.9436558987
C	-6.4785303161	2.50786931	1.0378551588	C	-7.1544008621	-24.8975983295	-5.8435827507
C	-5.0789951472	3.8820960495	2.4369731946	C	-6.5568483305	-17.2193025282	-4.4223402999
C	-7.5667491169	3.3241519438	1.326894121	C	-5.3411003304	-17.6922824962	-4.878528573
H	-6.6057261258	1.6807488725	0.3458604138	C	-9.3153045886	-39.1618414472	-7.7066637908
C	-6.1688620331	4.6909484057	2.7344928938	C	-7.9361391666	-38.7869620258	-7.7557518251
H	-4.0970545583	4.0993338274	2.8450014172	S	-5.4361100174	-38.267703661	-7.8224257313
C	-7.4177037783	4.4131469714	2.1823806301	S	-9.3380868147	-36.5873911627	-7.3030989342
H	-8.532889777	3.1125951286	0.876633352	F	-9.7116357653	-40.4158811772	-7.8676943849
H	-6.0431220877	5.5441045899	3.3958091347	C	-10.169478444	-38.1222439756	-7.4848882164
H	-8.2697430284	5.0479420578	2.4106859888	O	-12.1836073915	-39.3034208147	-7.5326460481
O	-1.9495330243	-0.0981184511	0.4662928649	C	-13.6060929591	-39.3216290568	-7.4315932731
O	-2.9053636072	2.5144738269	1.5299303579	H	-13.8948506619	-40.3625445435	-7.5760864784
Ir	-0.950366222	1.716542522	1.0735415867	H	-13.9262040941	-38.9660823404	-6.4486155016
C	-0.102214332	3.4537515776	1.5187116806	H	-14.0541995392	-38.6868510977	-8.2006649445
C	0.4603619215	3.8306470844	2.741192625	C	-11.6309388983	-38.095242418	-7.3765886299
C	-0.1224683221	4.4016704501	0.4561921572	O	-12.2565565404	-37.0770219157	-7.1679703154
C	0.9671312419	5.1098994967	2.9018066061	C	-7.6614001867	-46.4503716111	-10.0263633782
H	0.5118428027	3.1429454732	3.5785074395	C	-6.3454467539	-46.9709333564	-9.8999292152
C	0.4030175167	5.6781461469	0.6798131931	C	-7.0700514143	-49.1308357225	-10.621663346
C	0.9509864816	6.0604227756	1.8888008246	C	-8.3842470249	-48.6077042409	-10.7570470796
H	1.3524281928	7.0558446369	2.0333646381	C	-8.6956999708	-47.285389608	-10.4782232196

C	-0.6925541172	3.9275309533	-0.7963426786	C	-7.7296407422	-45.0805776787	-9.6366666937
C	-0.8163135334	4.6376649854	-1.9974323561	H	-8.6555296607	-44.5156022756	-9.623593591
C	-1.3626831078	4.0214463484	-3.111612657	C	-7.0143451595	-50.5170957311	-10.9516153741
H	-0.4793684706	5.6634664996	-2.0428743782	S	-9.5062174405	-49.831984931	-11.2817346982
C	-1.6434113149	2.0400287796	-1.8189599125	H	-6.1029802539	-51.1023308035	-10.8911193861
C	-1.7843161043	2.6962329976	-3.0291024001	S	-5.2346135519	-45.7612350192	-9.3211463703
H	-1.4566006872	4.5736784831	-4.042408326	C	-6.0296717796	-48.2881662009	-10.1992553097
H	-1.944070322	1.0079589141	-1.6760993993	C	-8.2237357654	-51.0363177599	-11.3282834847
H	-2.2136782547	2.1773769532	-3.8791271268	O	-4.755759939	-48.7559317493	-10.0453356958
C	0.4263309929	0.0588757479	3.0241345091	O	-9.9758369282	-46.824125551	-10.6019883754
C	-1.5604505102	0.9525224169	3.9001526445	C	-3.9820124203	-48.7189273133	-11.2387192713
C	0.6496377291	-0.6199646562	4.2290140546	H	-2.9994691128	-49.1183919211	-10.9802682313
C	-1.3839807413	0.3066407893	5.1111239668	H	-4.4339268515	-49.3378335783	-12.0237806984
H	-2.4086968105	1.5973645203	3.6987897038	H	-3.8737982894	-47.6914170346	-11.6076712717
C	-0.2565471052	-0.4961297539	5.2700191142	C	-10.2461178286	-46.2182412137	-11.860260231
H	1.5324303266	-1.2341514115	4.3351718687	H	-11.2905075182	-45.9013806165	-11.8310680907
H	-2.1140182698	0.4326569612	5.9031087626	H	-9.6027452753	-45.3450972354	-12.0262631472
H	-0.0813538996	-1.0228961834	6.2038030388	H	-10.1033487312	-46.9317161938	-12.6812807626
C	1.2777264926	0.0685030916	1.8434404488	C	-4.4883539069	-33.8368665336	-6.9940951054
C	2.4861063388	-0.621698327	1.706149712	S	-7.0195483025	-34.2246973779	-7.1755901007
C	0.8160998141	0.8692264036	0.7601929162	C	-4.6495982319	-35.2192991532	-7.1968404169
C	3.2599617911	-0.5551819265	0.5637936726	H	-3.5226905579	-33.3571408188	-6.8732985865
C	1.5993219612	0.9494582519	-0.3944556721	C	-5.9718368153	-35.6065099824	-7.3137879411
C	2.7889190628	0.2433982911	-0.4706500766	H	-3.8216345448	-35.9188410774	-7.2457387591
H	4.1928084706	-1.0997730288	0.4853907515	C	-6.71455605	-39.4399020967	-7.9117597302
H	1.2991149428	1.5537406774	-1.2440146684	C	-6.3599720605	-40.8178389694	-8.122561721
N	-0.6885806745	0.8303236555	2.890418768	C	-5.1345150311	-41.4023084265	-7.8503942554
N	-1.1187198119	2.6345244507	-0.738942037	S	-7.4266357651	-41.9797476003	-8.8561830968
F	3.5254952108	0.3259207492	-1.586072561	C	-5.0617252105	-42.7567091492	-8.2182196045
F	2.9458609815	-1.393383603	2.7092488565	H	-4.3235258073	-40.8661010848	-7.3687777806
F	0.3916797186	6.599554649	-0.302304391	C	-6.2309482017	-43.2343377399	-8.776956477
F	1.4980452956	5.457615454	4.0810785592	H	-4.1881306172	-43.378681841	-8.0541094103
C	-4.0604973605	-19.4418858743	-5.7624523792	C	-6.5243836481	-44.567295641	-9.2387378344
C	-5.3474916568	-19.0679706498	-5.2634402005	C	-6.5002478309	-36.9237178802	-7.5226989395
S	-7.7052303821	-18.5264866243	-4.4434588474	C	-7.8042914197	-37.3812405616	-7.5377005179
S	-3.7921181441	-16.9304353631	-5.120378008	C	-5.6800379237	-33.1414138966	-6.9488986386
F	-3.8010726845	-20.6662228302	-6.1976776719	C	-5.4039292942	-58.6479017809	-12.7673923619
C	-3.1403289936	-18.43559137	-5.7448198257	C	-6.7502449355	-58.1665736763	-12.7429424635
O	-1.318768325	-19.6056956568	-6.6209711113	S	-9.1973711917	-57.4365279961	-12.7799023268
C	0.0448811023	-19.6336562801	-7.0377192398	S	-5.1648902011	-56.1060878134	-12.2427196576
H	0.2217058667	-20.6507458948	-7.3870489356	F	-5.1138076262	-59.9174797763	-13.0113068917
H	0.2153498837	-18.9145712405	-7.8432894495	C	-4.4641646469	-57.6919740637	-12.5170357318
H	0.7072086032	-19.3924007226	-6.2020545997	O	-2.5550256206	-59.0281476209	-12.6662375382
C	-1.7341624706	-18.4213036408	-6.1581997233	C	-1.1365077976	-59.1650633141	-12.6101954223

O	-1.0360615503	-17.4320503636	-6.0820056959	H	-0.9376336038	-60.2176385479	-12.8109779824
C	-6.1271925416	-26.9813749676	-6.0927143531	H	-0.6591357926	-58.5325126512	-13.3632746036
C	-7.4969682016	-27.3584432134	-6.1147059267	H	-0.7617645307	-58.8835591314	-11.6224973895
C	-6.9187005225	-29.6560721958	-6.4274726838	C	-3.0031316315	-57.7868970561	-12.44726493
C	-5.5487951345	-29.2800030814	-6.3960781365	O	-2.2917710071	-56.8321460522	-12.2146403343
C	-5.1362167056	-27.9673576699	-6.2226053795	C	-7.8435884358	-66.0769164934	-13.2668862612
C	-5.9673628393	-25.5724715902	-5.9428760449	C	-9.1867751277	-66.378636548	-13.6181802423
H	-4.9987851932	-25.0841349004	-5.942878797	C	-8.733919666	-68.7244017224	-13.570332219
C	-7.0791059175	-31.0585495726	-6.6305223541	C	-7.3924364581	-68.4240098916	-13.2134157071
S	-4.5050983656	-30.6563141046	-6.6186242734	C	-6.9349847857	-67.1220776775	-13.0490067419
H	-8.0495939636	-31.5376739296	-6.7036582768	C	-7.6167204696	-64.6689213777	-13.1992148208
S	-8.5412427366	-25.9760305327	-5.9386352026	H	-6.6447600973	-64.2357341739	-12.9884764656
C	-7.9093285072	-28.6740696458	-6.2680871573	C	-8.9454415622	-70.1384910426	-13.6913804629
C	-5.8924604673	-31.7319191832	-6.7429955338	S	-6.442814964	-69.8746365214	-13.0384412073
O	-9.2370994804	-28.99225719	-6.302068339	H	-9.8929381211	-70.5788741188	-13.9793121533
O	-3.808840469	-27.6435192271	-6.2171481585	S	-10.1290370029	-64.9305072512	-13.8391354491
C	-9.7610284521	-29.4023353669	-5.0444508275	C	-9.6487384392	-67.6788202448	-13.762169413
H	-10.8167024805	-29.626031638	-5.209583989	C	-7.8234341296	-70.8548851346	-13.4325791037
H	-9.2498362161	-30.3002101265	-4.6754949953	O	-10.9464478059	-67.9231519329	-14.1163980607
H	-9.66827002	-28.6030262071	-4.2987824917	O	-5.6322773163	-66.8713785922	-12.7227616138
C	-3.2377640797	-27.5915492932	-4.9154612212	C	-11.8031261356	-68.1711446138	-13.009276676
H	-2.1865031747	-27.3299282358	-5.0510980015	H	-12.7984926063	-68.345487834	-13.4228959634
H	-3.7281419708	-26.8291057057	-4.2973203888	H	-11.479604454	-69.0564423108	-12.4474172512
H	-3.310500709	-28.563922133	-4.4127670491	H	-11.8351092407	-67.3081678169	-12.3324956105
C	-5.856473558	-7.6035891671	-1.5904644544	C	-5.409766847	-66.7268499427	-11.3256007419
C	-4.5360351051	-8.1016530955	-1.7517751895	H	-4.3408994186	-66.5418698671	-11.2017563502
C	-5.3644747906	-10.2577419514	-2.3659903296	H	-5.9776587304	-65.880332418	-10.9193782845
C	-6.6854966203	-9.7564154317	-2.2149809659	H	-5.6876714891	-67.6396694286	-10.7842565063
C	-6.949968536	-8.4462510495	-1.8444000704	C	-9.7351874515	-52.9027726217	-12.1631958278
C	-5.8586372688	-6.237908196	-1.1726629143	S	-7.3230175514	-53.6328731435	-11.6731487141
H	-6.7693007102	-5.6743758718	-1.0049423121	C	-9.6800511974	-54.2737591013	-12.4735697142
C	-5.3587653913	-11.6353943567	-2.7364190805	H	-10.6299969977	-52.2988648239	-12.2721343367
S	-7.8745179278	-10.9874536464	-2.541517067	C	-8.4327457684	-54.8330662797	-12.2677657898
H	-4.4467131106	-12.2086127341	-2.8640782547	H	-10.5252845936	-54.8382148244	-12.853252865
S	-3.3497047133	-6.885319778	-1.3778502667	C	-8.0192044398	-58.6988177446	-12.9635610855
C	-4.2713389468	-9.4076106894	-2.1416211251	C	-8.4848164445	-60.0222426003	-13.2823325145
C	-4.6073193574	-5.7097698013	-1.0228682553	C	-9.6874776647	-60.3476976134	-13.8856941714
O	-2.9874689071	-9.8572573323	-2.2645508589	S	-7.6202094107	-61.4691233164	-12.8526014925
O	-8.2350648411	-8.003336747	-1.6957432622	C	-9.9011807159	-61.7320372458	-14.00608408
C	-2.4729821707	-9.7684297545	-3.5877760208	H	-10.3784502439	-59.5979859604	-14.2567884444
H	-1.4507799482	-10.1494556999	-3.5464803965	C	-8.8644841347	-62.4899155211	-13.4991927274
H	-3.0629573343	-10.3773947867	-4.28420519	H	-10.7744742978	-62.1680338901	-14.4795451414
H	-2.462113712	-8.7288747364	-3.9380857934	C	-8.7313983526	-63.9254521711	-13.4746071489
C	-8.7681118952	-7.3994598719	-2.8674433889	C	-8.0205503978	-56.1920485408	-12.4734337739

H	-9.7886665039	-7.0984620025	-2.6220411921	C	-6.7628528568	-56.7642785419	-12.4702568856
H	-8.1852190244	-6.5163424225	-3.1582411459	C	-8.5339602296	-52.3873190593	-11.7194586171
H	-8.7883629226	-8.1084387519	-3.7044901268	H	-7.7114063425	-71.931473446	-13.4632607491
C	-6.6117273409	-12.1676369457	-2.874250516				

Table S6. The coordinate of **2** (255 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	-3.2126532331	-0.1548476844	0.1723882799	C	-7.0863972999	-13.4851236842	-2.9220317955
C	-4.000126709	2.125475351	0.9026663478	C	-8.3288819722	-14.0615862866	-3.0368093229
C	-4.1980722094	0.7875626905	0.5139672114	S	-5.8652885362	-14.7007407645	-3.1760792778
C	-3.629907956	-1.5512973955	-0.1570135312	C	-8.3013164239	-15.4398099208	-3.320335511
C	-2.7442460057	-2.3599222603	-0.8795054572	C	-7.0358292472	-15.9680186319	-3.4334352412
C	-3.0768582264	-3.6632819469	-1.212842878	C	-6.6699811368	-19.817134414	-4.220822602
C	-4.304102225	-4.2173328133	-0.8193969187	C	-7.1233214828	-21.1516126455	-4.4922621371
C	-5.1784813062	-3.4156785691	-0.0689980388	C	-8.4319532966	-21.5696695982	-4.6238385054
C	-4.8501318635	-2.1072814546	0.2491114203	S	-6.0764947722	-22.5349653092	-4.706228396
H	-5.2232070269	0.4466568803	0.480295432	C	-8.5882961336	-22.941776274	-4.8834850303
H	-1.786833569	-1.9434662129	-1.1750148126	C	-7.4033736059	-23.6320692076	-4.9603792425
H	-2.381301726	-4.2573970405	-1.8003969578	C	-7.18244477	-25.0317496714	-5.2027959813
H	-6.1108986063	-3.8366065822	0.295820546	C	-6.6545903495	-17.3201820255	-3.7087219866
H	-5.537685648	-1.5310199181	0.8604406955	C	-5.3930512353	-17.8760518985	-3.8144026687
C	-5.19596888	2.9804686206	1.1766754249	C	-9.0661293873	-39.0500842447	-8.3063890804
C	-6.458362729	2.7185685385	0.6307763633	C	-7.6841095437	-38.7216033122	-8.1396246568
C	-5.0368338491	4.1059180188	1.9946207983	S	-5.1767417524	-38.258948109	-7.8545115769
C	-7.5370344048	3.5503960198	0.911108332	S	-9.0863191814	-36.5074150239	-7.7573252789
H	-6.5973014612	1.879587964	-0.0445252418	F	-9.4760551748	-40.2771646938	-8.5992439018
C	-6.1172769539	4.9302853303	2.2838382302	C	-9.9199936714	-38.000223499	-8.1382246995
H	-4.0502246862	4.3216945041	2.3920582213	O	-11.9393180693	-39.1118355342	-8.5174222608
C	-7.3722296252	4.6537609942	1.745020264	C	-13.3633603501	-39.0892234747	-8.6040907313
H	-8.5080192796	3.3395832924	0.4710571518	H	-13.6563433841	-40.1106805699	-8.845694182
H	-5.9794331626	5.7945115903	2.9281428653	H	-13.800947722	-38.7778612582	-7.651977966
H	-8.2168422283	5.3006715664	1.9668044881	H	-13.6894215469	-38.3990185128	-9.3865952159
O	-1.962506197	0.0586911338	0.0695749924	C	-11.3824065712	-37.9331105463	-8.2211393125
O	-2.8822921701	2.700821467	1.0940306907	O	-12.0025320392	-36.9071181982	-8.0365165441
Ir	-0.9396727392	1.8738062884	0.6359461667	C	-7.6324828805	-46.459417098	-10.0192506513
C	-0.0698044651	3.6094469346	1.0444588203	C	-6.3265081577	-47.0150063462	-9.9460991201
C	0.5078869457	4.0004572255	2.2553656199	C	-7.1620157184	-49.1788322425	-10.5202249848
C	-0.089776983	4.5396513286	-0.0334948964	C	-8.4673181677	-48.6221107841	-10.5984223497
C	1.0299699751	5.2765348037	2.3899600155	C	-8.7193828346	-47.278111298	-10.3654201712
H	0.5598201347	3.3261890836	3.1034806846	C	-7.6338624849	-45.0707879655	-9.7043332656
C	0.4514474414	5.813857278	0.1639507021	H	-8.5382850305	-44.472076318	-9.6844561574
C	1.0146820429	6.2101719128	1.3613411125	C	-7.1680635602	-50.5782901265	-10.7859094778
H	1.4280857496	7.2034427725	1.4855318095	S	-9.6590222375	-49.8281377401	-10.9933023962

C	-0.6760356526	4.0507307024	-1.2727222751	H	-6.2722499686	-51.1890947298	-10.748572263
C	-0.8042275308	4.74231043	-2.4841049235	S	-5.1430461606	-45.8213068331	-9.4943543914
C	-1.3669666481	4.1133627652	-3.5828902574	C	-6.0711881058	-48.3547044955	-10.2008690424
H	-0.4581266214	5.763984243	-2.5496457862	C	-8.4157332677	-51.0729350016	-11.0611093217
C	-1.655034637	2.156256821	-2.2553135746	O	-4.8080017156	-48.8633305898	-10.1021673514
C	-1.8007847066	2.7939786399	-3.4747920832	O	-9.9869843501	-46.7738403405	-10.4318347877
H	-1.4643141427	4.6512647807	-4.5216935695	C	-4.0863946323	-48.8551790613	-11.3288079316
H	-1.9649327397	1.1298742245	-2.092418276	H	-3.1054232609	-49.2812988551	-11.1104906162
H	-2.2432644983	2.265708748	-4.3121958916	H	-4.5908257401	-49.4656186473	-12.0882341076
C	0.4353864515	0.2333554164	2.6023568629	H	-3.9644415015	-47.8336499634	-11.7095008923
C	-1.534425099	1.1626935722	3.4795424884	C	-10.3399690221	-46.2808544471	-11.7191394086
C	0.6609697416	-0.4286264195	3.8161317525	H	-11.3675790923	-45.9211242036	-11.6392471168
C	-1.3552436262	0.5343452252	4.6993124236	H	-9.6835227566	-45.4542095617	-12.0188903236
H	-2.3771015447	1.813583287	3.2743579981	H	-10.2887304858	-47.0741605249	-12.4749037365
C	-0.2353927233	-0.278186744	4.8621481666	C	-4.3049604415	-33.8414624397	-6.8307190784
H	1.537922537	-1.0506305079	3.9251918858	S	-6.8096041354	-34.2338650675	-7.0957228171
H	-2.0774197421	0.6810611006	5.4949241657	C	-4.4526834285	-35.2060620234	-7.1404692224
H	-0.0584180564	-0.791850487	5.8028677881	C	-5.7568278953	-35.6063211473	-7.3208223689
C	1.2773673732	0.2150671044	1.4149990075	C	-6.4561401408	-39.3898152867	-8.1942040792
C	2.477560274	-0.4895761995	1.279352696	C	-6.1214922918	-40.7577096382	-8.4711230246
C	0.8155116209	1.0034317314	0.3228493815	C	-4.860069069	-41.3179122035	-8.4600666615
C	3.2431663242	-0.4486609544	0.1302417452	S	-7.2756687909	-42.0008974805	-8.8922485324
C	1.5904976165	1.0578270144	-0.8388274392	C	-4.8209694858	-42.6860356174	-8.7777283968
C	2.7723442653	0.3386564893	-0.9129292011	C	-6.053330432	-43.2299163243	-9.0468251823
H	4.1699162671	-1.0037741623	0.0533033653	C	-6.388873585	-44.5801238636	-9.4087374202
H	1.2896916539	1.6521063045	-1.6952068692	C	-6.2536206596	-36.9097925795	-7.6421405847
N	-0.6721003944	1.0147968302	2.4651074732	C	-7.5557484418	-37.3350951108	-7.8296624974
N	-1.1142584184	2.7630898224	-1.1901606944	C	-5.4894600237	-33.1472280472	-6.763661245
F	3.5012325774	0.3964109822	-2.0349380646	C	-5.7317577315	-58.7501430378	-12.3428059259
F	2.9371415464	-1.2503533298	2.2908129922	C	-7.0756221969	-58.2611737907	-12.3629204798
F	0.4408739452	6.7188230634	-0.8333083557	S	-9.5256625724	-57.5030551342	-12.4319771787
F	1.575504527	5.6379660695	3.55834177	S	-5.4846230659	-56.2124111389	-11.8273963055
C	-4.0369883562	-19.7386721425	-4.1892680507	F	-5.4341614726	-60.0233990697	-12.5654171429
C	-5.3864998247	-19.2736347917	-4.1002953015	C	-4.7893588986	-57.8008640404	-12.0774991273
S	-7.8470217345	-18.5582795156	-3.972193626	O	-2.8832262228	-59.1469906542	-12.1785263047
S	-3.7937908554	-17.2017070112	-3.6683629932	C	-1.4662302346	-59.2895452361	-12.0911260451
F	-3.7357480297	-21.0043395086	-4.4480864027	H	-1.2677412693	-60.3439666723	-12.2819931951
C	-3.0932632605	-18.7752008747	-3.9873882324	H	-0.9704807534	-58.6630067122	-12.8372011133
O	-1.1785145257	-20.0876373649	-4.2463790767	H	-1.1122232532	-59.0042876801	-11.0969697122
C	0.2431533317	-20.2059752428	-4.2722539869	C	-3.3302523959	-57.9033575584	-11.9758254811
H	0.4437491764	-21.2563123356	-4.4824683444	O	-2.6214947029	-56.949271981	-11.7334417976
H	0.667246671	-19.5690901264	-5.052958116	C	-7.803547181	-66.0328077065	-13.9472565032
H	0.6702078844	-19.9170873088	-3.3083078367	C	-9.1561712157	-66.4048292019	-14.1697620563
C	-1.6290373811	-18.8529913467	-4.000800529	C	-8.5182643891	-68.6671439357	-14.6017763286

O	-0.9195364715	-17.8883091021	-3.8078595154	C	-7.1655037024	-68.2961033959	-14.3742225323
C	-6.097717081	-27.076789967	-5.5073230993	C	-6.7926469594	-67.0007580449	-14.0383343479
C	-7.4534404888	-27.4638329577	-5.6860011702	C	-7.6794065065	-64.6433964387	-13.6534717999
C	-6.8049791547	-29.7255421778	-6.1030373336	H	-6.7234880011	-64.1621217694	-13.4757206356
C	-5.4497087011	-29.3397414924	-5.9182556207	C	-8.6359389353	-70.0547275232	-14.9475835569
C	-5.0799107363	-28.0382296916	-5.6124299844	S	-6.0920644362	-69.6519698674	-14.5915719004
C	-5.9775220703	-25.683858803	-5.236944952	H	-9.5791261575	-70.5335697059	-15.18313824
H	-5.0214824503	-25.1919804953	-5.092363439	S	-10.2327704782	-65.0460768524	-14.0125474514
C	-6.9215869741	-31.109211367	-6.4208261461	C	-9.5303128143	-67.7042270088	-14.4833725284
S	-4.3626798822	-30.6814838197	-6.1395507822	C	-7.4365503173	-70.6867656516	-14.9719338547
H	-7.8734145143	-31.5890475329	-6.6226914407	O	-10.840782894	-68.020192717	-14.7082350333
S	-8.5367490068	-26.1120186331	-5.5167203938	O	-5.4823935987	-66.6692283187	-13.8397406568
C	-7.8249844996	-28.7699811371	-5.9702441616	C	-11.5217017362	-68.4930151878	-13.5528618401
C	-5.7158085138	-31.7578941453	-6.4713162313	H	-12.5473663746	-68.701116329	-13.8638281145
O	-9.1354582608	-29.1055168549	-6.1550975717	H	-11.0607973578	-69.4122988493	-13.1698735256
O	-3.7672950019	-27.694442734	-5.4562886465	H	-11.5279925528	-67.7356910066	-12.7590890426
C	-9.7865475318	-29.5551554348	-4.9722460649	C	-5.0569754492	-66.8042088022	-12.4892239197
H	-10.8143707061	-29.7874443816	-5.2571523632	H	-4.0033888131	-66.518656284	-12.468519087
H	-9.3039191905	-30.4561330571	-4.573248531	H	-5.6296213946	-66.142800432	-11.8267323489
H	-9.7884553478	-28.7751359203	-4.200967325	H	-5.1612795083	-67.8396055765	-12.1422589277
C	-3.3062090768	-27.7899104473	-4.1135869734	C	-9.9965679479	-52.9825245715	-11.6207035712
H	-2.2551417895	-27.4952239216	-4.1280382141	S	-7.5486424455	-53.6794224455	-11.4774657709
H	-3.8675899315	-27.1159754096	-3.4542555334	C	-9.9703874768	-54.3631190354	-11.8910494718
H	-3.3920165444	-28.816690081	-3.7372901745	C	-8.7128436454	-54.9210868545	-11.8580836896
C	-5.936086862	-7.5010178101	-1.6242262742	C	-8.3554513815	-58.7838537992	-12.5780772692
C	-4.6196448869	-8.0153853826	-1.7725912144	C	-8.8100811117	-60.1116724116	-12.8789728871
C	-5.4706484514	-10.1949543503	-2.2575368428	C	-10.1156231291	-60.5134649713	-13.0743887643
C	-6.7869918406	-9.6787965621	-2.1207011161	S	-7.7697768069	-61.5045065829	-13.0623630193
C	-7.0377838026	-8.3474568475	-1.8196825542	C	-10.2750008933	-61.8806472191	-13.3579117354
C	-5.9263167203	-6.115931287	-1.2763200573	C	-9.0953435053	-62.5828736924	-13.3913605804
H	-6.8321918163	-5.5394281821	-1.1281997538	C	-8.8786316051	-63.9819662218	-13.645171764
C	-5.4777816614	-11.5890830022	-2.5523928183	C	-8.335150377	-56.2824383691	-12.0888704965
S	-7.9907984227	-10.9143359646	-2.3575337558	C	-7.0794792606	-56.8608193462	-12.0903830408
H	-4.5695374832	-12.1707277115	-2.6700192636	C	-8.7613972639	-52.4338732853	-11.3697396858
S	-3.4229109535	-6.7882814237	-1.4725525378	H	-7.2476037811	-71.7258778285	-15.2108652478
C	-4.3681963391	-9.3419792408	-2.0937510352	F	-9.4742680263	-13.4003234405	-2.8978480509
C	-4.6708155979	-5.5890454441	-1.1645838483	F	-9.4162608954	-16.1533951759	-3.4628306786
O	-3.0910267969	-9.8125510681	-2.2073097501	F	-9.4840015546	-20.7621619781	-4.5162346802
O	-8.3166471106	-7.8864984144	-1.6770716593	F	-9.7899647179	-23.4901922384	-5.0344389941
C	-2.5739242049	-9.7527415676	-3.5311692499	F	-3.1087221301	-33.2988131673	-6.624976319
H	-1.5572091291	-10.1473035082	-3.4822959096	F	-3.406465326	-36.022519952	-7.244651671
H	-3.1724167032	-10.3651666725	-4.2174097548	F	-3.749911241	-40.6409744408	-8.1773756458
H	-2.5479811097	-8.7197756862	-3.8995292057	F	-3.6773777664	-43.3634705189	-8.8076395077
C	-8.8751958904	-7.3708744219	-2.8790639462	F	-11.1336662536	-52.2933160548	-11.6161835453

H	-9.8884757552	-7.0468136001	-2.6333667267	F	-11.0787717414	-55.0516936911	-12.1550701339
H	-8.2956913645	-6.5156838559	-3.2492482512	F	-11.1626461285	-59.6952787099	-13.0058485529
H	-8.9183651337	-8.1413143763	-3.6588983167	F	-11.4749719742	-62.4130358043	-13.5684455003
C	-6.7378434188	-12.1178302119	-2.6442929358				

Table S7. The coordinate of **3** (198 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	-2.1977540307	-1.0477834086	0.1539387063	C	-10.2961557294	-13.3422803498	-3.0569895596
C	-2.0903148418	1.3446432018	0.940080755	C	-10.7768925423	-11.9940224882	-2.9216349874
C	-2.7671419385	0.1801072978	0.5338172856	N	-9.0226495696	-13.7268139818	-2.9744555777
C	-3.098302974	-2.1939184209	-0.1769723461	N	-10.5791317542	-15.6216027561	-3.3925540024
C	-2.5674435231	-3.2749820552	-0.8915158158	C	-14.4898445372	-17.4360202355	-4.0264379028
C	-3.3535936104	-4.3664435196	-1.2260931499	C	-15.6569820479	-16.6285093759	-4.0860833167
C	-4.702349588	-4.4260485088	-0.8455680205	C	-17.0282233551	-18.5405972024	-4.5014731675
C	-5.2263067578	-3.3553975675	-0.1047786057	C	-15.8631072241	-19.3498849582	-4.4284185089
C	-4.4411286712	-2.259972855	0.2177663791	C	-14.6012272327	-18.827086189	-4.1872331736
H	-3.8462971247	0.2353522329	0.5259232632	C	-13.3154701698	-16.6602605244	-3.7976539743
H	-1.5218412965	-3.2403346643	-1.1794862666	H	-12.319456269	-17.0786784387	-3.7425303462
H	-2.9215078614	-5.1786714105	-1.8053908523	C	-18.1970794929	-19.3109657762	-4.7715567186
H	-6.2518853608	-3.4019557581	0.2498461643	S	-16.2391303967	-21.0279456769	-4.6877480745
H	-4.8754128606	-1.4701555951	0.8224821361	H	-19.1842111123	-18.8848850187	-4.8899592962
C	-2.8894020785	2.5652862413	1.2691038074	S	-15.2781027798	-14.9472506683	-3.8550621778
C	-4.1739902807	2.7931631368	0.7610049577	C	-16.9208356264	-17.152877852	-4.3118585415
C	-2.3136587305	3.5328328547	2.1017029592	C	-13.5617644958	-15.3179605354	-3.6733902318
C	-4.8711381604	3.9498465699	1.0930385697	C	-17.9525348733	-20.6541172221	-4.8898717603
H	-4.6236630568	2.0816410847	0.0749240781	O	-18.0113838245	-16.3342997018	-4.3822581058
C	-3.0149198382	4.6828693928	2.4425968789	O	-13.5059884954	-19.641385439	-4.1451754262
H	-1.3062106707	3.365580573	2.4690629049	C	-18.7549650148	-16.2607237011	-3.1720296638
C	-4.2977964099	4.8941285016	1.9413127969	H	-19.5837039126	-15.5759638448	-3.3623416997
H	-5.8631098269	4.1171755752	0.6820327788	H	-19.1506505749	-17.2435697358	-2.8880962005
H	-2.5577464448	5.4195890092	3.0977543116	H	-18.1374905672	-15.8694576242	-2.3539390442
H	-4.8454639962	5.7955223817	2.203251593	C	-13.1195846699	-20.0169386283	-2.8288613571
O	-0.9572153951	-1.2967782911	0.0187926944	H	-12.2473992005	-20.6644715075	-2.9379879985
O	-0.8361345512	1.4719976569	1.1076541638	H	-12.850690428	-19.1393679094	-2.2281442246
Ir	0.6678695344	0.0203583968	0.5601274715	H	-13.9234549472	-20.5677171093	-2.3247760788
C	2.1090432354	1.3291041298	0.9443643354	S	-22.4973953228	-20.602974393	-5.5483981421
C	2.8229281466	1.4733030199	2.1370649811	C	-20.7424458628	-23.9687688997	-5.6637505282
C	2.3874332564	2.2216479509	-0.1296206887	C	-18.4943447616	-23.0505893971	-5.2455005981
C	3.76834446	2.4788998147	2.2569588052	C	-19.378452299	-24.1207893768	-5.4888337793
H	2.6559895116	0.8142229839	2.9825107614	H	-17.4430427585	-23.2968712803	-5.1236609743
C	3.3524300082	3.217243897	0.0523234599	H	-18.9466962413	-25.1168440374	-5.535226823
C	4.0557041356	3.3707166017	1.2312536904	C	-21.2124245513	-22.6121325295	-5.5851872287
H	4.7991813054	4.1501199879	1.3439723937	C	-20.3021622511	-21.5100678808	-5.3300718087

C	1.6238165266	1.9945206545	-1.3477525909	C	-18.8921533603	-21.7287731893	-5.1524382416
C	1.7095555151	2.7072314948	-2.5506929213	N	-20.9186782956	-20.3291081955	-5.2861657391
C	0.9191486247	2.3413548701	-3.628336055	N	-22.4773364593	-22.2166136408	-5.7270108749
H	2.3965526189	3.5380244376	-2.6253155072	C	-23.5239930045	-26.4071263564	-6.2802000316
C	-0.0042882858	0.594570566	-2.2969781382	C	-22.5212281272	-27.4123608844	-6.2404692601
C	0.0445708659	1.2636080194	-3.5072232887	C	-24.1500381045	-29.1290712224	-6.5716774293
H	0.9874750585	2.8945435861	-4.560785555	C	-25.1512784703	-28.1227845737	-6.6232873019
H	-0.6548328194	-0.255489905	-2.1237505026	C	-24.8637138063	-26.7723296038	-6.4918943895
H	-0.5880409056	0.9439652179	-4.3280295602	C	-22.9816216791	-25.1038529837	-6.0800168576
C	1.4588582032	-2.0286452789	2.4642986851	H	-23.579259064	-24.2027907865	-6.0491704822
C	-0.0421641091	-0.4968586833	3.4193141439	C	-24.7006714715	-30.4369728157	-6.711922657
C	1.4873054285	-2.747147178	3.6664399418	S	-26.7319057301	-28.8113849715	-6.8501228191
C	-0.0463350663	-1.1685333808	4.6291189487	H	-24.1126132173	-31.3440253922	-6.6753772834
H	-0.6188604626	0.4054865633	3.2490060501	S	-20.9467070996	-26.7274466444	-5.9655503917
C	0.7340413682	-2.3166176947	4.7468253028	C	-22.8062049457	-28.7611955281	-6.3915448735
H	2.1016296404	-3.6332247974	3.7388394068	C	-21.622808924	-25.0978650872	-5.9022064778
H	-0.6473500379	-0.7972817976	5.4519411968	C	-26.061305629	-30.4439423127	-6.8734520893
H	0.757796117	-2.8747260512	5.6785135444	O	-21.8110037009	-29.6933237262	-6.3224960254
C	2.19859872	-2.3175469415	1.2443991382	O	-25.8606782227	-25.8400226992	-6.5277805257
C	3.0773952399	-3.3895479776	1.060065949	C	-21.3461410572	-30.1356410648	-7.5918430232
C	1.9949567627	-1.4030599959	0.1721829954	H	-20.5578524417	-30.8642723005	-7.3928037306
C	3.7649138208	-3.5986870843	-0.119723748	H	-22.149539577	-30.6138189817	-8.1654045378
C	2.6944955503	-1.6033125612	-1.0208386977	H	-20.9345737508	-29.3008758302	-8.1727273199
C	3.552801139	-2.6839220587	-1.143439586	C	-26.0333730503	-25.2335124592	-7.8026394561
H	4.4406471557	-4.4372538793	-0.2342651212	H	-26.8536027666	-24.5210523102	-7.6951505169
H	2.5836493842	-0.9297948849	-1.8639106135	H	-25.1260154958	-24.7024669864	-8.1157192072
N	0.6824961016	-0.9128804584	2.3721031783	H	-26.2951799319	-25.9809309416	-8.5619310233
N	0.7566721416	0.9482043489	-1.2525214031	S	-25.1924598473	-34.9376691834	-7.2485266788
F	4.2123055335	-2.8653999458	-2.2947816873	C	-28.8250264888	-33.8357508801	-7.3478871791
F	3.2871164725	-4.2753080118	2.0524382168	C	-28.3262004791	-31.4361601653	-7.0961050303
F	3.6340074872	4.0807303996	-0.9421233313	C	-29.2214977228	-32.5143092931	-7.248427729
F	4.4413091325	2.607216546	3.4076235063	H	-28.7585931787	-30.4419700867	-7.0227170424
C	-7.4331144447	-6.8604498882	-1.6804982676	H	-30.2805116109	-32.2748133031	-7.2914270788
C	-6.4100089946	-7.8427937125	-1.761116516	C	-27.4038166475	-34.0449274336	-7.2874998291
C	-8.0128725208	-9.5475240696	-2.251577564	C	-26.4814500941	-32.9341716588	-7.1338340482
C	-9.0330380289	-8.5610295325	-2.1870169926	C	-26.9518667286	-31.5794384573	-7.0316921685
C	-8.7668264879	-7.2264251952	-1.9175475172	N	-25.206123756	-33.3205602705	-7.1020401596
C	-6.9064792205	-5.5745311185	-1.3523098178	N	-26.7866592821	-35.2242350807	-7.3600648774
H	-7.5261046148	-4.6907104557	-1.2530763568	C	-30.7202885478	-37.0397456401	-7.8112912606
C	-8.5411133519	-10.8462885571	-2.5159943776	C	-31.894768334	-36.2503370545	-7.6910632099
S	-10.603928306	-9.2565829113	-2.4574666295	C	-33.2846159304	-38.1665357643	-8.016091429
H	-7.934744764	-11.7400038801	-2.5776477501	C	-32.1108486133	-38.9582126414	-8.1293947044
S	-4.8449750812	-7.1570582268	-1.429516396	C	-30.8338310045	-38.4222375033	-8.0214165088
C	-6.6743504675	-9.1744868246	-2.0500246688	C	-29.5342173985	-36.2531918075	-7.70116932

C	-5.5495775032	-5.5651133204	-1.1926422056	H	-28.5348514597	-36.6576774523	-7.7881325669
C	-9.9031510212	-10.8651339575	-2.6591478304	C	-34.4721497618	-38.9552771816	-8.1771891366
O	-5.6634986108	-10.0910615979	-2.0926457264	S	-32.4992041323	-40.6310147067	-8.4264351675
O	-9.7728807328	-6.30334768	-1.8445673861	H	-35.4731439395	-38.5408679875	-8.1483804443
C	-5.1848950598	-10.3589966731	-3.4047258598	S	-31.5077498886	-34.5728595841	-7.4420175543
H	-4.38627281	-11.095320912	-3.2957490433	C	-33.1704968775	-36.7890098877	-7.7794620337
H	-5.9783641704	-10.7707803976	-4.0404867867	C	-29.7772790194	-34.9214002772	-7.4972505829
H	-4.783416509	-9.4503172046	-3.8704108516	O	-34.2786045316	-35.9944464302	-7.6764188079
C	-10.0620123438	-5.6783431343	-3.0885335953	O	-29.7335071149	-39.2185418875	-8.1584534781
H	-10.8784554788	-4.9783438388	-2.8994943453	C	-34.7932815415	-35.9034242187	-6.354505675
H	-9.1898446638	-5.1308380193	-3.4679489841	H	-35.6618119903	-35.2436421253	-6.4065402131
H	-10.378939269	-6.4140620977	-3.8381187353	H	-35.1028529005	-36.8878848064	-5.9811608154
S	-8.9940279909	-15.3363516482	-3.1865805771	H	-34.0512502045	-35.4761213071	-5.6685328251
C	-12.6214598802	-14.2392428031	-3.430175584	C	-29.1613252755	-39.6305431325	-6.9234683502
C	-12.1464112464	-11.8508073607	-3.0549611303	H	-28.3033433138	-40.2563998283	-7.1767114636
C	-13.027522762	-12.9232915964	-3.2988437278	H	-28.8242940267	-38.7691108147	-6.3339590861
H	-12.5861729698	-10.8610537938	-2.967375778	H	-29.8781428102	-40.2146081345	-6.3328602938
H	-14.0842977388	-12.684506232	-3.3820303404	C	-34.1983321064	-40.2659675531	-8.3937267885
C	-11.2045836562	-14.4479541423	-3.3030660608	H	-34.9103963715	-41.065768262	-8.5546471691

Table S8. The coordinate of **4** (240 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	-17.4888544941	0.4395147057	-0.3649049362	S	7.7208841276	-11.6757435958	-3.5663342249
C	-19.5963519959	1.8203202133	-0.3269201288	C	6.6672747592	-9.222942113	-2.7532585442
C	-18.2021900926	1.6457721266	-0.2550418207	C	9.4729386889	-11.8010431278	-3.4583749759
C	-15.9960331853	0.4718619541	-0.3038718281	O	5.4012188311	-9.666327186	-3.0132068493
C	-15.3150035104	-0.7182320569	-0.0202412555	O	10.5934293447	-7.898933258	-1.9128549192
C	-13.9318578128	-0.7487435138	0.0606823165	C	4.926267044	-9.3125928421	-4.3064614344
C	-13.1713051049	0.4097543261	-0.1567034353	H	3.9177455124	-9.7230867708	-4.3867026972
C	-13.8530857029	1.594851521	-0.4747495366	H	4.8897520184	-8.2230625773	-4.4309865227
C	-15.2370475441	1.6258700906	-0.5400044328	H	5.5594756497	-9.7433304915	-5.0919867462
H	-17.6161924315	2.5408289149	-0.1026560435	C	11.2608469858	-7.3205061293	-3.027845841
H	-15.8956987528	-1.6211097219	0.1379802884	H	12.2471211886	-7.0160787829	-2.6719705251
H	-13.4328853863	-1.6809172567	0.313795068	H	11.3730336709	-8.0464606192	-3.8429849943
H	-13.2871357761	2.4931847324	-0.70347986	H	10.7197905824	-6.4419313072	-3.4004857894
H	-15.7240201287	2.554525737	-0.8209256891	C	6.5148048577	-5.7891377523	-1.4005793539
C	-20.163228792	3.1921812015	-0.1436494895	C	4.1783050539	-2.8031188829	-0.3904755147
C	-19.4875491031	4.211233839	0.5385692051	C	5.4814615764	-2.4467061365	-0.1021940778
C	-21.438036293	3.4582823213	-0.658645367	C	6.4219962624	-3.4455541897	-0.4218759799
C	-20.0646900361	5.4680280185	0.6851182562	C	5.8596548735	-4.5834187733	-0.9618961206
H	-18.5183827238	4.0178533763	0.988535761	S	4.1367023508	-4.4065578502	-1.0778831315
C	-22.0098818132	4.7171023589	-0.5214582263	H	5.7336851563	-1.4873488988	0.3294091797
H	-21.9699071375	2.6573043721	-1.1620428664	H	7.4890979745	-3.3375732513	-0.2567437948

C	-21.3236540718	5.7277147001	0.148863542	S	12.5024664794	-19.0313261535	-6.0649312106
H	-19.5317355128	6.2452100562	1.2262719283	C	15.5365471571	-17.0941305597	-4.8571038181
H	-22.9962418393	4.9097560625	-0.9349676748	C	14.2569757893	-15.104160922	-4.1673341068
H	-21.7716555714	6.7114899256	0.2608112257	C	15.4598075165	-15.818389088	-4.3235894083
O	-17.9859212959	-0.726816766	-0.4743036667	H	14.3258229869	-14.111582439	-3.729981676
O	-20.4596472394	0.9211550266	-0.5787605539	H	16.3728007489	-15.3234738005	-4.0030763875
Ir	-20.0743509894	-1.1961570377	-0.7488090603	C	14.2742267341	-17.655132091	-5.2553079161
C	-22.0193184653	-1.5741883056	-0.8522122553	C	13.0336344019	-16.9178470727	-5.0954140315
C	-22.7892119102	-1.7300730927	-2.0080777097	C	13.0146635713	-15.5946865964	-4.5335345542
C	-22.6658946489	-1.6510575609	0.4140857393	N	11.9685991246	-17.5981234182	-5.52004558
C	-24.1548863359	-1.9379656576	-1.9035398142	N	14.0939488794	-18.8617640723	-5.7925833581
H	-22.3438095009	-1.6915488508	-2.9965568234	C	11.7935526943	-14.8327442658	-4.3655847891
C	-24.0478328286	-1.8611841556	0.4546938118	C	10.4854518635	-15.2016453592	-4.613025279
C	-24.8164264812	-2.00610095	-0.6838518117	C	9.5503810028	-14.1893987498	-4.3213429511
H	-25.8852339522	-2.169785004	-0.6224048392	C	10.1219688363	-13.0268960285	-3.8475443767
C	-21.7953307452	-1.5121020689	1.5723430622	S	11.8478322101	-13.1947659268	-3.7655786208
C	-22.1624456795	-1.5682238327	2.9231743939	H	10.2256379407	-16.1800418559	-4.9943940326
C	-21.1957148693	-1.4424000496	3.9077711439	H	8.4798028893	-14.3079382553	-4.453425899
H	-23.2012665169	-1.7126253222	3.1837792401	C	25.3862396106	-19.0819329074	-4.2826228561
C	-19.5526781793	-1.2105993579	2.1978476474	C	25.1815821717	-17.7705775494	-3.7751946353
C	-19.8625382697	-1.2626501262	3.545452467	C	22.8281033047	-17.9280255045	-4.160507535
H	-21.4820015933	-1.4872171958	4.9547530841	C	23.0317606755	-19.2419501727	-4.6617258664
H	-18.5387894722	-1.0777349213	1.8367141614	C	24.284841739	-19.8340006058	-4.7208395199
H	-19.0759082433	-1.1639412354	4.2854570471	C	26.7651769235	-19.4448599467	-4.2722002052
C	-19.2966507272	-2.3163472564	-3.3155383105	H	27.1287521943	-20.3947286789	-4.6490827876
C	-19.8513466322	-0.0424815531	-3.5005261929	C	21.4560477489	-17.5447433492	-4.2204548913
C	-18.9916527403	-2.3511060185	-4.6822355035	S	21.535104045	-19.9639924168	-5.1826709829
C	-19.5659307915	-0.0249195793	-4.8544653608	H	21.1019870208	-16.5662454415	-3.9144571576
H	-20.202928042	0.8332957215	-2.9661520362	S	26.6833900444	-17.0309309032	-3.2963990855
C	-19.1255434413	-1.2051366562	-5.449479616	C	23.9260423246	-17.186491271	-3.6963629314
H	-18.6560198573	-3.2774227761	-5.1260945249	C	27.582750153	-18.4663434846	-3.7738162157
H	-19.6871052743	0.8918568661	-5.4209626006	O	23.7727378089	-15.9161421711	-3.2168601229
H	-18.8890883727	-1.2340891081	-6.509369786	O	24.4432243215	-21.0944874485	-5.2242524982
C	-19.2404629216	-3.4213455612	-2.3696117565	C	23.4492643107	-15.8624912472	-1.832778292
C	-18.8527995199	-4.7310798688	-2.6694433644	H	23.3637577321	-14.8043371715	-1.5777234603
C	-19.6326331631	-3.108610386	-1.037035809	H	22.4966071803	-16.367044121	-1.6280951192
C	-18.8419553365	-5.7420561024	-1.7281237374	H	24.2377874794	-16.3223246622	-1.2243143586
C	-19.6341572642	-4.128918986	-0.082094217	C	24.4232258974	-22.1124616157	-4.2310313614
C	-19.2420286366	-5.4084574087	-0.4402822405	H	24.5502194918	-23.0597882634	-4.7587875898
H	-18.5384589782	-6.748390596	-1.9891352932	H	25.2415762218	-21.9805135047	-3.5120651112
H	-19.9358319668	-3.9459624616	0.9438419049	H	23.467949461	-22.1201067565	-3.6916853206
N	-19.7188768667	-1.1482130794	-2.7555087767	C	20.6400962416	-18.5168116782	-4.7338089953
N	-20.485839937	-1.3280651815	1.2435763586	C	16.7901030106	-17.8070814888	-4.999710839
F	-19.2437481114	-6.3745463378	0.487158712	C	17.04061502	-19.0422598888	-5.5654279795

F	-18.4676725136	-5.0572078705	-3.9179288247	C	18.3994230551	-19.412016764	-5.5311795255
F	-24.6903776557	-1.9311298678	1.6360763363	C	19.2149249215	-18.4703485802	-4.9389516413
F	-24.8800601007	-2.0804571469	-3.0203208783	S	18.2770638048	-17.1082170278	-4.4113479349
C	-9.5025609661	1.0989910052	0.2378766743	H	16.2539406472	-19.6508514438	-5.9908407841
C	-9.3039926509	-0.2782576045	-0.0479494708	H	18.7761293855	-20.3451945667	-5.9372792027
C	-6.9329973278	-0.0272872001	0.1262028809	S	35.7269116697	-17.918393383	-2.4935091489
C	-7.1329684464	1.3479764516	0.4231515576	C	35.2075911371	-21.3943539989	-3.9309008231
C	-8.3942061308	1.9207154446	0.4945980499	C	32.7676186589	-21.1573042948	-4.1822034071
C	-10.8868404521	1.4493764396	0.2192964692	C	33.9660962528	-21.8865432948	-4.2974433262
H	-11.243013403	2.4523612183	0.4242417556	H	31.8562070736	-21.651170671	-4.508837586
C	-5.5480555838	-0.3685018494	0.1012550813	H	33.8937969893	-22.8944124626	-4.6976395201
S	-5.6183078654	2.1758982864	0.6548288864	C	35.1914498635	-20.0554544263	-3.4074195917
H	-5.1905716777	-1.3676975593	-0.1227222886	C	33.9549646783	-19.3037144212	-3.2870864023
S	-10.8169175769	-1.0883755432	-0.3367033049	C	32.6935765633	-19.866899339	-3.6850604121
C	-8.0422661942	-0.8560190399	-0.0988909265	N	34.1377378636	-18.0835131633	-2.7821790236
C	-11.7132396697	0.3985387323	-0.062072725	N	36.2563394034	-19.3710431442	-2.9891296757
O	-7.8818850296	-2.1803911436	-0.3947973623	C	31.4427059383	-19.1436644092	-3.5729703662
O	-8.5497972694	3.2511503408	0.7685832221	C	31.2106544131	-17.8458180999	-3.1605126913
C	-7.8757067046	-3.0249351967	0.7493804085	C	29.8503582053	-17.4808318017	-3.188883688
H	-7.7494004498	-4.0441870559	0.378930464	C	29.0151475966	-18.4895103186	-3.621651853
H	-7.0458206477	-2.7732545443	1.4218006218	S	29.9343805401	-19.9144010243	-3.9929999367
H	-8.8211890122	-2.9521377509	1.3009652816	H	32.0119846495	-17.1883123082	-2.8511079859
C	-8.7124580774	3.5315638799	2.1530898228	H	29.4883858985	-16.4980459745	-2.9047434702
H	-8.8172322738	4.6151328048	2.237824295	C	41.3198188856	-29.0613384211	-6.2057839177
H	-9.6105243828	3.043650317	2.5526657503	C	39.9889693219	-29.4815279474	-6.4691899384
H	-7.8383685669	3.2036511832	2.7293061345	C	39.123680409	-27.3621901274	-5.7796140872
S	3.4725062357	1.478421988	1.0902630638	C	40.455788752	-26.9405083915	-5.5222560668
C	2.9520343571	-2.0556591516	-0.1967539939	C	41.5540699413	-27.7605952552	-5.7365821502
C	0.4952450602	-1.8880446478	-0.289257992	C	42.267336418	-30.1054170758	-6.472735595
C	1.7025644234	-2.5906942127	-0.4621149784	H	43.3341415602	-29.9993167103	-6.3138491802
H	-0.4223475146	-2.415863934	-0.5355940243	C	38.1748243986	-26.3437474174	-5.4627691357
H	1.6308373118	-3.6134205844	-0.8227830167	S	40.5014647853	-25.3101875919	-4.9108380997
C	2.93505803	-0.7009043076	0.2838852035	H	37.1034317754	-26.4849979693	-5.5557500185
C	1.689542818	0.023810869	0.4627635897	S	39.944519955	-31.1302724134	-7.0322297712
C	0.4199475658	-0.583241474	0.1687853159	C	38.8905850863	-28.652746372	-6.2747446527
N	1.8728388345	1.2645860552	0.9146431191	O	37.622454404	-29.0969176658	-6.5236889578
N	4.0067339004	0.0231877209	0.6072397954	O	42.818944927	-27.3205476936	-5.4609675632
C	-4.7213637865	0.6884349408	0.3695446083	C	37.155619303	-28.7884519223	-7.8308981198
C	-0.8396245324	0.1130041051	0.3388798923	H	36.1454416664	-29.1968145043	-7.9014975032
C	-1.0791854834	1.415270743	0.7325188565	H	37.1250721549	-27.7038757297	-7.9950917879
C	-2.4477633674	1.7463069581	0.7797240985	H	37.7903860346	-29.2504743986	-8.5972173389
C	-3.281568246	0.7062871717	0.4259015624	C	43.4951894563	-26.7852756697	-6.5910543415
S	-2.3502791277	-0.7023249011	0.0246655435	H	44.4797329603	-26.4694999381	-6.2399986498
H	-0.277676226	2.0988469305	0.9784460223	H	43.6118816969	-27.5406665702	-7.3784754209

H	-2.8174170908	2.7239122163	1.0716836799	H	42.9588496489	-25.9200480928	-7.0003206863
C	9.0967991977	-9.625440473	-2.6912920005	C	38.7471232921	-25.193426345	-4.9931734297
C	7.7660914629	-10.0425519358	-2.964160351	C	36.4253630535	-22.1681216827	-4.0665974915
C	6.896934768	-7.940942817	-2.2292664616	C	37.7164641945	-21.8504645607	-3.6922455375
C	8.2281924057	-7.5207068339	-1.9640213475	C	38.6511142483	-22.8657755634	-3.9765929766
C	9.328770502	-8.3328244323	-2.1950408899	C	38.0957675575	-23.9779052628	-4.573547903
C	10.0432948796	-10.652203535	-2.9795269389	S	36.3887506776	-23.754343628	-4.7935582479
H	11.1088802935	-10.5369347401	-2.8131455327	H	37.964311789	-20.9077499586	-3.2230680168
C	5.9461573225	-6.9330708542	-1.892914216	H	39.7075505668	-22.7906059141	-3.7402807998
S	8.2688272615	-5.9044005278	-1.3169731971	C	41.6758082359	-31.241781637	-6.9174210415
H	4.8754259215	-7.07336408	-1.9945180628	H	42.1604925979	-32.1737514903	-7.1801168585

Table S9. The coordinate of **5** (240 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	-17.3436777077	0.0755734334	1.2564764285	C	10.021384871	-10.4746378427	-7.0921227798
C	-19.6185899062	1.1524759423	1.1575868851	O	5.8534238893	-8.4810334904	-7.0333322128
C	-18.2393780399	1.0933697967	0.8861568691	O	10.6893806099	-6.9286198592	-4.6882917665
C	-15.9181440967	0.1739389238	0.8198635671	C	5.6390855052	-7.9627533796	-8.3409675152
C	-14.9543199974	-0.5742668835	1.5062006827	H	4.6740353418	-8.3517691403	-8.671376392
C	-13.6175536742	-0.5212180175	1.1439949384	H	5.6091692182	-6.8659073934	-8.3306820572
C	-13.1932455721	0.2685011422	0.0648955271	H	6.4225106734	-8.2955196492	-9.0328591905
C	-14.1655147501	0.9928136382	-0.6426770062	C	11.4950811965	-6.0854598305	-5.503440803
C	-15.4988011429	0.9520063836	-0.2673133115	H	12.3877802999	-5.8547363953	-4.9189167618
H	-17.8247647668	1.9216671858	0.3292182491	H	11.7848683812	-6.5937371395	-6.4317976212
H	-15.2763580319	-1.2000059603	2.3321770741	H	10.9706291893	-5.1544274051	-5.750975844
H	-12.8882887993	-1.0902349502	1.7153101133	C	6.5036614239	-4.9749952709	-4.5667439828
H	-13.8747219552	1.5685046248	-1.5164413594	C	3.8514242987	-2.2372024631	-3.5567987382
H	-16.2243255325	1.4999309625	-0.8605673204	C	5.0222133045	-1.9731236134	-2.8929227354
C	-20.3904172346	2.3561825881	0.7200632157	C	6.057665834	-2.8911979896	-3.1830320278
C	-19.7922602437	3.6011318824	0.4906998965	C	5.708699092	-3.8850713865	-4.0627041357
C	-21.7761257657	2.2352250864	0.5578075148	S	4.0585149465	-3.648009169	-4.5581237268
C	-20.558264897	4.69117023	0.0918118475	S	14.5633188782	-15.6180271682	-11.4853192513
H	-18.7270750479	3.7336391012	0.6549420488	C	16.5727969052	-15.1758504854	-8.3107968402
C	-22.5395870204	3.3216846716	0.1487802803	C	14.8625932847	-13.8621882485	-7.1338037425
H	-22.2392129428	1.2755669253	0.7640890262	C	16.1318786779	-14.4821312932	-7.20068331
C	-21.9325207356	4.5533108501	-0.0883473477	H	14.5899195947	-13.353811058	-6.2129080892
H	-20.0808031439	5.6534732755	-0.0722322337	H	16.789559322	-14.394402762	-6.3401077033
H	-23.6125738137	3.2089232801	0.0185796935	C	15.6623682076	-15.2399187442	-9.4150430915
H	-22.5291299165	5.4051288571	-0.4038488884	C	14.3731902318	-14.5883653301	-9.3544588469
O	-17.6052992392	-0.9393096268	1.9780910063	C	13.9565075188	-13.8882540029	-8.1760899347
O	-20.317550252	0.249193341	1.7161712197	N	13.6649626962	-14.7176595842	-10.4761684244
Ir	-19.5694083466	-1.5546160159	2.6362230505	N	15.8784797623	-15.8727598817	-10.5679803245
C	-21.3800504961	-1.9850163842	3.3229284782	C	12.6688104356	-13.2186238795	-8.0973729679

C	-22.3349884218	-2.8123440432	2.7259068748	C	11.4369401098	-13.6176909979	-8.5491991329
C	-21.7128410064	-1.3272667719	4.5411768668	C	10.4003540283	-12.7040433428	-8.249829706
C	-23.5798712703	-2.9639095164	3.3146439678	C	10.8040842276	-11.591294589	-7.555268339
H	-22.1280814721	-3.3452743736	1.8039027113	S	12.5214339213	-11.6791135369	-7.2949907426
C	-22.9864856216	-1.5184121086	5.085833403	C	24.6540154316	-20.2257526595	-5.0520365584
C	-23.93859922	-2.3268743968	4.4959469474	C	23.7660340832	-20.0603560205	-3.9552712991
H	-24.91717133	-2.4582478506	4.9410118237	C	22.2016801243	-18.8944552734	-5.3352526367
C	-20.6576881258	-0.5086632028	5.1201697521	C	23.0890638529	-19.0612556435	-6.4323084029
C	-20.7069684805	0.2219866563	6.3143234586	C	24.3011840043	-19.7267189605	-6.3153190096
C	-19.5942520566	0.9313514945	6.7367469067	C	25.8449270836	-20.9083948708	-4.6687438601
H	-21.6166586947	0.2212476254	6.8976509254	H	26.6573119387	-21.1084945295	-5.3591505499
C	-18.4357283622	0.176958009	4.7962757312	C	21.0332588327	-18.1680952575	-5.7074625971
C	-18.4315926608	0.9110026715	5.9693341708	S	22.4675737755	-18.3222369322	-7.8806658106
H	-19.6338050328	1.4962712211	7.6638071648	H	20.2481313206	-17.9141940115	-5.0033220793
H	-17.5703167256	0.1074038894	4.1464860077	S	24.4176563357	-20.7420584738	-2.4919505948
H	-17.53882701	1.4497740367	6.2673505844	C	22.5435705882	-19.4149118857	-4.0775220146
C	-19.1634894109	-3.9468216386	1.0347348523	C	25.8691136741	-21.2558023008	-3.3447750868
C	-20.1567843656	-2.229144763	-0.2198027244	O	21.7159343576	-19.2551017569	-3.0025184167
C	-19.1556512716	-4.7682882177	-0.0997944365	O	25.1423016988	-19.8598190678	-7.3835233995
C	-20.1746594073	-3.0011864597	-1.3680828488	C	20.7904318843	-20.3216641928	-2.8281870848
H	-20.5416024579	-1.2157585006	-0.1916663212	H	20.2027000683	-20.0766051089	-1.9414246578
C	-19.6602145417	-4.2941239339	-1.2998743283	H	20.1253721214	-20.4128122475	-3.6962574504
H	-18.7548074092	-5.7690413619	-0.0253914012	H	21.3090685833	-21.2750701225	-2.6695860828
H	-20.5811890853	-2.5939764952	-2.2873240193	C	24.9187703324	-21.0410825388	-8.1445604137
H	-19.6535667512	-4.9326718881	-2.1786842825	H	25.6410387165	-21.0206568086	-8.962938442
C	-18.6975778601	-4.284073492	2.3719165355	H	25.0792591102	-21.9393273333	-7.535032843
C	-18.1467952828	-5.5103144747	2.7575228984	H	23.9021802224	-21.0613678382	-8.556004726
C	-18.8395330902	-3.2569593241	3.347695441	C	21.0201671117	-17.8002280733	-7.026109304
C	-17.737834257	-5.7729767703	4.0505823768	C	17.8696478585	-15.8312675	-8.3481378719
C	-18.4356884046	-3.5188109829	4.6597060983	C	18.7832763071	-15.9232254836	-9.3668110693
C	-17.8979229686	-4.7543432066	4.9815126149	C	19.9619592025	-16.6175428743	-9.009757484
H	-17.3159696718	-6.732973173	4.321498898	C	19.9892563286	-17.0655693022	-7.7127905452
H	-18.5310067754	-2.7742696235	5.442983324	S	18.4976414962	-16.6287018012	-6.932080345
N	-19.6666586474	-2.6840756211	0.9413162248	S	30.5680206342	-26.9299118287	0.1175722988
N	-19.5113528125	-0.5072117084	4.384060306	C	32.9555666938	-25.1236568751	-2.1947910097
F	-17.5113005812	-4.9887486773	6.2420886884	C	31.371550742	-23.3574224973	-2.8319000062
F	-17.9935915936	-6.5001784504	1.8574804784	C	32.6390535083	-23.980910954	-2.9030064748
F	-23.3344692139	-0.9042418848	6.232770492	H	31.2145565427	-22.4504568988	-3.4094988769
F	-24.4861053314	-3.7564839202	2.7282343198	H	33.3887105335	-23.5427230318	-3.5562957057
C	-9.777161774	1.0831076172	-1.2627598285	C	31.917335955	-25.6571631207	-1.3642887115
C	-9.3601411369	-0.1505393592	-0.6939865318	C	30.6156204195	-25.0309868587	-1.3065570186
C	-7.135246004	0.1692620372	-1.5055009195	C	30.3376409895	-23.8413206382	-2.0544714433
C	-7.5498219786	1.4062201545	-2.0672914284	N	29.7581536469	-25.6711098473	-0.5117733436
C	-8.8485168922	1.8809655585	-1.9473560134	N	32.0181905025	-26.7342201116	-0.5855286932

C	-11.1654392866	1.3281791658	-1.0349965898	C	29.0320503024	-23.2026508122	-2.0205072683
H	-11.6688167542	2.2223275408	-1.3839758275	C	28.1857143554	-22.9807841635	-0.9647719103
C	-5.7635940457	-0.1026377368	-1.7830523605	C	27.0063275565	-22.2867683071	-1.3204554494
S	-6.2511226027	2.195730291	-2.9159427606	C	26.9204340592	-21.9516719527	-2.6486125057
H	-5.2670903236	-1.0130692567	-1.4646273956	S	28.336449495	-22.5365508892	-3.4720997666
S	-10.6844502206	-0.9667455578	0.086204624	C	42.9804806214	-25.8188796551	-2.9016116878
C	-8.0561848344	-0.615308583	-0.7944254746	C	42.6346029166	-24.4410741387	-2.8727316671
C	-11.7878475536	0.3378866386	-0.3290570256	C	40.3122619506	-24.9738816007	-2.6855744363
O	-7.688462393	-1.8155325968	-0.254587444	C	40.658206376	-26.3509963972	-2.7094720902
O	-9.2193662613	3.0675178412	-2.515221803	C	41.9722828355	-26.7880743192	-2.8053936242
C	-7.2057463165	-1.7177494085	1.0796947785	C	44.3961190274	-26.0069038779	-3.0437011738
H	-6.9611493576	-2.7343692317	1.3938720754	H	44.8655039964	-26.9814642555	-3.1101007989
H	-6.3058536897	-1.0915771698	1.1295442824	C	38.9011352282	-24.7859731218	-2.5945578346
H	-7.97015082	-1.3033007213	1.748480206	S	39.2501942706	-27.3708348594	-2.6204799803
C	-9.0920691424	4.1831314053	-1.6422104867	H	38.436552249	-23.8056791236	-2.5880252856
H	-9.4085667308	5.058290282	-2.2131708044	S	44.0471835713	-23.4307097318	-3.0206488328
H	-9.7333234253	4.069284107	-0.7589725478	C	41.3213132944	-24.0028906119	-2.75558453
H	-8.0526369702	4.3163165753	-1.3177101718	O	41.0166231851	-22.6708008068	-2.7468233185
S	2.8506672111	2.2110287009	-3.332287733	O	42.2646588687	-28.122753722	-2.8441314304
C	2.5677488318	-1.5576936531	-3.5010702503	C	40.9996559136	-22.0967262321	-1.4457442465
C	0.1112146321	-1.6061587696	-3.5113988553	H	40.7552039091	-21.0408934305	-1.578310017
C	1.3712753063	-2.2474851912	-3.5317631442	H	40.2393765118	-22.5728968163	-0.8136160759
H	-0.7790745823	-2.2272777685	-3.5602744019	H	41.9790393848	-22.1859635493	-0.959727209
H	1.3913501921	-3.3335529655	-3.5621571716	C	42.5627975309	-28.6798154077	-1.5703285136
C	2.4688020052	-0.1295916559	-3.4455892112	H	42.770943379	-29.7383636924	-1.7383875045
C	1.1803520703	0.5251390694	-3.4025513399	H	43.4425793007	-28.1992538956	-1.123899829
C	-0.0338899685	-0.2338493952	-3.4483850657	H	41.7118500736	-28.5800487445	-0.8850748934
N	1.2673451509	1.8525782599	-3.3197112899	C	38.2001368216	-25.9600252934	-2.5442937268
N	3.4931046314	0.7230523629	-3.4291500493	C	34.2729061787	-25.7345383941	-2.2607876909
C	-5.1534012537	0.8792186743	-2.516269859	C	34.6291393455	-27.0576103231	-2.3112683133
C	-1.3394887709	0.4029815924	-3.4003000876	C	36.0240962288	-27.2654558853	-2.4133230002
C	-1.7869004051	1.5480059486	-4.0083058972	C	36.7706883158	-26.1146496143	-2.451650481
C	-3.1495333237	1.8284643635	-3.7561417022	S	35.7045731759	-24.7449445815	-2.3389782226
C	-3.7840785984	0.9065499566	-2.9618561235	C	45.0712355267	-24.8331169046	-3.1119453275
S	-2.6434376532	-0.3228930448	-2.5008002442	H	46.1390627179	-24.6964436108	-3.2283960878
C	9.4279313709	-8.478220489	-6.0366829073	F	-3.7441207841	2.8977825459	-4.2786791976
C	8.1878049944	-8.8500020271	-6.6221080182	F	-1.074916838	2.3189790446	-4.8151914131
C	7.1171443968	-6.9258877901	-5.6935028974	F	7.2562078615	-2.7844421109	-2.6158593319
C	8.3574612535	-6.5535856856	-5.108861971	F	5.2032164958	-1.0064023908	-2.0070352812
C	9.514196361	-7.3017526607	-5.276320029	F	9.1420493197	-12.9428052019	-8.609343479
C	10.4517053413	-9.427919286	-6.3217109483	F	11.1748376432	-14.7646995869	-9.1556205078
H	11.4628081183	-9.3372795145	-5.9394066672	F	18.6543304807	-15.3799945684	-10.5670037601
C	6.080300659	-6.0058966402	-5.3619057642	F	20.9541156412	-16.789363547	-9.8791125256
S	8.2141969474	-5.0942419152	-4.1705986178	F	26.0817232661	-21.9824693522	-0.4135987219

H	5.0533177803	-6.1321831076	-5.687620068	F	28.4270318913	-23.3074483601	0.2951395934
S	8.3134170224	-10.3493002325	-7.4976321062	F	33.7876784759	-28.0795338362	-2.3291636675
C	7.0364221304	-8.0897862107	-6.4735394004	F	36.5377916059	-28.4908140243	-2.48157187

Table S10. The coordinate of **6** (198 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	-2.1211563903	-1.0367020597	0.0254189704	N	-9.3703927897	-13.7014092975	-1.954875816
C	-1.8937994827	1.4301231214	0.4802046668	N	-10.9621988697	-15.567812921	-2.3481300843
C	-2.6302377062	0.2485845949	0.2763395953	C	-14.7931484216	-17.36979069	-3.1126454323
C	-3.0703305184	-2.182264343	-0.1267096546	C	-15.9782564433	-16.591973948	-3.1884919824
C	-2.5917952035	-3.3636287638	-0.7068484787	C	-17.2801737891	-18.5341739362	-3.6873010531
C	-3.4224749347	-4.4568691858	-0.8931670818	C	-16.0935625784	-19.3121927136	-3.6018693648
C	-4.7664787132	-4.4162088209	-0.494303403	C	-14.8569506022	-18.7603493106	-3.3083809104
C	-5.237867298	-3.2439147962	0.1167000971	C	-13.6481474657	-16.5680573732	-2.8453942266
C	-4.4072582632	-2.1479729054	0.2918922818	H	-12.6447985553	-16.9642056228	-2.776683266
H	-3.7053011684	0.3412722528	0.3297196197	C	-18.4167133476	-19.3300467006	-4.0149631386
H	-1.5514047458	-3.4035054396	-1.0121665104	S	-16.4100902556	-20.9923149448	-3.9210880129
H	-3.0302865045	-5.3492517549	-1.3745612808	H	-19.4125062196	-18.9292524782	-4.1485817367
H	-6.2594816957	-3.2055898595	0.483746479	S	-15.6553909795	-14.9062856004	-2.9242524382
H	-4.8035721539	-1.2721490968	0.7960647282	C	-17.2200044654	-17.1496487083	-3.4627164894
C	-2.6311131408	2.7118320793	0.7060444755	C	-13.9303974195	-15.2308862071	-2.711148668
C	-3.9533567409	2.9146527377	0.2924153666	C	-18.1253087405	-20.6600596826	-4.1699496023
C	-1.9558668056	3.7636284874	1.3377713346	O	-18.3349395416	-16.36726489	-3.5531537073
C	-4.5882607172	4.1305555381	0.5215398653	O	-13.7393772837	-19.5430200417	-3.255740401
H	-4.4848669566	2.1331053162	-0.2420738776	C	-19.0822841677	-16.2870203956	-2.3455874785
C	-2.5936595093	4.9747514247	1.575940357	H	-19.9310688407	-15.6325814864	-2.5531738313
H	-0.9220323245	3.6123474989	1.6311253257	H	-19.4479091731	-17.275129974	-2.0396614155
C	-3.9136869367	5.1616363335	1.1709877916	H	-18.479379552	-15.8573799306	-1.5360129138
H	-5.6113995652	4.2752580385	0.1851772229	C	-13.3702692596	-19.9297005033	-1.9376910103
H	-2.0580488178	5.7776970896	2.0753053494	H	-12.4755526308	-20.547181345	-2.0382353855
H	-4.4123005768	6.1100033363	1.3527138684	H	-13.1432830996	-19.0550001028	-1.3158792727
O	-0.8976757323	-1.3468496305	-0.1347287768	H	-14.1669325562	-20.5149708122	-1.4618330298
O	-0.6275093983	1.5323237732	0.533295637	S	-22.6757859624	-20.7730819687	-4.7913779094
Ir	0.7941362418	-0.0274036414	0.0752199339	C	-20.7786961197	-24.0405195197	-5.2165045324
C	2.2901941845	1.2733240825	0.1428786384	C	-18.5597970847	-23.0337413628	-4.722114054
C	3.1233728709	1.5489055882	1.2305748669	C	-19.4075022832	-24.1059268117	-5.0542216718
C	2.47318624	2.0124779379	-1.060467821	C	-21.2972792048	-22.711340912	-5.0116273916
C	4.0902840115	2.5354937687	1.1258775701	C	-20.4401419574	-21.5893662872	-4.6656884605
H	3.0335869265	1.0076206942	2.1663560625	C	-19.0182392863	-21.7494626962	-4.5138725578
C	3.4650278647	2.997464423	-1.1043222869	N	-21.1096369683	-20.4491793151	-4.5148423386
C	4.2850714544	3.2815695739	-0.0297375479	N	-22.5788988516	-22.3629353147	-5.1108958324
H	5.0465481573	4.0491617288	-0.092268636	C	-23.5118371708	-26.4668393629	-6.0286223894

C	1.5976593562	1.6431741491	-2.1629464085	C	-22.4941787449	-27.4498884027	-6.1436996821
C	1.5805210215	2.1877732454	-3.4535647541	C	-24.112460947	-29.1408187481	-6.629521956
C	0.7006845101	1.6913422923	-4.4016205733	C	-25.1295727812	-28.1537247923	-6.5221284165
H	2.2606127318	2.9913477967	-3.6972604665	C	-24.8552854997	-26.8256738541	-6.237029001
C	-0.107950812	0.1503498716	-2.7743491412	C	-22.98024896	-25.1905602339	-5.6898795564
C	-0.1598037841	0.6490181965	-4.064027182	H	-23.5899399372	-24.3120860229	-5.5319586707
H	0.6898638024	2.1141212987	-5.4022598566	C	-24.6480669844	-30.4301379104	-6.9175792589
H	-0.7415805888	-0.6631026243	-2.4386587295	S	-26.7080157527	-28.8376506458	-6.7809686708
H	-0.8581665166	0.2280350924	-4.7789885195	H	-24.0441154768	-31.3218416372	-7.0184349667
C	1.7009619621	-1.8174755169	2.1780459057	S	-20.921234089	-26.7827562166	-5.83535809
C	0.3515596007	-0.0967882269	3.033167797	C	-22.7692099957	-28.7761349059	-6.4494980041
C	1.8218699295	-2.3590535177	3.4643354493	C	-21.6135722718	-25.1800299619	-5.5561088936
C	0.4427009234	-0.589360524	4.3230703211	C	-26.0132449547	-30.4405743139	-7.0335088582
H	-0.2070730741	0.7998458555	2.7880104591	O	-21.7675851591	-29.7002734081	-6.5327523479
C	1.1912139501	-1.745183164	4.5346261276	O	-25.8665136557	-25.9150272577	-6.1243775586
H	2.4115832419	-3.2529409387	3.6093968187	C	-21.2654377601	-29.8844522857	-7.8506195137
H	-0.0616015504	-0.076676601	5.1348216785	H	-20.4729141185	-30.6315436729	-7.7756660581
H	1.2866949594	-2.166107776	5.5315283169	H	-22.0500690569	-30.2489855097	-8.5253332597
C	2.3132205491	-2.3074037206	0.9515294183	H	-20.8503424581	-28.9504200054	-8.2491289775
C	3.1364922803	-3.4328262969	0.846249565	C	-26.0717567534	-25.1354231043	-7.296148372
C	2.0411032727	-1.5426778955	-0.2184205181	H	-26.9037484662	-24.4636819801	-7.0759288452
C	3.7059124449	-3.8343037314	-0.3465892941	H	-25.1805550691	-24.5452517798	-7.5424448318
C	2.6219143463	-1.9374555131	-1.426757741	H	-26.3318723223	-25.771574446	-8.1513048664
C	3.4305095136	-3.0617236708	-1.4677372484	S	-25.1056978043	-34.8574346916	-7.9126238115
H	4.3410612244	-4.7099861094	-0.3985345966	C	-28.7602703401	-33.8112989387	-7.8490589911
H	2.4563247789	-1.383671609	-2.3448956449	C	-28.2631651782	-31.4296664811	-7.3368797531
N	0.9553116341	-0.6919163719	1.9956343196	C	-29.1331189346	-32.5047639484	-7.5958088436
N	0.73634122	0.6338171302	-1.8528962644	C	-27.3304469159	-33.9919991016	-7.8259577054
F	3.9757333399	-3.4302672566	-2.6340539405	C	-26.4129896093	-32.8953301344	-7.563346135
F	3.4073367048	-4.1809669086	1.9324857395	C	-26.8906424572	-31.562730358	-7.3062559142
F	3.6579107551	3.7187398111	-2.2251704013	N	-25.1354372831	-33.2670421196	-7.5895729076
F	4.8772992907	2.7910848632	2.178707701	N	-26.6993965307	-35.1461798378	-8.0348083765
C	-7.5888359569	-6.8236722759	-1.0664932572	C	-30.5349266634	-37.0250925854	-8.5906993678
C	-6.5986095444	-7.8427680501	-1.057891103	C	-31.7451373909	-36.2987401933	-8.4427535976
C	-8.2545655046	-9.5283193922	-1.4147951712	C	-33.037409072	-38.2496143039	-8.9324723536
C	-9.2425650803	-8.507756622	-1.4383965802	C	-31.8252321457	-38.9777777374	-9.0749253833
C	-8.9340600836	-7.164752224	-1.2770735036	C	-30.5782742131	-38.3939209511	-8.9003273935
C	-7.0176430601	-5.5313761403	-0.858973497	C	-29.3911215154	-36.1973373163	-8.3980105287
H	-7.6055219384	-4.6207956359	-0.8451734083	H	-28.3745996149	-36.553337441	-8.4891781405
C	-8.8207796895	-10.8247930587	-1.5908869408	C	-34.1837614433	-39.0792302337	-9.1706407676
S	-10.832753947	-9.171016561	-1.6784056238	S	-32.1301199039	-40.6427895686	-9.4928933875
H	-8.242950055	-11.7391136567	-1.5819277049	H	-35.2029906388	-38.7130294263	-9.1323343346
S	-5.0111208378	-7.1836654669	-0.7891678908	S	-31.4460393443	-34.6275219533	-8.0756174103
C	-6.9053201498	-9.1846287854	-1.2332933073	C	-32.993005503	-36.8895351219	-8.5995948087

C	-5.6597799941	-5.5532816321	-0.7060452132	C	-29.696935666	-34.8922165798	-8.1057363901
C	-10.1805924434	-10.8094801291	-1.7560160278	O	-34.143574073	-36.1613211128	-8.4698316281
O	-5.9262025719	-10.1341611801	-1.1923747793	O	-29.4382931717	-39.1278387034	-9.0655765319
O	-9.911577579	-6.2096616241	-1.2887238906	C	-34.6388141744	-36.110916242	-7.1386328901
C	-5.4473670298	-10.5272441222	-2.4729680245	H	-35.5430573009	-35.4994595806	-7.1688934515
H	-4.6733682785	-11.2759455454	-2.293976538	H	-34.8871851618	-37.1149980753	-6.7714283504
H	-6.2490780664	-10.9670075834	-3.0788821838	H	-33.9103907026	-35.6496068747	-6.4602050938
H	-5.0140575561	-9.6746304145	-3.010334448	C	-28.8759325897	-39.5996212243	-7.8480670762
C	-10.1468518656	-5.649869501	-2.5749184583	H	-27.9863731554	-40.1706275001	-8.1215894275
H	-10.9439258611	-4.9143277416	-2.4493981147	H	-28.5891680974	-38.767573001	-7.1932210635
H	-9.2473633735	-5.1540082206	-2.9611556043	H	-29.5795286321	-40.2520899545	-7.3159972071
H	-10.4686897008	-6.4182242583	-3.2887532275	C	-33.8455890886	-40.357836241	-9.4698907902
S	-9.3732737248	-15.3152272831	-2.125938711	H	-34.5165994823	-41.1763683706	-9.6987869943
C	-12.9810042352	-14.1613262721	-2.4543842991	F	-14.6125827627	-12.4710034774	-2.4583904206
C	-12.4404411381	-11.7583542856	-2.1138991933	F	-18.7826678058	-25.279708277	-5.2196168458
C	-13.3262078213	-12.8276329784	-2.3415074876	F	-30.4344710922	-32.184022705	-7.5823536669
C	-11.5652130497	-14.381393924	-2.2977862957	H	-12.893741263	-10.7734164104	-2.0590070489
C	-10.6318065504	-13.2918992771	-2.0652784717	H	-17.5042425254	-23.2742305705	-4.6416098615
C	-11.0788062129	-11.9272447264	-1.971789282	H	-28.7391019007	-30.4712355774	-7.1539099752

Table S11. The coordinate of 7 (240 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	-17.4056599642	0.6547311999	-1.4352095066	C	6.6052592133	-9.8363413193	-0.2430439265
C	-19.4099209096	2.0311930255	-2.0947074091	C	9.4663836879	-12.4035266199	-0.7263421297
C	-18.0599367476	1.861464455	-1.7362469171	O	5.3464582133	-10.36620517	-0.2787754113
C	-15.9370434416	0.6711005141	-1.1566968858	O	10.5169450602	-8.2395719863	-0.0856988685
C	-15.3658573504	-0.4444608575	-0.5319845194	C	4.73237429	-10.2960518981	-1.5599810304
C	-14.0079493981	-0.4947339702	-0.2598869693	H	3.7444817052	-10.7482740345	-1.4525690426
C	-13.1621092217	0.5659793735	-0.6161660098	H	4.6250782644	-9.2557791268	-1.891803439
C	-13.7310107296	1.6737177372	-1.2634864402	H	5.3107438918	-10.854427783	-2.3064645324
C	-15.0914691095	1.726649816	-1.5229340816	C	11.0362639446	-7.8516386198	-1.3519756933
H	-17.4592296695	2.7592028821	-1.7031919658	H	12.0343153	-7.4503798002	-1.1652216222
H	-16.0118273573	-1.2747849295	-0.266273046	H	11.1074711815	-8.7108729775	-2.0307321775
H	-13.597381235	-1.3630397849	0.2495474709	H	10.4122214829	-7.077637937	-1.8155186059
H	-13.0909928182	2.4849760098	-1.5981757071	C	6.3951158526	-6.2086499814	0.4175816997
H	-15.4847554884	2.5850488884	-2.0583598628	C	4.0089807544	-3.1432115135	0.9529121821
C	-19.9227089257	3.415096425	-2.3355608634	C	5.3058189828	-2.7334489812	1.2125776326
C	-19.3260101145	4.5536391554	-1.780689432	C	6.2620889053	-3.7519771514	1.0529470295
C	-21.064903552	3.5735344449	-3.130076644	C	5.7185641224	-4.9610067822	0.6700539561
C	-19.8478149759	5.8184776218	-2.0295642941	S	4.0003771603	-4.8307030774	0.4976979173
H	-18.4680042025	4.4539651652	-1.122554402	H	5.5411779856	-1.7213286601	1.511334585
C	-21.5793584669	4.8382142808	-3.3878140723	H	7.3235812246	-3.6082727962	1.2265899253
H	-21.5410810357	2.6861469682	-3.5347227565	S	12.5964619402	-19.9100391264	-2.1659360925

C	-20.9707737912	5.96583377	-2.840309603	C	15.632434453	-17.6266068217	-2.0502802015
H	-19.3795081252	6.6914431732	-1.5828762906	C	14.3094338632	-15.5770096341	-1.5710000966
H	-22.460931584	4.9448119024	-4.0142851378	C	15.5084345042	-16.2718649963	-1.8005980259
H	-21.3750565162	6.9551858101	-3.0372312747	H	14.4081484668	-14.5113842055	-1.3878172646
O	-17.9456555902	-0.4932473079	-1.3372572617	C	14.3623417478	-18.3064197607	-2.0509458964
O	-20.264101865	1.1089995981	-2.2869482246	C	13.1091737098	-17.6086148144	-1.8158192047
Ir	-19.977007565	-0.9917558876	-1.8693466383	C	13.0723672937	-16.1913550984	-1.5697883406
C	-21.8894079323	-1.3626083537	-2.2483505459	N	12.0496153646	-18.4132040425	-1.8584804753
C	-22.4423932342	-1.7854662146	-3.4600041381	N	14.1900614512	-19.6105270565	-2.2597532021
C	-22.7592903342	-1.122698506	-1.1471086076	C	11.8416602957	-15.4632939686	-1.3441168334
C	-23.8136344922	-1.9472469975	-3.5720374323	C	10.5485311199	-15.9373709199	-1.2352923743
H	-21.822712356	-1.9917073307	-4.3261368039	C	9.596638319	-14.9251283143	-1.0078881765
C	-24.1350283343	-1.3028521147	-1.3222819043	C	10.1404841474	-13.6588130965	-0.9396390293
C	-24.6894559224	-1.7114042273	-2.5197776397	S	11.859321711	-13.7275657377	-1.1692017398
H	-25.7590106393	-1.844115545	-2.6264630188	H	10.311496095	-16.9896678982	-1.3175133087
C	-22.1074405461	-0.7143807831	0.0884609933	H	8.5354713654	-15.1170290319	-0.887518551
C	-22.7165323165	-0.4375101992	1.3190557168	C	25.4925475559	-19.2604299616	-3.3558409834
C	-21.9398144533	-0.0852966367	2.4110418774	C	25.3456215383	-17.9228725111	-2.8993431516
H	-23.7917484803	-0.5044551587	1.4044032088	C	22.9757575731	-18.1820507729	-2.7280314411
C	-20.0029094645	-0.2903931581	1.0388998698	C	23.1240114908	-19.5232252025	-3.1742687492
C	-20.5551254186	-0.0111436544	2.2766676077	C	24.3581140174	-20.0780219848	-3.4794182423
H	-22.4139776514	0.1279935381	3.3648910579	C	26.8539887134	-19.5785219226	-3.6349476174
H	-18.9347804524	-0.2591034191	0.8542325663	H	27.1693908872	-20.5461994218	-4.0100400463
H	-19.9121717678	0.2568958912	3.1078392106	C	21.6086954737	-17.8486728347	-2.4962009156
C	-18.8080888269	-2.7194437857	-3.8921764647	S	21.5843430928	-20.3263850542	-3.2995034437
C	-19.2015108833	-0.5601554238	-4.7260669786	H	21.2867956155	-16.8669528602	-2.166175688
C	-18.2617840462	-3.0944483202	-5.1263026178	S	26.8791079176	-17.1007060707	-2.8306840463
C	-18.6748856425	-0.8813867885	-5.964765058	C	24.1137808137	-17.3745891262	-2.5735612571
H	-19.5989518553	0.4223997485	-4.4962528289	C	27.7152627434	-18.5407067373	-3.3998173788
C	-18.1946864863	-2.1744991888	-6.1603459892	O	24.0119633324	-16.0781592319	-2.154265568
H	-17.8995370555	-4.103806505	-5.2597402005	O	24.4607649464	-21.3664018959	-3.9227785487
H	-18.6442043559	-0.1339388425	-6.7499156844	C	24.0190373707	-15.9326487328	-0.7393622958
H	-17.7713674451	-2.4671749389	-7.1170271689	H	23.9374818249	-14.8623493385	-0.5398803505
C	-18.985157665	-3.5557499957	-2.7137837334	H	23.1698764033	-16.4563042625	-0.2827106691
C	-18.6202058973	-4.9015103591	-2.6080406467	H	24.9522500169	-16.314898141	-0.3073574908
C	-19.5987045677	-2.9200317605	-1.5971775818	C	24.6917911592	-22.3109319838	-2.8846603872
C	-18.8380786676	-5.6480198564	-1.4662807053	H	24.7411502646	-23.2901212633	-3.365042073
C	-19.8320217221	-3.6720335	-0.4425993021	H	25.6383198612	-22.1077790991	-2.368023856
C	-19.4505668468	-5.0032181287	-0.3990618506	H	23.8739960829	-22.3034741712	-2.153497783
H	-18.5467690759	-6.6897644188	-1.4127736264	C	20.7456919242	-18.8817893581	-2.7456436853
H	-20.3069981588	-3.238753261	0.4313653243	C	16.8937519155	-18.2984507969	-2.2888746121
N	-19.262831636	-1.4462801301	-3.7230503936	C	17.1014378327	-19.6396413689	-2.5627444447
N	-20.7519355163	-0.627191694	-0.0197539009	C	18.4539610571	-19.9741546419	-2.7501081599
F	-19.6758211689	-5.709647582	0.7161545262	C	19.3096415661	-18.8991978825	-2.6225843142

F	-18.029375219	-5.5289492387	-3.6427280878	S	18.4235379495	-17.4525218076	-2.2731322984
F	-24.9853640421	-1.0777961747	-0.302504155	H	16.2873386353	-20.3487060437	-2.6207736949
F	-24.3296518471	-2.3478895869	-4.7410054657	H	18.7958858148	-20.9811568619	-2.9660008158
C	-9.5262002837	1.2013361644	0.069533426	S	35.9024993108	-17.6437913306	-4.0753547279
C	-9.37378304	-0.2112178564	0.0725972911	C	35.2100347635	-21.110907684	-5.4699064078
C	-7.0207622182	-0.0108013189	0.4416358466	C	32.7562191284	-20.9792681401	-5.0927768114
C	-7.1760881614	1.4017497509	0.4554921421	C	33.9271668806	-21.6250881755	-5.5224469899
C	-8.4064596132	2.0194591375	0.2853420569	H	31.8353313384	-21.5416537228	-5.2135969823
C	-10.8802647516	1.5865539626	-0.1717411417	C	35.2500588984	-19.7852040874	-4.9073355393
H	-11.2024726651	2.6209763518	-0.2057132557	C	34.0515511811	-19.097022232	-4.4561936635
C	-5.6589301495	-0.3962890245	0.6193074213	C	32.7528990854	-19.709553057	-4.5492253792
S	-5.6483937982	2.2083662801	0.6777292805	N	34.3006852724	-17.8836535984	-3.9688781382
H	-5.3343091083	-1.4311800784	0.6289604312	N	36.3521230443	-19.0564202641	-4.7391682622
S	-10.8897180356	-1.0122306248	-0.223915062	C	31.5386366472	-19.0532227895	-4.1122713717
C	-8.1456317286	-0.8299544604	0.2637998844	C	31.368839038	-17.8007727647	-3.554321809
C	-11.7273348819	0.5282605712	-0.3414438452	C	30.0271497933	-17.4973612586	-3.253143671
O	-8.0287606232	-2.1908026915	0.2376618291	C	29.1451532231	-18.5089221722	-3.5732742272
O	-8.5142482212	3.3821683863	0.2847370198	S	29.9962622622	-19.8545930226	-4.2637887787
C	-8.1581550222	-2.8010634454	1.5158605103	H	32.2004685587	-17.1332269595	-3.3726003724
H	-8.0525988497	-3.8758421217	1.3556835648	H	29.7109131417	-16.5606983928	-2.805869049
H	-7.3746821778	-2.4533991412	2.201046088	C	41.163695988	-28.2902774736	-9.2952446202
H	-9.1407909566	-2.5927542504	1.956876319	C	39.880257493	-28.8669405738	-9.1031041188
C	-8.822975971	3.9301313493	1.5600491604	C	39.025950472	-26.8116735086	-8.2297961912
H	-8.8746537997	5.0125168607	1.4259434997	C	40.3096057892	-26.2346695037	-8.4248197154
H	-9.7882505222	3.5594141972	1.9274090242	C	41.3747526296	-26.9452051443	-8.9597599679
H	-8.0431644049	3.6904172893	2.2935991301	C	42.0970155854	-29.240423418	-9.8292782185
S	3.3455241476	1.2823118446	1.9854348855	H	43.1366812287	-29.0084371325	-10.0288280693
C	2.7975265721	-2.3507140639	1.0134113802	C	38.1086769162	-25.8827433814	-7.6515074783
C	0.3343821046	-2.1130019338	0.7755501912	S	40.3459307689	-24.573132531	-7.9035259429
C	1.5338844139	-2.8428187735	0.7417043134	H	37.0893922314	-26.1443574076	-7.3887261626
H	-0.5639727346	-2.6699385628	0.5272899645	S	39.8612387857	-30.5433690215	-9.5792846061
C	2.7824237241	-0.9526388864	1.3604636474	C	38.8076862215	-28.1494544024	-8.5873756408
C	1.5535414829	-0.1771017762	1.4014319297	O	37.5908845168	-28.7425998842	-8.4004861791
C	0.2789534221	-0.7708368914	1.0963369945	O	42.6001929273	-26.3596173005	-9.1204582441
N	1.7519631163	1.0943175973	1.7419304006	C	36.6986391465	-28.5738575611	-9.4946860498
N	3.8553633051	-0.2279738728	1.6729984713	H	35.7772640013	-29.0931901489	-9.2235050368
C	-4.8079010159	0.6649809013	0.7662383804	H	36.4828073115	-27.5123721525	-9.670225899
C	-0.963310233	-0.0271242247	1.1145483575	H	37.1096730925	-29.0142407328	-10.4116456981
C	-1.1864270078	1.3062174471	1.3993784903	C	42.7897523747	-25.7811503472	-10.4049381794
C	-2.5411512888	1.6811133096	1.3066057086	H	43.7914247649	-25.3463653548	-10.4026995663
C	-3.3785974443	0.6439915287	0.9518625839	H	42.7211871441	-26.5398490293	-11.1949169872
S	-2.4687713257	-0.8146245026	0.7192740416	H	42.0508349304	-24.9934481571	-10.5981063605
H	-0.3842280945	1.9802377325	1.668647682	C	38.6549678543	-24.6501581599	-7.4209200751
H	-2.9008256776	2.6851078273	1.506553137	C	36.3894300942	-21.8173810404	-5.9270445746

C	9.047961026	-10.134157924	-0.3580349145	C	37.7017568822	-21.3765678406	-5.9132510671
C	7.7220845006	-10.6431406676	-0.4031958181	C	38.6165849665	-22.3107246794	-6.4310219082
C	6.813806706	-8.4682386619	-0.0074948512	C	38.0257075517	-23.4849476689	-6.8494611595
C	8.1397291599	-7.9584084506	0.034844089	S	36.3120487772	-23.425674771	-6.6085110785
C	9.2558996481	-8.761961432	-0.1462371248	H	37.9787814697	-20.4036126697	-5.5316651447
C	10.0171137099	-11.1640071018	-0.54048203	H	39.6860817312	-22.1350023163	-6.4837274094
H	11.0859430409	-10.9824176582	-0.5054161028	C	41.5387335295	-30.4598898251	-10.0294058643
C	5.8452320439	-7.4466379723	0.2197855196	H	42.0245342165	-31.3487383339	-10.4120945142
S	8.15272925	-6.244288276	0.3411703553	F	33.7407413423	-22.8552012532	-6.0253497473
H	4.7792201136	-7.6412989278	0.2650742529	F	16.6154471823	-15.5143683134	-1.7656849569
S	7.7079964016	-12.363026291	-0.6743687092	F	1.3984094949	-4.1347478107	0.4054226959

Table S12. The coordinate of **8** (240 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	-27.603300636	0.1600360991	0.8470917645	O	2.2354318861	1.6754095904	-1.0890258525
C	-30.0344162139	0.7610679751	0.5671690261	C	-1.1924921717	-0.0693605213	-6.0994319628
C	-28.6551843158	0.9660922395	0.3787531256	H	-1.8482395972	-0.6647498922	-6.7375678174
C	-26.196870093	0.5431459537	0.5172597547	H	-1.6421552606	0.9170045867	-5.9290852053
C	-25.1626544835	0.0179989932	1.3014012721	H	-0.2207433785	0.0574848396	-6.5922319216
C	-23.8406855821	0.358398602	1.0620592435	C	2.7714285	2.9272402697	-1.5017584285
C	-23.4980065949	1.2258221289	0.0143389453	H	3.3757646087	3.2920623791	-0.6690460025
C	-24.5318560529	1.7186617174	-0.7972812318	H	3.4033081696	2.8112551784	-2.3913437206
C	-25.8543406034	1.3894783014	-0.5456093995	H	1.9737627218	3.6487328366	-1.7169279817
H	-28.3747041775	1.8409481409	-0.1901860181	C	-2.3134272335	2.0332614428	-1.83652586
H	-25.41891432	-0.6606305843	2.1084492221	C	-5.9533415825	3.3912973077	-1.1857663654
H	-23.0627699063	-0.0378126193	1.7100099563	C	-5.1125766197	3.9341812282	-0.2467919311
H	-24.2902972604	2.3450963032	-1.6510586341	C	-3.7691418869	3.5207200228	-0.3824012646
H	-26.6216549543	1.7683438063	-1.2136565511	C	-3.5474478797	2.6480698319	-1.4184600953
C	-30.9974615603	1.765116091	0.0179302855	S	-5.0481654966	2.3376093287	-2.2369829748
C	-30.6403269869	3.0887686056	-0.2665294839	S	9.5121151487	-6.4824524355	-4.8414613396
C	-32.3226988586	1.3657942678	-0.1959288455	C	11.4116576487	-3.2991625843	-4.0875292239
C	-31.5795959859	3.9830391851	-0.768549498	C	9.4218314785	-1.8477075652	-4.1950504044
H	-29.6321122825	3.4382026159	-0.0655474863	C	10.8125384975	-2.0641103827	-4.008518176
C	-33.2583973337	2.2565136951	-0.707246057	C	10.5174330898	-4.3787997977	-4.392349989
H	-32.6022611242	0.3471130008	0.0529596596	C	9.0983630229	-4.1604245092	-4.5674521076
C	-32.8892575705	3.5682221897	-0.9981376786	C	8.5235191801	-2.848751914	-4.4806584239
H	-31.2888598249	5.0096799068	-0.9744321028	N	8.4209044852	-5.2790661053	-4.8105537814
H	-34.2805182174	1.9279796582	-0.875496235	N	10.8752450687	-5.651386855	-4.5398269042
H	-33.6212072719	4.2672800343	-1.3939162204	C	7.1042228753	-2.6073906833	-4.6729160807
O	-27.7080465861	-0.8708872189	1.5854097946	C	6.2636026695	-3.1750929255	-5.597474183
O	-30.5788688533	-0.2346935121	1.1408446866	C	4.9227483044	-2.7463756794	-5.4828938043
Ir	-29.5500852455	-1.8042361396	2.2075367294	C	4.7027854081	-1.8389114883	-4.4768201553
C	-31.2757546698	-2.5309990755	2.8630490056	S	6.2016177764	-1.513478248	-3.6612157311

C	-32.0290101982	-3.5603617747	2.2916632267	C	21.3865830646	-1.954544244	-4.642410156
C	-31.7815634124	-1.8759197728	4.0215122914	C	20.7636280091	-0.9023624749	-5.3661744235
C	-33.2485356308	-3.910999555	2.847452278	C	18.5964415752	-1.7621786181	-4.8441525381
H	-31.6837108473	-4.0971678626	1.4141293646	C	19.2191307206	-2.8143879987	-4.1203168207
C	-33.0200986881	-2.2737250028	4.5348897913	C	20.5975063096	-2.9205250853	-3.9987886896
C	-33.7743215391	-3.2837673316	3.9700802746	C	22.8078024557	-1.8617248513	-4.6948399775
H	-34.7299561135	-3.5723424391	4.3900902369	H	23.4635306022	-2.5878064948	-4.2262600198
C	-30.92640361	-0.8380264241	4.5784146846	C	17.176288454	-1.878280668	-4.8271192752
C	-31.1696050941	-0.057781444	5.7162928323	S	18.0485013186	-3.9122324645	-3.4462240455
C	-30.2303502656	0.8730480836	6.1296988942	H	16.522393748	-1.1834196209	-5.3431761273
H	-32.0912337806	-0.1939952793	6.2638676394	S	21.9349442415	0.1613191739	-6.0914472122
C	-28.8565863449	0.2317533149	4.2915034305	C	19.3848531172	-0.7831321029	-5.4681885386
C	-29.0468454876	1.0235771871	5.4102057808	C	23.2545559241	-0.7888754981	-5.4183825839
H	-30.4201551869	1.4765618236	7.0128081851	O	18.8121618184	0.2305736967	-6.1822530783
H	-27.9599544616	0.2878811379	3.6840394587	O	21.1702376971	-3.9503521898	-3.3084697612
H	-28.2845850837	1.7369512517	5.7037632113	C	18.5466078817	1.3960578898	-5.4103941237
C	-28.6305125733	-4.1578754178	0.7726620715	H	18.1051809906	2.1234683039	-6.0943236546
C	-29.8985135472	-2.7465792165	-0.6103350705	H	17.8405771349	1.17934446	-4.5987992767
C	-28.4232021122	-5.0262182631	-0.3068798845	H	19.4696132195	1.8086379362	-4.9849644532
C	-29.7263716978	-3.5728124833	-1.7069071818	C	21.3857215253	-3.6673133626	-1.9307664484
H	-30.4770366769	-1.8303842195	-0.6540584524	H	21.8322223321	-4.5650310931	-1.4989798314
C	-28.9702155418	-4.7317547637	-1.5454402868	H	22.0704907409	-2.8192001341	-1.8047260579
H	-27.8379718481	-5.9227820422	-0.1601759793	H	20.4408738493	-3.447240736	-1.4189204415
H	-30.1749092423	-3.3092128174	-2.6584536656	C	16.7293492969	-2.9626460676	-4.1211822359
H	-28.8090919047	-5.4066149979	-2.3813333332	C	12.8351349625	-3.5034583213	-3.8834588776
C	-28.1595495029	-4.3208729297	2.1404420564	C	13.4569840618	-4.5248555326	-3.2099524485
C	-27.3950770875	-5.3907887731	2.6161971029	C	14.8667855008	-4.4425007855	-3.2316648427
C	-28.5399856866	-3.2909281979	3.0470312363	C	15.3596374655	-3.3581913133	-3.9138710297
C	-26.9970823217	-5.4978550655	3.9346889003	S	14.034906522	-2.4219102839	-4.5356208621
C	-28.1490808256	-3.3977193413	4.3844986378	S	30.4037621779	2.8896739673	-4.9996191379
C	-27.3936460963	-4.4833948928	4.7968814509	C	31.4519839812	-0.7437843953	-4.8899607942
H	-26.4063593069	-6.3389985977	4.2759903866	C	29.1865475577	-1.6189162083	-5.3165374578
H	-28.4221003247	-2.6465029592	5.1181501182	C	30.5752481846	-1.787312489	-5.0723197017
N	-29.3663885397	-3.0262229513	0.5870470292	C	30.8569467239	0.5588478116	-4.9788172577
N	-29.7657653503	-0.6650669477	3.8856063875	C	29.4395765331	0.730021161	-5.2108380184
F	-27.0226998701	-4.5692229795	6.0808441108	C	28.56843748	-0.3936672557	-5.4027002505
F	-27.0124602536	-6.3765562653	1.7825432221	N	29.0600789485	2.0048216668	-5.2268640284
F	-33.5303865916	-1.6693940508	5.6248429412	N	31.5124196874	1.7102152917	-4.8599763275
F	-33.9619613049	-4.895555547	2.2862213696	C	27.1473697739	-0.2376594835	-5.6592253524
C	-20.2402045976	2.8396620959	-0.9191679845	C	26.5267064587	0.6926671095	-6.4549378177
C	-19.6126885047	1.713863129	-0.3202911071	C	25.1176768851	0.5988960494	-6.4434265417
C	-17.4477817162	2.5807827535	-0.842027738	C	24.6242134806	-0.4078660303	-5.6516869431
C	-18.0745765997	3.7094390507	-1.4342805801	S	25.9471257692	-1.249994279	-4.9043885325
C	-19.4538113701	3.8608911551	-1.472355367	C	40.8587476334	-4.3092292039	-5.6020865898

C	-21.6639227262	2.7496891622	-0.8525786405	C	40.0252379805	-5.1180463543	-6.420734239
H	-22.3209613018	3.5184203801	-1.2425198865	C	38.1022528246	-3.8303243624	-5.8241671263
C	-16.027336779	2.6564892657	-0.9355304108	C	38.9354541533	-3.0212945278	-5.0068348033
S	-16.9087789252	4.8229565957	-2.0903535803	C	40.3024731579	-3.235800886	-4.8930857974
H	-15.3701324617	1.8784798181	-0.5618663762	C	42.2217854326	-4.7571419967	-5.6270939928
S	-20.7890118069	0.58429158	0.2879454431	H	43.0138684709	-4.2903144015	-5.0534248958
C	-18.2330560618	1.5708125321	-0.2650567231	C	36.7390418117	-3.4148714504	-5.7629894799
C	-22.1123004269	1.617809299	-0.2331355021	S	38.0267924245	-1.7839148089	-4.1862963058
O	-17.6537077343	0.4700377967	0.2995049662	H	35.9435940107	-3.9237769472	-6.2970308775
O	-20.0277057564	4.9521786304	-2.061984743	S	40.9352271933	-6.3928044841	-7.1857742346
C	-17.4063558814	0.6041648632	1.6937641521	C	38.6610653869	-4.8901573328	-6.5528368509
H	-16.9541741807	-0.3352979771	2.0175842095	O	37.8797077011	-5.692652082	-7.3350986723
H	-16.7150715954	1.4326399836	1.8938367326	O	41.0728599211	-2.4476657295	-4.0845338477
H	-18.3382098975	0.7703994706	2.2481670185	C	37.7788870232	-5.2545991011	-8.6844397292
C	-20.2500272554	6.034654307	-1.1665911975	H	37.1427749954	-5.9793616958	-9.1963780007
H	-20.6981535306	6.8357656093	-1.7577294265	H	37.321436855	-4.2587953364	-8.743249684
H	-20.9357461913	5.745723576	-0.3600506841	H	38.7633169096	-5.2278336324	-9.1676731611
H	-19.3080173616	6.387944923	-0.7292560327	C	41.6336159821	-1.323237932	-4.7501276678
S	-8.3611219407	7.2551850531	-0.8923063611	H	42.2085088511	-0.7765563579	-3.9999909028
C	-7.3746280947	3.6335504011	-1.3621588098	H	42.2983432296	-1.6371280956	-5.5649748924
C	-9.6677411302	2.8596049535	-1.8324289724	H	40.8500136988	-0.6710353231	-5.1553408692
C	-8.2743671585	2.6396206221	-1.6670932866	C	36.5374412375	-2.3379725103	-4.9432970409
C	-7.9488767138	4.9419856085	-1.2345413215	C	32.8687030932	-0.9340055598	-4.6339358366
C	-9.3697838408	5.1634878989	-1.3878172266	C	33.6752262725	-0.2383383278	-3.768322901
C	-10.2664695248	4.0914737935	-1.7120118192	C	35.025846507	-0.6499077164	-3.7962320811
N	-9.7270321329	6.4311134281	-1.2011211205	C	35.2874965858	-1.6739712604	-4.671667405
N	-7.2692968531	6.0541855653	-0.9686570341	S	33.8170959805	-2.1279400472	-5.4775148976
C	-15.585007783	3.7898549471	-1.5627512091	C	42.3973732218	-5.8395797592	-6.4243931123
C	-11.6926283302	4.3021875307	-1.8879689067	H	43.3200970306	-6.3752425433	-6.6092928945
C	-12.3224867101	5.3434324471	-2.5221116756	F	31.000705004	-3.048459082	-5.0288952608
C	-13.7318071569	5.2707245194	-2.469018716	F	11.5319032513	-0.9743533819	-3.7453783251
C	-14.2169872999	4.1727744872	-1.803310459	F	-7.868776285	1.3816392883	-1.8282259012
S	-12.8850438323	3.2131839452	-1.2342753783	F	-10.3897087722	1.7775438161	-2.1168495649
C	1.9597118418	0.1660654801	-2.9460307056	F	9.0169195885	-0.5845953506	-4.0726314655
C	1.1025369153	-0.446809932	-3.8992329918	F	28.4889764376	-2.7441719046	-5.4603113258
C	-0.786838541	0.7248705973	-3.0234532497	F	35.9390537914	-0.0825193117	-3.0126115273
C	0.0708125131	1.3388601262	-2.0713658945	F	33.2684520699	0.702408207	-2.9311773494
C	1.4343005134	1.0843592771	-2.0240191733	F	27.1433962022	1.5821674262	-7.2160774166
C	3.3052474992	-0.2829727362	-3.0807122887	F	24.361673173	1.4221752729	-7.1647470952
H	4.1057571684	0.0530790624	-2.4303690389	F	15.6242757397	-5.3468914691	-2.6169411917
C	-2.1402941529	1.1402462408	-2.8595996181	F	12.8411425494	-5.4898656781	-2.5465594045
S	-0.8059546407	2.399347198	-1.0054447949	F	6.6316094704	-4.0107627291	-6.5549634705
H	-2.9505667132	0.7642600351	-3.4751294005	F	3.9793808439	-3.1909809809	-6.3086920078
S	1.96911096	-1.5528605922	-4.9266193731	F	-2.824399665	3.9482899079	0.4509112302

C	-0.2567020946	-0.1744015212	-3.9617891887	F	-5.4823375594	4.7356953491	0.7390130889
C	3.4748163838	-1.192503977	-4.0897157649	F	-11.7147401839	6.3211084694	-3.1748146147
O	-1.0599985649	-0.7892966684	-4.8792307526	F	-14.4960120435	6.1984101313	-3.0395439853

Table S13. The coordinate of **9** (198 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	-2.0937181965	-0.984231003	-0.0706577069	N	-9.3677991784	-13.3623641881	-2.9936454552
C	-1.8457964757	1.4605798369	0.4875493007	N	-10.8996493456	-15.2785970474	-3.3720485608
C	-2.5891156626	0.3095492231	0.1662365344	C	-14.7005710436	-17.247578158	-3.8103607306
C	-3.0584424592	-2.0888391461	-0.3556189068	C	-15.9209769946	-16.5614856259	-3.5707878521
C	-2.5825358975	-3.2433476708	-0.9884465316	C	-17.1763360536	-18.5467625393	-4.0105902169
C	-3.4289796045	-4.3030974353	-1.2718330312	C	-15.9554444157	-19.2336542848	-4.2451809718
C	-4.7846612984	-4.2598726543	-0.9133452693	C	-14.7194341952	-18.6121340085	-4.1425840745
C	-5.2542297191	-3.1133757697	-0.2531242117	C	-13.5733862098	-16.3896208101	-3.6725672801
C	-4.4096864201	-2.0470220437	0.0125559737	H	-12.5544648193	-16.7141178878	-3.8296878718
H	-3.6599225404	0.4367062198	0.0901610078	C	-18.3050615604	-19.3953005367	-4.1899316829
H	-1.5312823718	-3.2928753792	-1.2525700778	S	-16.2259505017	-20.8925665588	-4.6813539377
H	-3.036002221	-5.1740101537	-1.7905189457	H	-19.3266695963	-19.0605762861	-4.0774021513
H	-6.286001481	-3.0734545443	0.0836694786	S	-15.6512840188	-14.8878368594	-3.1919024493
H	-4.8027197679	-1.1924710837	0.5548274668	C	-17.1561525144	-17.1878552649	-3.6551965065
C	-2.5627122313	2.7642998847	0.6374102604	C	-13.90169503	-15.0996431489	-3.337335213
C	-3.8004343885	3.0255332031	0.0374095276	C	-17.9760843096	-20.6809758227	-4.541656731
C	-1.9541944976	3.7746732926	1.3923813157	O	-18.3114545182	-16.4935174949	-3.4373235095
C	-4.4212137265	4.2588727907	0.2039105815	O	-13.5668954898	-19.2983496145	-4.3970161898
H	-4.2709151546	2.2756276795	-0.5914875571	C	-18.7915382129	-16.5831638524	-2.1014341653
C	-2.5798165633	5.0028334843	1.5676988456	H	-19.702144957	-15.982269176	-2.0614507961
H	-0.9814980783	3.5779847887	1.8318512326	H	-19.0253047146	-17.6211589914	-1.833702038
C	-3.8172867319	5.2483388078	0.9760407158	H	-18.058036589	-16.1822398313	-1.3909807105
H	-5.37682301	4.4497945857	-0.2769854911	C	-12.9438678669	-19.8291532223	-3.233690547
H	-2.0986838642	5.7733453258	2.1642179573	H	-12.0506187071	-20.354708585	-3.5768338755
H	-4.3053265736	6.2102541456	1.1086976243	H	-12.6548663149	-19.0302748734	-2.5395075273
O	-0.8702945113	-1.3325906257	-0.1093129426	H	-13.6068973194	-20.534770486	-2.7179283208
O	-0.595640039	1.515319144	0.7133574056	S	-22.5554708932	-20.9224298751	-4.2428413678
Ir	0.8104770297	-0.1070567635	0.4657680891	C	-20.7390359395	-24.0737346161	-5.3438055439
C	2.3277156166	1.1080458468	0.8630289386	C	-18.4946010109	-23.0304452903	-5.2047237536
C	2.950108395	1.3083794443	2.0980526958	C	-19.3675728643	-24.1165986557	-5.4648986836
C	2.7748859821	1.8652471149	-0.2571820494	C	-21.2206458767	-22.7835451764	-4.9148577475
C	3.9694866	2.239432359	2.2133930641	C	-20.3249535853	-21.6695947626	-4.6470221776
H	2.6546157256	0.7500417331	2.9799071275	C	-18.8943137745	-21.7773100258	-4.7955409347
C	3.8070459535	2.7913491711	-0.0774027039	N	-20.9697955728	-20.5729852585	-4.2599324545
C	4.4204819371	3.000734276	1.1424392115	N	-22.4991469069	-22.4730728071	-4.7214891554
H	5.219261059	3.7238212192	1.252106215	C	-23.5453725884	-26.5002255849	-5.8306620932

C	2.1035158652	1.5789749171	-1.5166009517	C	-22.5614717911	-27.4261741083	-6.2687491793
C	2.3542155707	2.1594600157	-2.7665354225	C	-24.2273925478	-29.105654118	-6.6065531345
C	1.6362033932	1.7457537632	-3.8770593418	C	-25.2122448897	-28.1773894004	-6.1756500489
H	3.1107768667	2.9263671977	-2.852451282	C	-24.8972650105	-26.8807847252	-5.7960327486
C	0.4574016898	0.2127976432	-2.4856926495	C	-22.9717538247	-25.2496098113	-5.4663175074
C	0.6701156109	0.7510682103	-3.7426748238	H	-23.5474968051	-24.4164474666	-5.0886322009
H	1.8328397711	2.196749281	-4.845627576	C	-24.795323369	-30.370257886	-6.9293453329
H	-0.2724713439	-0.567204966	-2.2981323692	S	-26.8005324063	-28.8798288004	-6.1787534665
H	0.0911447028	0.396519684	-4.5883702296	H	-24.2125354573	-31.2193826404	-7.2574575384
C	1.2182227104	-2.0127634774	2.6228508112	S	-20.9669311158	-26.7397567347	-6.2178219278
C	-0.1976665827	-0.2586729184	3.2787623992	C	-22.8787949837	-28.7172729013	-6.6652811439
C	1.0640943047	-2.6055289779	3.8826131868	C	-21.6084392449	-25.2035802216	-5.6209508501
C	-0.3794198187	-0.80080353	4.5388600425	C	-26.1571632554	-30.4198906248	-6.7638889645
H	-0.6605669287	0.6718620473	2.969613875	O	-21.9052458313	-29.5889415477	-7.0611863948
C	0.2644481219	-1.9994880174	4.8382647471	O	-25.8678715765	-26.0219557022	-5.3666927177
H	1.5755947711	-3.5330202887	4.0966462106	C	-21.7058184909	-29.6262113038	-8.4689268434
H	-1.0101372128	-0.2932695813	5.2604396648	H	-20.9062678724	-30.3479854496	-8.6467962948
H	0.1464090514	-2.460393523	5.8148582342	H	-22.6154823161	-29.9514463264	-8.9889649298
C	2.034353266	-2.4896006798	1.5158553506	H	-21.402120172	-28.6435540117	-8.8505796325
C	2.8160278775	-3.6491547315	1.5217518212	C	-26.362872962	-25.1583709264	-6.3826146473
C	2.0241227334	-1.6729925544	0.3494851147	H	-27.1283096311	-24.5382566695	-5.9120433086
C	3.5883448456	-4.035940064	0.4437333625	H	-25.5664470279	-24.5176634374	-6.7811860953
C	2.8111141786	-2.0529393349	-0.7410537135	H	-26.8112450116	-25.7313743508	-7.2036764502
C	3.5663628223	-3.2125369752	-0.6749054784	S	-25.2271606782	-34.6525416664	-8.2956036251
H	4.1856000206	-4.9387960027	0.4764692973	C	-28.8588327635	-33.8803102206	-7.4853206248
H	2.8485753671	-1.459957133	-1.64878833	C	-28.3831261518	-31.5480749923	-6.7933916169
N	0.5709615958	-0.8451518246	2.3514070446	C	-29.2520939529	-32.6452221643	-7.0197750466
N	1.1461113728	0.6153709854	-1.4093473664	C	-27.4388559639	-33.9579193982	-7.726953318
F	4.311702437	-3.5661039048	-1.7298699533	C	-26.5478686009	-32.8315525995	-7.4974443262
F	2.8418073371	-4.446067813	2.6070095851	C	-27.0224487608	-31.5611792185	-7.0064072946
F	4.2480389081	3.5274981906	-1.1151929753	N	-25.2804768067	-33.1113983993	-7.7868092147
F	4.553066256	2.4230347611	3.4046316282	N	-26.8006040879	-35.0351422524	-8.1748096919
C	-7.6309049787	-6.6143087462	-1.5869904286	C	-30.5780860288	-37.104692369	-8.2968757474
C	-6.6422978242	-7.6299640842	-1.6981038623	C	-31.7812306746	-36.4732954864	-7.8871829466
C	-8.3169705064	-9.2844934535	-2.104559603	C	-33.045539248	-38.4371740002	-8.3946421162
C	-9.3047684769	-8.2702509009	-2.0017612317	C	-31.8393865277	-39.0713688451	-8.7989594215
C	-8.9840804439	-6.9407373368	-1.7572342592	C	-30.607451379	-38.4339153206	-8.7484520294
C	-7.0494272999	-5.3411885935	-1.3037076179	C	-29.4564684649	-36.2331608083	-8.1877376418
H	-7.6382843281	-4.4380003734	-1.1933104384	H	-28.4522359702	-36.5148156928	-8.4716984348
C	-8.8916351195	-10.5653705316	-2.3392274665	C	-34.1776003153	-39.3045599832	-8.5528521956
S	-10.9060181228	-8.9173197486	-2.1887980084	S	-32.1324062475	-40.6975825093	-9.354622533
H	-8.3106711115	-11.4724401372	-2.4287496133	H	-35.1938998682	-39.0071950119	-8.322274661
S	-5.0442047449	-6.9913114454	-1.4406368369	S	-31.5047809188	-34.8351633931	-7.3816038285
C	-6.9587844349	-8.9535097993	-1.9628608843	C	-33.0105279012	-37.1196088117	-7.9192709346

C	-5.6871295365	-5.3725094015	-1.2010934821	C	-29.77284265	-34.9870660219	-7.7084092913
C	-10.2614547774	-10.5480329803	-2.4206625532	O	-34.1549733986	-36.4777114952	-7.5351966428
O	-5.9809169229	-9.9030780304	-2.0400018598	O	-29.4735633259	-39.072189668	-9.1622547149
O	-9.9546301292	-5.9847981444	-1.6443756037	C	-34.4673204433	-36.6440786593	-6.158351432
C	-5.5648754954	-10.1945146168	-3.3684169566	H	-35.3861348446	-36.0815990037	-5.9805443395
H	-4.7820561501	-10.950985434	-3.285765056	H	-34.631806502	-37.7016753699	-5.915549967
H	-6.3948173657	-10.5904213	-3.966687219	H	-33.6683721198	-36.2478848494	-5.5193457653
H	-5.1594189886	-9.3010049483	-3.859156901	C	-28.7319953586	-39.6686358585	-8.1057393253
C	-10.3139716276	-5.3863715683	-2.8832918848	H	-27.8672607557	-40.1473183222	-8.5695237669
H	-11.0948365004	-4.6572091411	-2.6580146008	H	-28.3906403792	-38.9147828986	-7.3854551432
H	-9.4554866822	-4.8762930595	-3.3385316412	H	-29.3305957845	-40.4240923347	-7.5816913474
H	-10.7045508734	-6.1320145105	-3.5867758862	C	-33.8339588669	-40.5211049256	-9.0436387331
S	-9.3098714004	-14.9540994355	-3.3098378285	H	-34.495893373	-41.3497405355	-9.2624248161
C	-12.982359833	-13.9965324514	-3.118932265	F	-13.1272751919	-10.4513204461	-2.413345592
C	-12.5091257978	-11.6105391627	-2.6421646206	F	-14.6787084596	-12.3916193337	-2.7979689173
C	-13.3840715036	-12.7043322982	-2.8614032245	F	-17.203915042	-23.3094253368	-5.3897062811
C	-11.5474746826	-14.1393639854	-3.1464355875	F	-18.7512058465	-25.2330348349	-5.8539304793
C	-10.6500651012	-13.0174787706	-2.9217849059	F	-28.9924583189	-30.4520693662	-6.3403522741
C	-11.1338207558	-11.6853676232	-2.6536025661	F	-30.532161224	-32.3955657654	-6.7413299211

Table S14. The coordinate of **10** (240 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	-17.6112740808	0.7593442416	-1.1791030546	C	9.501092967	-12.2720794443	-1.3461734306
C	-19.5894177027	2.1749433163	-1.8342367743	O	5.3466797857	-10.2847719145	-0.9842917141
C	-18.2429395595	1.9791880798	-1.4761636167	O	10.4719627812	-8.2202518896	-0.1117892095
C	-16.142679531	0.7467951804	-0.9009355369	C	4.8425149987	-10.066119453	-2.2964556934
C	-15.5911136641	-0.3845499035	-0.2869651137	H	3.850577709	-10.5212994693	-2.3244227142
C	-14.2341048814	-0.4618637426	-0.0167823296	H	4.7602165656	-8.9942333173	-2.5158784985
C	-13.369579188	0.5869375071	-0.363486771	H	5.4835312622	-10.5399157237	-3.0501684426
C	-13.9190066175	1.7110626389	-0.999102383	C	11.1107154517	-7.7216033419	-1.2809164642
C	-15.278447169	1.7905867218	-1.2573955606	H	12.0867491655	-7.3497646138	-0.9630444931
H	-17.6262789867	2.8658577251	-1.4398218314	H	11.2459562364	-8.5139938248	-2.0276337109
H	-16.2517408789	-1.2055126808	-0.0283185943	H	10.5345486989	-6.901424423	-1.7268699485
H	-13.8385282322	-1.3423108918	0.483567112	C	6.3141287964	-6.2529352319	0.3043298474
H	-13.2645385758	2.5139713442	-1.3259656635	C	3.8630845662	-3.2842946814	1.0458190883
H	-15.6561033661	2.6612112571	-1.7842625897	C	5.1439417311	-2.8810877481	1.3823823082
C	-20.0774579446	3.5693296447	-2.0659404319	C	6.1212600172	-3.8674469123	1.1608474346
C	-19.4623074015	4.6926540918	-1.5003607282	C	5.6099772711	-5.0438533411	0.6516592663
C	-21.2150925301	3.7539701184	-2.8612941747	S	3.8955647419	-4.9239122539	0.4413925192
C	-19.961639932	5.9683948738	-1.7394575157	H	5.3534425077	-1.8967314812	1.7776488064
H	-18.6076143496	4.572324155	-0.8413646477	H	7.17498657	-3.7238769669	1.3762512556
C	-21.7070599422	5.0295155277	-3.1092540102	S	12.6489928719	-19.672731827	-3.119927244
H	-21.7056075625	2.8782755765	-3.2742068498	C	15.7153190996	-17.4370281291	-2.9266055973

C	-21.0802950812	6.1418224459	-2.5509937933	C	14.4077303984	-15.4020906187	-2.3923663072
H	-19.4792811498	6.8293572078	-1.2844933299	C	15.6175417798	-16.0923360706	-2.6385903406
H	-22.585352806	5.1567099616	-3.7365000871	C	14.433257027	-18.0964990754	-2.9509508512
H	-21.467186489	7.1395842475	-2.7402970574	C	13.1896954401	-17.3869720878	-2.6964584315
O	-18.1735439695	-0.3781741978	-1.0842889764	C	13.1541794426	-15.9757020194	-2.4033188202
O	-20.4598657039	1.2692928526	-2.0324714371	N	12.1225855564	-18.1775842358	-2.766401338
Ir	-20.2126665718	-0.8378939683	-1.6231183989	N	14.2460490624	-19.3892387525	-3.2005351356
C	-22.1305874942	-1.1697262318	-2.0099186446	C	11.9310541215	-15.2427998019	-2.1498755859
C	-22.6878558613	-1.575431534	-3.2254725961	C	10.63665082	-15.733501809	-2.1336360475
C	-22.9993344956	-0.9186908268	-0.9102891028	C	9.6667312411	-14.7546463094	-1.8556914526
C	-24.0615667914	-1.7104418016	-3.3425790916	C	10.1971272316	-13.4969825972	-1.6522016992
H	-22.0696031907	-1.788714719	-4.0908874451	S	11.9204341889	-13.526725344	-1.8171569672
C	-24.3776556207	-1.0720224009	-1.0904191702	H	10.4125519007	-16.7753553058	-2.3160502854
C	-24.9360349953	-1.4638960251	-2.2916642532	H	8.6044584188	-14.966492537	-1.7923048023
H	-26.0075700148	-1.5757324475	-2.4022944741	C	25.5572921423	-19.1657870659	-4.2354066838
C	-22.3439944804	-0.5273308438	0.3289903994	C	25.4173891283	-17.8079523722	-3.8399791558
C	-22.9514392389	-0.2443406254	1.5590080631	C	23.0462079769	-18.0465102798	-3.6589787093
C	-22.1714077116	0.0901276824	2.654215156	C	23.1869974882	-19.4061581526	-4.0473871823
H	-24.0278900683	-0.2926495944	1.6413059125	C	24.4179807346	-19.9809536396	-4.3266924485
C	-20.2347146968	-0.1441242554	1.2864891855	C	26.9167039897	-19.5021724129	-4.5042320508
C	-20.785321666	0.1405349998	2.5237267497	H	27.22542093	-20.4806721452	-4.85597466
H	-22.6442225628	0.3082047092	3.6076623485	C	21.6810609083	-17.6960907269	-3.4425395948
H	-19.1657221743	-0.1313308903	1.1047169121	S	21.643673398	-20.2069724736	-4.1359338212
H	-20.1400472618	0.3942757897	3.3575861189	H	21.3650503595	-16.6977782922	-3.1596455447
C	-19.0637068582	-2.5815350612	-3.6440594128	S	26.9563933225	-16.9944221546	-3.8004247446
C	-19.4098523405	-0.4124872172	-4.4733155102	C	24.1882993983	-17.2388744494	-3.5399933351
C	-18.5137736353	-2.9622649962	-4.8748321002	C	27.7833722194	-18.4593969719	-4.3158576309
C	-18.8785946593	-0.7389973513	-5.7086424803	O	24.0914652711	-15.925074627	-3.1779149194
H	-19.7907753905	0.5765168208	-4.2432642379	O	24.5095556954	-21.2874894562	-4.7152681519
C	-18.420623009	-2.0400773098	-5.904828549	C	24.1143473053	-15.7164999476	-1.7709596153
H	-18.1689011717	-3.9776354054	-5.0086453508	H	24.0365114853	-14.638213526	-1.6186861275
H	-18.8271552604	0.0105834249	-6.4906679891	H	23.2693084225	-16.2176450359	-1.2824474116
H	-17.9942566836	-2.3370888025	-6.8588158235	H	25.0515545275	-16.0808795601	-1.3323424649
C	-19.2659406906	-3.4182888978	-2.4701107388	C	24.7739021965	-22.1858395272	-3.6445200191
C	-18.9300321631	-4.7718316329	-2.3673859343	H	24.8139863304	-23.1844936257	-4.0838512861
C	-19.874153975	-2.7741458143	-1.355413191	H	25.7335259897	-21.958324552	-3.1637015376
C	-19.1717319958	-5.5181320068	-1.2303030761	H	23.9765162872	-22.1490710649	-2.8919633151
C	-20.1315385303	-3.5257752551	-0.205718287	C	20.8127706787	-18.7344091045	-3.6480815488
C	-19.7784081242	-4.8648314465	-0.1649270136	C	16.9681280082	-18.1174613772	-3.1807452213
H	-18.9027064142	-6.5659501396	-1.1789488793	C	17.1595694718	-19.4538107308	-3.4872172731
H	-20.6042126172	-3.0861310424	0.6662826582	C	18.5081917598	-19.7993662421	-3.6804089127
N	-19.4962789296	-1.3008744476	-3.4741447532	C	19.3765023288	-18.7377511301	-3.5256740184
N	-20.9868406291	-0.464052069	0.2248466891	S	18.5077471502	-17.2904581618	-3.1388876186
F	-20.026865198	-5.570876928	0.9456202546	H	16.3371802581	-20.1512542489	-3.5654874246

F	-18.3453240323	-5.4074421887	-3.4005712022	H	18.8381998562	-20.8037216225	-3.924762008
F	-25.2267507857	-0.8361203425	-0.072027636	S	35.9089447375	-17.4565596815	-5.2124804226
F	-24.5814582284	-2.0947715801	-4.5153556161	C	35.4264004185	-21.1949080573	-5.6908677563
C	-9.7227265918	1.1455822055	0.3311847644	C	32.9730481177	-21.0921368267	-5.3628305462
C	-9.5948032555	-0.2690615232	0.3032331817	C	34.1813675879	-21.7821995309	-5.6168409103
C	-7.2383571116	-0.1183311505	0.6742645175	C	35.3832250037	-19.7692815256	-5.4792094769
C	-7.3692061096	1.2960618832	0.7211484684	C	34.1408902912	-19.0597928549	-5.2182086524
C	-8.5888765867	1.9386944871	0.5651295091	C	32.8679479557	-19.7336758495	-5.1529952886
C	-11.0703665685	1.5592122012	0.0998121404	N	34.3201733283	-17.7525544396	-5.0522518292
H	-11.3751403565	2.5994315861	0.0889242414	N	36.441426674	-18.9640091047	-5.4981177045
C	-5.8832804492	-0.5318225029	0.8427596996	C	31.615828825	-19.0531022363	-4.8948184457
S	-5.8271177951	2.0699499941	0.9606964008	C	31.4141105692	-17.70008555	-4.6825565099
H	-5.5759888487	-1.5719060703	0.8310965362	C	30.068555747	-17.3595992678	-4.4591436573
S	-11.1246043226	-1.0375850709	-0.0073954421	C	29.2134697834	-18.4421025226	-4.4968430803
C	-8.3776476684	-0.9132414502	0.479354373	S	30.0908631682	-19.9027995482	-4.8050489359
C	-11.9353870124	0.5193705919	-0.0911945742	H	32.2266521435	-16.9869191708	-4.6948423534
O	-8.287431911	-2.2751994061	0.4221548476	H	29.7299370133	-16.3433667276	-4.286051251
O	-8.6742762379	3.3029008914	0.5965080176	C	41.8047849154	-28.7627205931	-7.5928598079
C	-8.3998637634	-2.9101290118	1.689724173	C	40.514885966	-29.3315136072	-7.4205510914
H	-8.3184105025	-3.9830088153	1.5046862198	C	39.5539175278	-27.1758905581	-7.0394513216
H	-7.5950174389	-2.5922763011	2.3644838985	C	40.8433696016	-26.6070165678	-7.218945863
H	-9.368431619	-2.6927069599	2.1568482334	C	41.9650627286	-27.3723462599	-7.5028230737
C	-8.9621636658	3.8252635951	1.8871550636	C	42.7985299668	-29.7683928774	-7.8380969941
H	-8.9980817387	4.9112490472	1.7792243126	H	43.851095443	-29.5482279713	-7.9730952454
H	-9.9297129981	3.4608567567	2.2549744865	C	38.5730001878	-26.1824147344	-6.7422870123
H	-8.1794218984	3.5561290304	2.6072785116	S	40.8094642285	-24.8767012603	-7.0252622326
S	3.0909918845	1.0337397793	2.4075820803	H	37.5343484005	-26.4205192971	-6.539787883
C	2.6372108326	-2.5186633742	1.138317481	S	40.5633269084	-31.067642929	-7.5649134996
C	0.1858252836	-2.2885608275	0.8642689357	C	39.3876765939	-28.5630663684	-7.1556669359
C	1.3975376713	-3.0147874232	0.7956550739	O	38.1653282356	-29.1461746716	-6.9758093622
C	2.5836060741	-1.1518273425	1.594071481	O	43.1916545098	-26.7864557168	-7.6500651393
C	1.3378971952	-0.4041928143	1.6624248902	C	37.3884978162	-29.2266062436	-8.1642921316
C	0.0718267114	-0.9798777971	1.2822691331	H	36.4515539509	-29.7137114507	-7.8869622543
N	1.5069636515	0.8377131732	2.1070447534	H	37.1769741994	-28.2283449134	-8.5678653282
N	3.6341579501	-0.43904208	1.9900924448	H	37.8980250282	-29.8242287463	-8.9303505555
C	-5.0140507173	0.5105092555	1.0145368458	C	43.531198327	-26.5042198221	-9.0013087773
C	-1.1825118735	-0.2570848809	1.3291173388	H	44.5195604998	-26.0405339195	-8.9802075474
C	-1.3912630502	1.0585066703	1.7059829069	H	43.570110914	-27.422355787	-9.6010809983
C	-2.7375982219	1.4585357817	1.6319031184	H	42.8122502584	-25.80996305	-9.4540294764
C	-3.5846531841	0.4582237691	1.2013006379	C	39.0790865871	-24.9120873768	-6.703700035
S	-2.7000562954	-0.9917878301	0.8687761952	C	36.6479345266	-21.9275110318	-5.9522676941
H	-0.5837347161	1.7009177965	2.0288284486	C	37.9361804235	-21.4276055318	-6.0328303387
H	-3.0837362692	2.4506505182	1.9023919481	C	38.9055720216	-22.4097983971	-6.3016345665
C	9.0423132815	-10.0625547731	-0.7388836285	C	38.3813521213	-23.6796096022	-6.4317189656

C	7.7269886329	-10.5559202892	-0.9537022456	S	36.6626830554	-23.654648488	-6.2225937932
C	6.7779106996	-8.444349007	-0.3610078416	H	38.1572470047	-20.3780014615	-5.8969000361
C	8.093133161	-7.949291761	-0.1500915464	H	39.9652853834	-22.1945851615	-6.3911096067
C	9.2247921168	-8.728552668	-0.3407333036	C	42.2771079244	-31.0201554917	-7.8540282127
C	10.0286467395	-11.0675062843	-0.9658532705	H	42.8095386065	-31.9503804333	-8.0079466685
H	11.0898459631	-10.8999356731	-0.8164847495	F	34.0432936506	-23.0989092394	-5.7899800179
C	5.7887442447	-7.454551552	-0.0881024566	F	16.7137511427	-15.3326210774	-2.5753378957
S	8.0722457064	-6.2869556462	0.3683524345	F	1.2691182672	-4.268013988	0.3536829891
H	4.7238705533	-7.6482779188	-0.1586815103	F	-0.8939962276	-2.9729066912	0.4791065285
S	7.7446734635	-12.2285763184	-1.4363243998	F	14.5528745332	-14.0994792125	-2.1377498348
C	6.5962473357	-9.7707263714	-0.7827883004	F	31.8859305946	-21.8669649032	-5.3353163444

Table S15. The coordinate of **11** (240 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	26.2669176552	-5.5135813887	-0.9853384118	O	1.5203386913	-0.2027960563	1.0665731235
C	28.691597242	-5.8944002295	-1.5543809549	O	-2.0554864256	2.4683742522	-2.3057112723
C	27.4244922555	-5.3167962429	-1.7575243189	C	2.0584297197	0.6001875757	2.1107449844
C	25.0168733892	-4.7869416375	-1.3621995835	H	2.7213057283	-0.0484930828	2.6865527856
C	23.7906513114	-5.2952649531	-0.9175979876	H	2.6311747226	1.4438990656	1.7056287515
C	22.5968349113	-4.6780472662	-1.2558287046	H	1.2652337283	0.9838854349	2.764092552
C	22.5833659115	-3.512471892	-2.0363243535	C	-2.2917457239	3.8278018819	-1.9580606439
C	23.8161755461	-2.9805500821	-2.4463856482	H	-2.9923429675	4.217045515	-2.6993117372
C	25.0075296573	-3.6103562543	-2.1228015921	H	-2.733911278	3.9078275765	-0.9569029875
H	27.3309750968	-4.6526688841	-2.6051200542	H	-1.36449203	4.4128340142	-1.9905835076
H	23.7933534064	-6.1897992695	-0.3033205753	C	2.540902607	2.0109311661	-2.5221060915
H	21.6586219091	-5.1166923808	-0.9252091975	C	6.112673082	2.4199316764	-4.1353116019
H	23.8395371419	-2.0477822137	-3.0022166551	C	5.2060282827	3.1079080834	-4.9034048912
H	25.9417134013	-3.1530185284	-2.4340723933	C	3.8825951617	3.0441509563	-4.4149579793
C	29.7862742631	-5.5954301167	-2.5283080094	C	3.7371127623	2.3015921333	-3.2700353556
C	29.5428185017	-5.1847852	-3.8445229571	S	5.2849958472	1.669002478	-2.798134326
C	31.1123680784	-5.7597725111	-2.1092588831	S	-9.49590103	-0.2731914198	6.2373417826
C	30.5988377675	-4.9286951109	-4.7125008682	C	-11.0649978611	-0.6079823526	2.8110767807
H	28.5239154699	-5.0948963838	-4.2090704084	C	-8.9147442861	-0.5733866668	1.5862268317
C	32.1673492947	-5.4931440337	-2.9732356224	C	-10.3235594625	-0.5941045044	1.6485908182
H	31.295910386	-6.1053963904	-1.0969772997	H	-8.4654830381	-0.6231501403	0.599137082
C	31.9140691891	-5.0741916864	-4.2777923451	C	-10.2809430811	-0.5199744949	4.0084810576
H	30.3932853837	-4.6210949957	-5.7342763887	C	-8.8354028224	-0.4920755971	3.9686690319
H	33.1908622098	-5.6168962629	-2.6296039226	C	-8.1313123281	-0.5502794227	2.7210318422
H	32.7382043802	-4.8700673523	-4.9561475924	N	-8.2767927157	-0.3515552134	5.169146672
O	26.139277013	-6.301293148	0.0057370177	N	-10.7725377395	-0.4017356878	5.240444809
O	29.0358430956	-6.6394500865	-0.5833195387	C	-6.6815769638	-0.5409467319	2.6542580182
Ir	27.7237944427	-7.4309596521	0.9381136516	C	-5.7631728746	-1.1662920803	3.4594295339
C	29.1920341039	-8.5520462537	1.6626097345	C	-4.4254974858	-0.9778724312	3.0442189544

C	30.0545303103	-8.2368885022	2.716116883	C	-4.2822114135	-0.2151743661	1.9117833265
C	29.3743377871	-9.7870570289	0.9777413391	S	-5.8542229458	0.2919829664	1.3670037757
C	31.0697942968	-9.1140698394	3.0612758805	C	-20.7526662846	0.9419295205	0.4654428697
H	29.9527806732	-7.3140509429	3.277396135	C	-19.9622996456	1.6969641073	-0.4421437886
C	30.4182586277	-10.6302583044	1.3713892871	C	-17.9509014231	0.9239990625	0.5909359896
C	31.2803025459	-10.3204669131	2.4052539666	C	-18.7415764883	0.1681604358	1.4980682798
H	32.0797419602	-10.9932445212	2.6902120235	C	-20.1283248071	0.15458486	1.4450868567
C	28.4203501681	-10.0604758298	-0.0869737869	C	-22.1458467697	1.118606682	0.2247610885
C	28.3557473025	-11.2010890132	-0.8977295238	H	-22.9121824495	0.6404952908	0.8255326931
C	27.3608633321	-11.3130715807	-1.8555024475	C	-16.5583237763	0.7794902136	0.8579616628
H	29.0856143721	-11.9866601603	-0.7640005709	S	-17.7570043348	-0.6909681966	2.6478831264
C	26.5375253519	-9.1818963363	-1.1795207076	H	-15.7922259686	1.2971068192	0.2906347833
C	26.4288119673	-10.2882736311	-2.0034510054	S	-20.9475842174	2.6006845193	-1.5568909144
H	27.3119123852	-12.1987811077	-2.4825941741	C	-18.5753259343	1.6920533202	-0.4042770682
H	25.8477831425	-8.3466013904	-1.2314106897	C	-22.4130767534	1.96542916	-0.8174205654
H	25.6332368261	-10.3389531121	-2.7387102967	O	-17.8442967823	2.4408759202	-1.2820581527
C	27.1616608339	-5.8663937111	3.3214285107	O	-20.8668804948	-0.5684133492	2.3381751652
C	28.7989779844	-4.8422708157	1.9864219251	C	-17.4593126376	1.7347024043	-2.4557444621
C	27.2267342289	-4.7940692381	4.2203160603	H	-16.8991277592	2.4422186711	-3.0700606393
C	28.9046725001	-3.7624890096	2.8453739382	H	-16.8211678195	0.8766039208	-2.2097053235
H	29.3957941863	-4.9322911382	1.0854859084	H	-18.3368887532	1.383202066	-3.0121014475
C	28.0968131728	-3.7428694768	3.9802571157	C	-21.122632754	-1.9048826374	1.922484361
H	26.596275417	-4.800295633	5.0979702934	H	-21.7059983736	-2.3683823165	2.720380337
H	29.6021055635	-2.9619182753	2.6245587702	H	-21.6976847821	-1.9238532053	0.9880385082
H	28.1465241026	-2.9124986007	4.6789154498	H	-20.1888316911	-2.463035864	1.7824912672
C	26.3358681673	-7.0603742006	3.4296355369	C	-16.2912718585	-0.0513670236	1.9128455322
C	25.4435661596	-7.3419569553	4.4688719475	C	-12.5143849294	-0.68668163	2.8403524285
C	26.4882740318	-8.008863113	2.3786763377	C	-13.30399495	-1.3780687368	3.7255466337
C	24.7059174299	-8.5085565251	4.5257164552	C	-14.6880996464	-1.2181114779	3.4976229519
C	25.7526779795	-9.1956619711	2.4348484322	C	-14.9964018938	-0.4098312379	2.4320933444
C	24.8856385036	-9.4191189869	3.4920730316	S	-13.5262364326	0.1558610366	1.6987220343
H	24.0232432432	-8.7013424574	5.3440986804	S	-29.4557416757	5.8144715292	-2.1954484708
H	25.8407915599	-9.9556125969	1.6656438784	C	-30.5602224915	2.275868965	-1.4363436357
N	27.9539259163	-5.857145187	2.2128656297	C	-28.2641214536	1.3710151462	-1.2496773559
N	27.5004992449	-9.0693810198	-0.2546156046	C	-29.6677223014	1.2591346688	-1.1701499693
F	24.1835053888	-10.5588777377	3.5297262051	H	-27.6877405976	0.4705031925	-1.0611731497
F	25.2707550243	-6.4625289884	5.4738290086	C	-29.9422147523	3.531883124	-1.7490911623
F	30.6218718216	-11.8014880986	0.7384987715	C	-28.5046615555	3.6707688205	-1.8335417758
F	31.8915729292	-8.7958899201	4.0695665952	C	-27.6413148071	2.5500579729	-1.6007429694
C	19.7640337623	-1.575485039	-3.5837442624	N	-28.1078545935	4.9178406836	-2.0789242852
C	18.9511771051	-2.0995368879	-2.5424274747	N	-30.589877712	4.6806313073	-1.9341858374
C	17.0422182315	-0.9291404489	-3.3764317568	C	-26.1961469666	2.6626438778	-1.6768150875
C	17.853363105	-0.4076604229	-4.4193457773	C	-25.4147672448	3.3606802189	-2.5625481929
C	19.1986222654	-0.7256412465	-4.5459826981	C	-24.0279016853	3.1887418645	-2.3504910549

C	21.1135510033	-2.0313899202	-3.4819756141	C	-23.7100512116	2.3546627549	-1.3074292635
H	21.8826309274	-1.7528433993	-4.1929610627	S	-25.1778483259	1.7883671974	-0.5662846805
C	15.7007556139	-0.4558994079	-3.4642919732	C	-39.7158215022	-0.6497559894	1.6248494975
S	16.9520264425	0.64917871	-5.4686216727	C	-38.7565076076	-1.2677087681	2.4714119893
H	14.9330319121	-0.7277768356	-2.7476852126	C	-36.9631424247	-0.2126755124	1.2953544741
S	19.8733289658	-3.1150331413	-1.4714848655	C	-37.9220976861	0.4076866611	0.4514019595
C	17.600972959	-1.7991605087	-2.4276170734	C	-39.2877550383	0.2125083679	0.6059546755
C	21.331961482	-2.8632271924	-2.4205096497	C	-41.0536542988	-1.0429635995	1.9639757102
O	16.8433758783	-2.3023715397	-1.4081463	H	-41.9303100512	-0.7028691704	1.4252166328
O	19.956400508	-0.1992367447	-5.5540128514	C	-35.6304370671	0.1373341672	0.9265503558
C	16.2513949055	-3.5619222472	-1.7019480395	S	-37.1656259449	1.3951747406	-0.7661955427
H	15.6907511193	-3.853376673	-0.8116219325	H	-34.7565140822	-0.254300685	1.4360631018
H	15.5685337606	-3.4867849554	-2.5578288063	S	-39.52326701	-2.3034591812	3.6454096589
H	17.0151205593	-4.3196730758	-1.9159089627	C	-37.3904785339	-1.055321209	2.3313374816
C	19.9772043832	-0.9988412898	-6.7302610299	O	-36.4869378657	-1.6744067877	3.1484455353
H	20.6006999163	-0.4678124112	-7.452233912	O	-40.1815335814	0.8135219802	-0.235924827
H	20.4093867821	-1.9870381261	-6.5281249848	C	-36.192843501	-0.9443311085	4.3328545603
H	18.9684552549	-1.1240220816	-7.1427663045	H	-35.4753004805	-1.5455190104	4.89484661
S	9.2068384839	5.5206056402	-5.4246074417	H	-35.7484788125	0.030628227	4.0954927145
C	7.5463125115	2.3009859916	-4.3317613619	H	-37.0941739667	-0.7912660721	4.9391279273
C	9.6382626631	0.9786886889	-4.3090929387	C	-40.6672892557	2.0605845994	0.2439809948
C	8.2558152017	1.1442749601	-4.0865818096	H	-41.3580527015	2.4345194287	-0.5144183208
H	10.051485046	-0.0072979506	-4.120181595	H	-41.1989385441	1.9383241187	1.1962136627
C	8.3516104585	3.3982264546	-4.7838310531	H	-39.8494499624	2.7794891032	0.3781514389
C	9.772381151	3.2524993434	-5.0153346776	C	-35.5699483026	0.9867817414	-0.1445099033
C	10.4302567837	1.9975250207	-4.7954588828	C	-32.0020133065	2.1146750575	-1.3836092129
N	10.367048959	4.3868189636	-5.3790679454	C	-32.9473902381	2.6754086627	-2.2061226994
N	7.9145782787	4.6405403802	-4.9812377989	C	-34.2750804326	2.3488369512	-1.8528372613
C	15.4904893325	0.3846177954	-4.5241867472	C	-34.3837078466	1.5240420437	-0.7615456101
C	11.8527290481	1.8200035202	-5.0216299236	S	-32.794441416	1.149750915	-0.1673360406
C	12.6539424649	2.3133447249	-6.0203834952	C	-41.0921121796	-1.904180502	3.0103622657
C	13.9933394339	1.8680487961	-5.9430317259	H	-41.969178017	-2.3567802806	3.4557934636
C	14.2529865051	1.0217408171	-4.8938182721	F	-30.135519592	0.0518781975	-0.831027819
S	12.79441502	0.7937787495	-3.9748298916	F	-10.9569389547	-0.6328653355	0.4701493853
C	-1.6411120592	1.1177025584	-0.3544174152	F	7.6092698373	0.0666395021	-3.6263456374
C	-0.7116457383	0.4504719284	0.4877600415	F	14.899915392	2.2411997436	-6.8418816461
C	1.1121158076	1.152374469	-0.8870038144	F	12.2508793605	3.0801509602	-7.0201496039
C	0.1835606872	1.8261192298	-1.7255655657	F	5.4846785481	3.7459100935	-6.0292292705
C	-1.181015012	1.8308107427	-1.472440043	F	2.8795523301	3.6474430868	-5.0477649415
C	-2.9821404654	0.9340880182	0.0910365359	F	-3.4115420388	-1.5251918037	3.7082853336
H	-3.8380313984	1.3441626215	-0.4344228917	F	-6.0489038429	-1.9362747265	4.4963453683
C	2.4467220602	1.2757908812	-1.3710276266	F	-12.8602380073	-2.1710118819	4.688194389
S	0.9737593656	2.589678581	-3.0759145049	F	-15.592281053	-1.8305119307	4.2579299738
H	3.2961058063	0.8090750934	-0.8837886426	F	-23.12890065	3.786285049	-3.1275259971

S	-1.5057495946	-0.3761373955	1.7972085964	F	-25.8623930775	4.0870353377	-3.5735866916
C	0.6548705133	0.4659822866	0.248592743	F	-32.6910668591	3.4204865172	-3.2700061327
C	-3.0776916302	0.1685346271	1.2222988718	F	-35.3109040598	2.80475072	-2.5530524774

Table S16. The coordinate of PTB7Ir/PC₇₁BM (311 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	23.6886728155	2.064239032	-0.4681376462	C	9.7317750362	-7.684341666	0.2606816669
C	26.1379865991	1.902581981	0.0971860285	O	8.5923968199	-9.722330599	0.2769552562
C	24.8064647005	1.4489204529	0.1214961182	C	8.6078145263	-11.1459379269	0.1989115174
C	22.3542290354	1.405870168	-0.338678777	H	7.5672783923	-11.4541248184	0.2993610003
C	21.2038869343	2.1954600101	-0.4525402724	H	9.0160523823	-11.4741676765	-0.760741501
C	19.9409449916	1.6381991832	-0.330715921	H	9.2142095662	-11.5687444182	1.0043880905
C	19.7794498118	0.2617934071	-0.1121792828	C	9.7953559412	-9.1464186953	0.1740034384
C	20.9326796397	-0.5317704804	-0.0177189463	O	10.8350209176	-9.7533062098	0.0243383296
C	22.1953181522	0.0301421045	-0.1293501144	C	5.0679845041	-2.7450554164	1.6141185815
H	24.6199912144	0.5340087282	0.6663730185	C	4.4472640695	-3.8021282509	0.8946943118
H	21.3202632618	3.2562494946	-0.6496884649	C	2.275790954	-2.9665858236	1.4453307482
H	19.0641769308	2.2726265752	-0.4336800912	C	2.8993028551	-1.9129423655	2.1678440389
H	20.8339700341	-1.5981784726	0.1640622966	C	4.2764392391	-1.7793754077	2.2566870271
H	23.0650420909	-0.6174203323	-0.0715746169	C	6.4871402687	-2.8550368593	1.5943093555
C	27.1741819953	1.1397777785	0.8589058393	H	7.1425929758	-2.179522807	2.1327360902
C	26.8643659419	0.3224117233	1.9525880567	C	0.854699387	-2.8932775246	1.522284497
C	28.5145327257	1.2718327463	0.4755555538	S	1.7246126976	-0.858426218	2.9016640206
C	27.8677892859	-0.3586106108	2.6333532247	H	0.199619154	-3.6354438556	1.0792801709
H	25.8384444636	0.2403483658	2.2989527976	S	5.6232941534	-4.8953838367	0.2235297169
C	29.5154725905	0.5822397432	1.1486919152	C	3.067933497	-3.9235786727	0.7919472458
H	28.7528386496	1.9290216031	-0.3547117846	C	6.941806914	-3.941767142	0.8904540061
C	29.1951090434	-0.2376296306	2.2290161403	C	0.4055567015	-1.8291421839	2.2600289495
H	27.6123539042	-0.9805462081	3.4870990188	O	2.4949400777	-4.9592879601	0.1103223267
H	30.5499123546	0.6880389122	0.8328384275	O	4.8387805237	-0.7678573598	2.979979255
H	29.9777299122	-0.7735698859	2.7594557091	C	2.2846088346	-4.6899645563	-1.2707581678
O	23.6702883421	3.1776001591	-1.0836307437	H	1.8355293731	-5.5902533042	-1.6946400837
O	26.5851828944	2.9008108141	-0.5512165344	H	1.6037508371	-3.8403532906	-1.4075814547
Ir	25.4041522579	4.3356592641	-1.6532758313	H	3.2315662216	-4.4794272732	-1.7827823968
C	27.0223643787	5.4238885232	-2.0193921351	C	5.1770855376	0.3771751756	2.2059895765
C	27.8361728961	5.3706801618	-3.1543956021	H	5.6084429126	1.1000182193	2.900931989
C	27.376450116	6.3140700166	-0.9661302511	H	5.9131839921	0.1285307036	1.4312732605
C	28.9687753554	6.1650494816	-3.2271234374	H	4.2875483436	0.8108495122	1.7327617845
H	27.6054116455	4.7168788735	-3.9889927645	C	16.6936846301	-1.8780780832	-0.0883331387
C	28.5322723582	7.0900785434	-1.0978800317	C	16.0202173534	-0.7379436871	0.4276112633
C	29.3463894372	7.0357580407	-2.2125422442	C	13.941494999	-1.9152400177	0.4701633677
H	30.2354536631	7.6495279554	-2.288659525	C	14.6130266366	-3.0529491323	-0.0526886338

C	26.4656296539	6.3350176836	0.1689398485	C	15.9741494707	-3.0595206404	-0.3238254316
C	26.5609303125	7.1264676102	1.3207309987	C	18.0797749267	-1.615237136	-0.3163270099
C	25.5839908681	7.0422678604	2.2997843816	H	18.7533624014	-2.3410878465	-0.7575791471
H	27.3986863987	7.7999603611	1.4318080102	C	12.5520623552	-2.1621167756	0.6665568686
C	24.466172391	5.4064716447	0.9763362638	S	13.512996738	-4.378140668	-0.3122195657
C	24.5110329737	6.1699833023	2.1296124561	H	11.8712302405	-1.4207433876	1.0700084431
H	25.6586289149	7.6578803082	3.1917521641	S	17.1061702286	0.6082581463	0.6151861618
H	23.6638558777	4.7072876359	0.7673366315	C	14.6650366236	-0.7404501599	0.7263236369
H	23.7241745449	6.0780572049	2.8702240521	C	18.4535570811	-0.3417735642	0.0068679327
C	24.6406007846	3.7814943105	-4.4020388621	C	12.168358108	-3.4268778523	0.305194275
C	26.0947900912	2.1395649565	-3.565811954	O	14.0480937368	0.3759040747	1.214204264
C	24.5554813298	3.0857617886	-5.6148925838	O	16.5832956417	-4.1688222042	-0.8390322904
C	26.0490369605	1.4177030006	-4.7454792231	C	14.0042473143	0.429337026	2.6361260022
H	26.688227476	1.8275437479	-2.7135736509	H	13.4981013881	1.3619068145	2.8931779062
C	25.2589679314	1.9043093301	-5.7847640688	H	13.4417315116	-0.4171007437	3.0483715574
H	23.9398049133	3.4824857967	-6.4093993832	H	15.0147419189	0.4323462448	3.0629912993
H	26.6181929746	0.4994227986	-4.8399450773	C	17.1221726991	-5.0364127548	0.1510205048
H	25.1925969408	1.3664398758	-6.7262476486	H	17.5644142317	-5.878182895	-0.3854531519
C	23.9990949084	5.0428854333	-4.0619958497	H	17.8958515356	-4.5292583668	0.7414066158
C	23.1687558288	5.787927229	-4.9053070605	H	16.3387772449	-5.4047469719	0.8247412461
C	24.2763722061	5.5388237236	-2.7567282932	C	10.8458813368	-3.9896610266	0.3722728291
C	22.6089912472	6.9933886287	-4.5289684837	C	9.2217860505	-0.6041579354	10.0005679893
C	23.7221409112	6.7630020643	-2.3730080645	C	10.5070127845	-0.6769902716	10.7491723116
C	22.9079877638	7.4563728785	-3.2537226503	C	11.5327652294	-0.3178505611	9.7288986015
H	21.9698900366	7.5502030145	-5.2030933852	C	10.8683436673	0.2182062121	8.5727227405
H	23.9119286585	7.1909520632	-1.3942243254	C	9.8213700755	-6.8714682148	4.9509685011
N	25.4118401212	3.279992189	-3.3968870487	C	9.6029211585	-7.5630616644	6.2014671661
N	25.4115900993	5.4830486851	0.0302291353	C	10.8935531752	-7.8227680364	6.8006989199
F	22.3799245346	8.6258205319	-2.8703401689	C	11.9087390349	-7.2856546551	5.9211885996
F	22.8818620481	5.3428288562	-6.1435090517	C	11.2453692854	-6.6997106837	4.77825602
F	28.8980410294	7.9369454463	-0.116463452	C	9.4488245934	0.0452486167	8.7420362288
F	29.7422751518	6.0997731357	-4.3184690895	C	8.2379760799	-1.5729617594	10.0875965076
C	-15.1306535268	-5.2139409371	-2.3224674701	C	10.7672964642	-2.072971345	11.510769823
C	-13.2039199986	-4.160807638	-1.5029118184	C	12.701213292	-1.0366101446	9.5432892024
C	-14.5546421336	-3.9644487039	-1.9280379456	C	11.4301122598	0.1084987243	7.2976108132
C	-14.9847464342	-2.6455543731	-1.804849627	C	8.9503003321	-5.8537778259	4.5649914954
S	-13.6759814821	-1.6782336336	-1.2081970412	C	8.5231266669	-7.2126605102	7.0081272609
S	-12.6975890877	-5.8257341184	-1.6090919601	C	11.0482397718	-7.7202451185	8.1800830683
F	-16.3799099369	-5.3111133616	-2.7489713473	C	13.0349531697	-6.6684711388	6.4606540967
C	-14.2807782764	-6.2749962309	-2.219709788	C	11.7372963973	-5.5181746371	4.2258904872
O	-15.7153820107	-7.949910086	-2.9887585751	C	8.6430967571	-0.2288608807	7.633794355
C	-15.957968721	-9.3202041681	-3.3006877424	C	8.4781042812	-2.8321210777	10.7842303257
H	-16.9880722142	-9.3600296037	-3.6542554246	C	11.9942488774	-2.8073257847	11.1075621562
H	-15.2700867749	-9.6651308732	-4.0772678379	C	13.2710873994	-1.1801042694	8.2297523647

H	-15.8309614478	-9.9448199794	-2.4125065311	C	10.5969414256	-0.1980947091	6.1604762498
C	-14.4861887038	-7.6935341598	-2.5287052727	C	7.8415961153	-5.4881136853	5.4101763222
O	-13.6218267247	-8.5311810153	-2.3772611664	C	8.6914858822	-7.0991365369	8.436154839
C	-17.930773604	-0.3751870334	-2.0133142964	C	12.2141330839	-7.0739312788	8.7335872907
C	-18.4177400854	-1.2279226049	-3.0397508418	C	13.5328829627	-5.4409113697	5.8894582304
C	-20.3768718907	0.1162955592	-3.2987484592	C	10.8310016557	-4.4684702526	3.8312566449
C	-19.8886172623	0.9705658158	-2.2732635463	C	9.4665623825	-4.6327918827	3.9983291959
C	-18.6770784108	0.7495728246	-1.6312134076	C	7.6302306775	-6.1531321385	6.6058858628
C	-16.6908509037	-0.8403571424	-1.4872360788	C	9.9270482181	-7.3512226284	9.0109016193
H	-16.1784409315	-0.35598146	-0.663191953	C	13.1851939177	-6.5567991538	7.8910214003
C	-21.6524842794	0.5534668382	-3.7893890666	C	12.8963886616	-4.8784934283	4.7957861708
S	-21.0037811896	2.2696476885	-1.9466504633	C	9.2326314408	-0.3635847749	6.3247163881
H	-22.2085902638	0.028478415	-4.5571785599	C	7.4271802629	-1.8848358216	8.9389580682
S	-17.3449690863	-2.5671992271	-3.325070868	C	9.6949413494	-3.0884907885	11.3728958697
C	-19.6211834232	-0.9965171748	-3.6926411042	C	12.9338262886	-2.2959190374	10.2409721539
C	-16.240108985	-1.9905874683	-2.0836469371	C	12.6562579325	-0.6081224467	7.1261335979
C	-22.0909132931	1.6753198192	-3.1666503764	C	7.6140698554	-1.2170808297	7.7373033314
H	-23.0210786401	2.2013897359	-3.3416051448	C	7.7996732723	-3.8804463976	10.0607655801
O	-20.0684899189	-1.8498484101	-4.6618698528	C	11.6967668171	-4.2114167047	11.0439857046
O	-18.2433146638	1.5765892893	-0.6344371199	C	13.8638616874	-2.4886046774	8.1174967622
C	-19.6829693274	-1.4736434285	-5.9778757551	C	11.325195813	-1.0822066955	5.2816444457
H	-20.0898536956	-2.2343403241	-6.6470688291	C	7.6637818156	-4.0560636275	5.3444421551
H	-20.0940048092	-0.4919481541	-6.2454032399	C	7.8905882896	-5.9941484192	8.9074378701
H	-18.5908553974	-1.4460567192	-6.0786860409	C	11.8142056614	-6.3298621985	9.9026939142
C	-17.4306655476	2.6501605146	-1.0928206918	C	14.0050913366	-4.5932111382	6.9593483445
H	-17.1667375876	3.2350418001	-0.2095000604	C	11.4406440685	-3.1923533413	4.1331781011
H	-16.5167522644	2.2774885195	-1.5726112723	C	8.6634219395	-3.5281045911	4.4716251806
H	-17.976035002	3.2855287885	-1.801445434	C	7.2371173922	-5.4097291905	7.7800995251
C	-3.3780980847	0.2792606524	4.5500570068	C	10.4053534098	-6.5007461204	10.0729346265
C	-1.4947999462	-0.6457359953	3.5086162024	C	13.7920417151	-5.2822752911	8.1918916575
C	-2.9200771626	-0.5429594269	3.4723068312	C	12.713279763	-3.4466288481	4.7305193608
C	-0.9589499483	-1.463167219	2.5322735793	C	8.5453807246	-1.417313291	5.6171939989
C	-3.5012933487	-1.2929642568	2.4518451858	C	7.148395643	-3.298773658	8.9320674259
S	-2.2482082956	-2.068091676	1.5379778299	C	10.2901874281	-4.3819466989	11.2092886567
S	-0.7844829581	0.2541914288	4.8223388127	C	13.6510860746	-3.1748026985	9.350207423
F	-4.6635438459	0.5274469746	4.7517938671	C	12.5972121532	-1.338165866	5.8800109006
C	-2.3797160065	0.7760188778	5.3345925656	C	7.5484065388	-1.9478055703	6.4920515082
O	-3.690106178	1.9971045368	6.8346940433	C	8.3012760479	-5.2038255398	10.0087865639
C	-3.7909750612	2.8499174342	7.9730650812	C	12.4548996876	-5.1204679699	10.2617385067
H	-4.8571369993	3.0325732163	8.1064481413	C	13.9104259451	-3.1827042624	6.8830401378
H	-3.3698098263	2.3632326429	8.8568130638	C	10.663761247	-2.070100818	4.5085355853
H	-3.2583956075	3.7886570292	7.7987695939	C	9.2198259349	-2.2441406145	4.6837910256
C	-2.4391437177	1.6512534693	6.5094611568	C	6.9786075281	-4.0187294085	7.7231575514
O	-1.4502465384	2.0142873321	7.1106527946	C	9.6029713403	-5.4649776405	10.6045769307

C	-6.7194517951	-2.4874574788	1.0066204256	C	13.4791072	-4.5794131019	9.3813149457
C	-7.2941516218	-1.2795220809	1.4867195725	C	13.2456953097	-2.586982504	5.722098939
C	-9.4167764527	-1.858091083	0.5531315332	C	7.1927353453	-3.3169362137	6.4562770192
C	-8.8411364573	-3.0674411024	0.0759009528	C	10.6257609596	-0.7606400394	12.2500391208
C	-7.5149526703	-3.4053453011	0.3016181421	C	9.3375850163	-0.5816951189	13.0213218131
C	-5.3399884074	-2.5841915378	1.3432899452	C	11.7461293898	-0.1102329077	13.0748438776
H	-4.7233628967	-3.4340660953	1.0719462793	C	8.5675424018	0.5704065969	12.8502408384
C	-10.7906242722	-1.7459704444	0.1931366143	C	8.9640245558	-1.5063926133	13.9985139816
S	-9.9974244831	-4.0136091734	-0.8184063755	H	11.4016598325	0.9160591612	13.2659331942
H	-11.4073918472	-0.8982064675	0.4704591361	H	11.7115914163	-0.6095096981	14.0537138031
S	-6.1251879703	-0.303621232	2.3270386877	C	13.1961062641	-0.0523965437	12.6082314096
C	-8.6292926907	-0.9577152108	1.2875763838	C	7.4369349831	0.7880698167	13.6322145818
C	-4.869904156	-1.5044337522	2.048542126	H	8.8514543707	1.2984735238	12.0940724149
C	-11.2522462121	-2.8153694364	-0.5288857948	C	7.8337610257	-1.2907181018	14.7816091587
O	-9.1524224875	0.2149950809	1.7541104134	H	9.5590409142	-2.405317798	14.1418681984
O	-6.9866186225	-4.568264647	-0.1800441967	H	13.6061348932	-1.053792811	12.4539428628
C	-9.6915938024	0.1167001041	3.0674453627	H	13.2857070082	0.4702003668	11.6524008286
H	-10.064748327	1.1107425593	3.3215066306	C	14.0469881826	0.6702166758	13.6442677773
H	-10.516912987	-0.6055834835	3.1020615407	C	7.0660777243	-0.1435075729	14.5984103286
H	-8.9222053632	-0.1795706116	3.7909368021	H	6.8431069327	1.6856817662	13.4829378056
C	-7.1114389304	-5.6695126843	0.7134866395	H	7.5515838915	-2.0223706604	15.5337616392
H	-6.66445924	-6.5271656005	0.2073872881	H	13.6803174482	1.6898986109	13.8246576242
H	-6.5774905847	-5.4769181383	1.6524594157	H	14.0047401161	0.1683554948	14.6203666936
H	-8.164112919	-5.8844803368	0.9337766266	C	15.4953391875	0.764458562	13.2315637933
C	-12.5767141391	-3.0148178747	-1.0539038445	H	6.1808521568	0.0235372495	15.2058563638
C	8.6635991161	-6.854088158	0.431596405	O	15.9618983461	0.3379386361	12.2018833284
C	10.4152325931	-5.3013990939	0.3031702396	O	16.2212077536	1.3962641621	14.1690701038
C	9.0037736341	-5.4650147045	0.4552457355	C	17.6062005951	1.5349637014	13.8622862717
C	8.3278065346	-4.2636098484	0.6521985879	H	18.0733117546	0.5547448232	13.7334988172
S	9.4643807681	-2.9585805413	0.5825900723	H	17.7419950138	2.1116656778	12.9432553912
S	11.254440486	-6.8200683346	0.1330289398	H	18.0460417246	2.0593216529	14.7109584602
F	7.4150034965	-7.2742628844	0.5619276602				

Table S17. The coordinate of PTB7Ir/PC₇₁BM (311 atoms) calculated by PBE0-D2 functional.

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	23.8716677294	1.8630011502	-0.7617884935	C	9.6984857815	-7.4616961005	0.4092287087
C	26.3578573681	1.4530499489	-0.7298438748	O	8.5339273883	-9.4826842413	0.5300985222
C	25.0144087941	1.0652453032	-0.5768437375	C	8.531746585	-10.9084208744	0.5163065313
C	22.5218091024	1.2435736747	-0.5992696365	H	7.4892157485	-11.1990676824	0.6445546259
C	21.4236657661	2.0831348641	-0.376340192	H	8.9227525242	-11.2844458109	-0.4329191547
C	20.1478295922	1.5654336479	-0.2190657775	H	9.1444405402	-11.3018386073	1.3318453314
C	19.9158519789	0.1836740349	-0.2925101205	C	9.7421794864	-8.926940521	0.3865332364
C	21.0159345959	-0.6559438857	-0.5272063676	O	10.7724051934	-9.5531301377	0.2509669267

C	22.2911016847	-0.1359440488	-0.6815925529	C	5.097771425	-2.3925399372	1.5195599884
H	24.843830037	0.0384695554	-0.286092525	C	4.4713555662	-3.5006794435	0.887085981
H	21.5905601798	3.1547571286	-0.3416558285	C	2.3033514926	-2.6153170385	1.366453601
H	19.3134000052	2.2444021893	-0.0620661491	C	2.9314656684	-1.5058745846	1.9953654015
H	20.8691129679	-1.7310076131	-0.5747219541	C	4.3092741468	-1.3715298831	2.0752851491
H	23.110148075	-0.8177762069	-0.8882605417	C	6.5164508183	-2.5136588942	1.5100027078
C	27.4346951599	0.4587998738	-0.4320977287	H	7.1764685247	-1.8013113953	1.9926299473
C	27.2434072523	-0.6395723803	0.4148476302	C	0.8831739062	-2.5298454793	1.4354947738
C	28.696401703	0.6525056848	-1.0079664251	S	1.7602239336	-0.3861889088	2.6325726579
C	28.2818927819	-1.5305390536	0.663651033	H	0.225870861	-3.3046472432	1.0560794112
H	26.2889875172	-0.786072153	0.9116313477	S	5.6393828577	-4.6491842062	0.3021643768
C	29.7305838444	-0.24384271	-0.7679507313	C	3.092187107	-3.6257549832	0.7947830956
H	28.8482698121	1.5211422046	-1.6406812271	C	6.9644111883	-3.65445668	0.8918013351
C	29.526029663	-1.3405424501	0.0669580714	C	0.4371067033	-1.4025761088	2.0754528612
H	28.120397295	-2.3722843019	1.3317112789	O	2.5193703404	-4.7134146288	0.1992389901
H	30.7011730774	-0.0842979898	-1.2300423692	O	4.8735396867	-0.3021216502	2.7082173101
H	30.3354726366	-2.0397715646	0.2592213398	C	2.2674937927	-4.5393503748	-1.1901771237
O	23.8517357387	3.1079587994	-1.0245869242	H	1.8226308816	-5.4724612046	-1.5412820564
O	26.7778314219	2.5788649843	-1.1464271687	H	1.5689837886	-3.7111529441	-1.3642657869
Ir	25.5645987606	4.3261593494	-1.5196410891	H	3.1970014745	-4.3486449819	-1.7405641116
C	27.1900979284	5.4213360907	-1.8267868749	C	5.2300174508	0.7630063044	1.8345532302
C	27.7954859583	5.7097144903	-3.0529591808	H	5.6607181271	1.5442348416	2.4635874449
C	27.7924845729	5.9161801407	-0.6351823769	H	5.9715145987	0.4372845783	1.0943763041
C	28.9659371003	6.4500674916	-3.0862806718	H	4.3491834884	1.1575002349	1.3132583287
H	27.3715377809	5.3659339025	-3.9905445916	C	16.74088681	-1.8196165746	-0.3026215435
C	28.9747797618	6.6564309789	-0.7333208167	C	16.1651026278	-0.7424871283	0.4235138526
C	29.5836702032	6.936933243	-1.9411069075	C	14.0425019514	-1.8391073988	0.4728378611
H	30.4987047847	7.5144208863	-1.987586368	C	14.6204409173	-2.9187305737	-0.2478374538
C	27.0882692194	5.6038746578	0.5998598452	C	15.9537578845	-2.933079499	-0.6322851655
C	27.4449426632	5.9815290985	1.9007725967	C	18.1134800348	-1.5754802221	-0.6120720271
C	26.6409816872	5.6206233031	2.9700207452	H	18.7100398777	-2.2554258883	-1.2093014711
H	28.3470720509	6.5557645543	2.0563355334	C	12.6610768636	-2.0634480271	0.7474561038
C	25.1745555885	4.5333621698	1.4389632815	S	13.4484353328	-4.1620421365	-0.5848283042
C	25.4800924557	4.8849204499	2.7420417936	H	12.0435966976	-1.3668724425	1.3035673488
H	26.9185818785	5.9153293764	3.9781143967	S	17.3275008112	0.5203269989	0.7095082997
H	24.2879743957	3.9653895238	1.1792385946	C	14.8377070555	-0.7388360384	0.8292492602
H	24.8224048504	4.5866521023	3.551102448	C	18.5753185016	-0.3780700653	-0.1430680399
C	24.3165647468	4.6918091403	-4.1191104243	C	12.2000791249	-3.2574380871	0.2614739977
C	25.7287961948	2.8164346985	-4.0975910945	O	14.3138638831	0.3167678696	1.5187311757
C	23.9739867436	4.4160159621	-5.449084654	O	16.4711989867	-3.9807355432	-1.3406867032
C	25.4264225495	2.5030215367	-5.4110656545	C	14.3487279719	0.1487983739	2.9323042183
H	26.419975273	2.2308965066	-3.5014512894	H	13.8800205422	1.0371363392	3.3598467925
C	24.528465632	3.3214605156	-6.0927935166	H	13.7902216154	-0.743753115	3.2393537866
H	23.2783502432	5.0649729786	-5.9616493958	H	15.3812250724	0.0693578203	3.2943861311

H	25.884613607	1.6393556101	-5.8803608195	C	17.0452621611	-4.9943430929	-0.5242629424
H	24.2619147016	3.1094000942	-7.1243502064	H	17.4087810598	-5.7675557846	-1.2039526281
C	23.8552348695	5.8034964298	-3.3005404553	H	17.8825266788	-4.599401185	0.0650894403
C	22.9684418535	6.8038480938	-3.7110938801	H	16.2997602637	-5.4269855483	0.1541652828
C	24.3825577785	5.8522588809	-1.9788199526	C	10.8641729992	-3.7861250387	0.3607411199
C	22.5847263959	7.8463284685	-2.8899884977	C	9.105325637	-0.5783593954	10.2174200587
C	24.0061724855	6.9094779552	-1.1459866529	C	10.360036043	-0.7488222927	11.000786724
C	23.1247179249	7.8721756705	-1.610282429	C	11.4331231126	-0.3613242799	10.0412961653
H	21.8968160254	8.6083792988	-3.2349384454	C	10.8291707982	0.2749108909	8.9029649712
H	24.3874926603	6.9991967305	-0.134301725	C	9.6624205026	-6.5151060032	4.7785607773
N	25.191049658	3.8718820414	-3.4714652929	C	9.375593963	-7.2800187741	5.9713901787
N	25.9524255938	4.8774300491	0.4037575625	C	10.6345961023	-7.6262208602	6.5939654938
F	22.7698062954	8.8766957706	-0.7988281566	C	11.6980712558	-7.0696474828	5.786567696
F	22.447098562	6.7825260861	-4.9525379434	C	11.0966395486	-6.3855133793	4.6644125145
F	29.5731237102	7.1322405464	0.3755530535	C	9.3994812035	0.1436600595	9.0135634382
F	29.5370198856	6.714182965	-4.2685410829	C	8.0857466643	-1.513462255	10.2066768024
C	-15.1251107389	-5.6284425631	-1.6340250979	C	10.5449145591	-2.2003188503	11.6745069315
C	-13.1932732439	-4.438816682	-1.047764913	C	12.5817885811	-1.1090450677	9.8461028346
C	-14.5447349631	-4.3269267974	-1.5002618511	C	11.4311860371	0.2290360784	7.6424389108
C	-14.9701468223	-3.008240419	-1.6441343094	C	8.8415200386	-5.4424304532	4.4341092404
S	-13.6557418368	-1.9459769113	-1.2574316141	C	8.281306898	-6.9428815581	6.7642298055
S	-12.6918245558	-6.0926245711	-0.8172014598	C	10.7444701006	-7.6211743675	7.9814140156
F	-16.3758466092	-5.8056203351	-2.0296675619	C	12.82557687	-6.5322886951	6.4029711595
C	-14.2780585401	-6.6500875978	-1.3215918395	C	11.6484485431	-5.1886141442	4.20991852
O	-15.7197797441	-8.4402305775	-1.7357048433	C	8.6237448934	-0.0251835322	7.8639321839
C	-15.9682293907	-9.8442636221	-1.7637131027	C	8.2569551365	-2.8236923933	10.8246158898
H	-16.998962482	-9.9505722307	-2.1013416281	C	11.7584531484	-2.9517751003	11.2629452216
H	-15.282840779	-10.342124226	-2.4547955813	C	13.1915909405	-1.1864782115	8.5451362459
H	-15.8424892322	-10.2767547977	-0.7675570826	C	10.6282500975	0.0304274555	6.4604639033
C	-14.489004802	-8.1010226555	-1.3377484735	C	7.7168126162	-5.0922349424	5.2647590907
O	-13.6275261062	-8.8942260559	-1.0208978101	C	8.4037605908	-6.9305521598	8.201436892
C	-17.8996592373	-0.8072975568	-2.3148975001	C	11.9122909282	-7.0570273471	8.6152232242
C	-18.4056363742	-1.8575746057	-3.1264879089	C	13.3862073771	-5.2893012615	5.9326534276
C	-20.3557552501	-0.5801389854	-3.6532540569	C	10.7939146404	-4.082560626	3.8575741442
C	-19.8479025204	0.4718489839	-2.8436563747	C	9.4196356845	-4.2065483126	3.9689503498
C	-18.6308756441	0.3824354133	-2.1806410031	C	7.440772095	-5.8265179595	6.4053963971
C	-16.6584084319	-1.1604439344	-1.7111957064	C	9.6086142854	-7.2662192123	8.7980443714
H	-16.133325751	-0.5135131644	-1.0169407042	C	12.9298365596	-6.5218153405	7.8417178138
C	-21.6327790169	-0.2459969816	-4.2157631069	C	12.808638266	-4.632317253	4.8591799401
S	-20.9471220884	1.8238374944	-2.7989007657	C	9.2539363975	-0.0944558125	6.568569442
H	-22.2023524063	-0.9194496952	-4.8453906329	C	7.3057768774	-1.7179222312	9.0134836033
S	-17.3475454115	-3.2384228911	-3.1229770317	C	9.4429162832	-3.1637160963	11.4339529675
C	-19.614626669	-1.7604154675	-3.8026360121	C	12.7457410769	-2.4197410967	10.4643741446
C	-16.2233369889	-2.4173785067	-2.0474935123	C	12.6368593182	-0.5194912428	7.463110454

C	-22.053723005	0.989690083	-3.8491336231	C	7.5579214417	-0.9793229452	7.866559583
H	-22.9809839336	1.4754289288	-4.1262730516	C	7.5684716446	-3.7956543607	10.0096599138
O	-20.0812983216	-2.7983458926	-4.5593712963	C	11.4142730769	-4.336349989	11.0949817172
O	-18.1762421974	1.4025887671	-1.3942759876	C	13.7423768778	-2.5055591925	8.3642842609
C	-19.6999599468	-2.7251048185	-5.9273113015	C	11.3551228614	-0.8199777376	5.548030778
H	-20.1238784312	-3.6064368684	-6.4126909964	C	7.5915002097	-3.6532238487	5.2899162414
H	-20.0975104471	-1.8184618289	-6.4008169043	C	7.6260035522	-5.8301484409	8.7197318811
H	-18.6083504503	-2.7388041702	-6.0360302814	C	11.4976811246	-6.3772933162	9.8179586442
C	-17.3576219385	2.3377268296	-2.0860919305	C	13.8498587853	-4.5324678727	7.0720565103
H	-17.0731005746	3.0972855417	-1.3552635565	C	11.4364710975	-2.8527983039	4.2644740623
H	-16.4558518244	1.8552647111	-2.483994104	C	8.6391621452	-3.1060339126	4.4880030638
H	-17.906018278	2.8111439339	-2.9097694718	C	7.0333824231	-5.1484792378	7.6137479791
C	-3.3443045219	0.9897560362	4.0764561676	C	10.0787080959	-6.5064183426	9.9302430301
C	-1.4612109858	-0.0634484271	3.1625994793	C	13.570096914	-5.2934963284	8.2476288963
C	-2.8878230756	0.0203206512	3.1284692958	C	12.6780313696	-3.1935195415	4.8848582715
C	-0.9268579856	-1.011123404	2.3104552189	C	8.5558322454	-1.0730378507	5.7696060768
C	-3.4721025503	-0.8776983211	2.2382057236	C	6.9777171791	-3.1167214171	8.902056158
S	-2.2215472624	-1.7686202793	1.4335811662	C	9.9976636978	-4.4649144266	11.2027771133
S	-0.748053503	1.030324666	4.3181268006	C	13.4628321846	-3.2636603769	9.5403052068
F	-4.6305925782	1.2520510865	4.2530069196	C	12.595448659	-1.1625394772	6.1692448729
C	-2.3436407878	1.6080098412	4.765927248	C	7.5109412969	-1.623015493	6.5733156091
O	-3.6516423428	3.0280669594	6.0812390867	C	8.0246251873	-5.130532774	9.8849505327
C	-3.7502887653	4.0414305237	7.0796692346	C	12.1672058038	-5.2190061634	10.2784356471
H	-4.8167873499	4.2347832404	7.1938985254	C	13.8074226054	-3.1173946304	7.0878626128
H	-3.318192623	3.6956692366	8.0225241909	C	10.6870802925	-1.7293403388	4.6892212911
H	-3.2265898093	4.9468756847	6.7616660852	C	9.232603651	-1.8607172644	4.8046514479
C	-2.4003796686	2.6490093306	5.7969339815	C	6.8252101735	-3.748258221	7.6424913956
O	-1.4093591934	3.1073130742	6.3250974254	C	9.2943010581	-5.4790915833	10.5041351354
C	-6.6925198953	-2.3188027019	1.0462667122	C	13.240480893	-4.6598090111	9.4708078995
C	-7.2730068511	-1.0510872004	1.3216523011	C	13.2051544402	-2.421427719	5.9489777594
C	-9.3983371085	-1.7931329732	0.518234214	C	7.107993705	-2.9724225139	6.4333194938
C	-8.8173590951	-3.0625671869	0.2489332372	C	10.4237165298	-0.9350218768	12.4954947459
C	-7.4864566879	-3.3481343852	0.5150688118	C	9.1165890813	-0.7592454123	13.2351817631
C	-5.30921782	-2.3481272314	1.3800216723	C	11.5364177723	-0.3804298366	13.3971095802
H	-4.687554957	-3.2271295354	1.2497625209	C	8.3941971181	0.4298125448	13.1173637894
C	-10.7761681422	-1.7530241762	0.1567892389	C	8.6778032002	-1.7311948655	14.1364450382
S	-9.9728957181	-4.155189257	-0.4599741768	H	11.2238216854	0.6452755971	13.6394785798
H	-11.3987521905	-0.8754642475	0.2922306963	H	11.4473602591	-0.9361274763	14.3415259218
S	-6.1050634939	0.0598307492	1.9755049542	C	13.0041073275	-0.3524915972	12.9862269521
C	-8.6121179077	-0.7761665661	1.0821335868	C	7.2464416487	0.6385118991	13.8765782885
C	-4.8426264302	-1.1622756224	1.889841622	H	8.7296457936	1.194567413	12.4208688786
C	-11.2346098239	-2.933246856	-0.3672865788	C	7.5305287147	-1.5244728426	14.8968274086
O	-9.139589092	0.4559621986	1.3465467081	H	9.2353812782	-2.6593075169	14.2379236369
O	-6.9531600043	-4.5721304052	0.2309314779	H	13.3801891172	-1.3578947582	12.7807455332

C	-9.6816823093	0.5760922099	2.656798611	H	13.1502169256	0.2268724129	12.0708982407
H	-10.0596662313	1.5968943828	2.7403918839	C	13.8420656833	0.2662392305	14.0973372707
H	-10.5040700033	-0.133938874	2.8104106777	C	6.8107321041	-0.3394830944	14.7668841965
H	-8.9128824905	0.4083565073	3.4209650042	H	6.6905666506	1.565915879	13.7691395911
C	-7.0496697797	-5.5043359207	1.3026313777	H	7.1975151027	-2.2924530471	15.5896416928
H	-6.6000306689	-6.4318803254	0.94348368	H	13.511975774	1.2881342234	14.3282231277
H	-6.5032669771	-5.1481135555	2.1849124392	H	13.7385979995	-0.2927982332	15.0372310933
H	-8.0959137127	-5.6883089622	1.5753849216	C	15.3090254708	0.3193717045	13.7477909767
C	-12.5613417084	-3.2285018081	-0.8393340203	H	5.9124264404	-0.1791955152	15.356684064
C	8.6431149375	-6.6105089764	0.5575814829	O	15.8008932603	-0.0760719297	12.7174933212
C	10.4122816303	-5.0909951617	0.3424621756	O	16.01977702	0.8725513916	14.7446648296
C	9.0006167001	-5.2257471353	0.5168325201	C	17.4213750136	0.9643020746	14.5025454148
C	8.3462466581	-4.0049820795	0.6713891223	H	17.851922204	-0.0285160802	14.3457978567
S	9.5049005722	-2.7232630937	0.5412552994	H	17.6212711669	1.5767850079	13.6190708202
S	11.2307544052	-6.6256395589	0.2251975502	H	17.8455964804	1.4284597446	15.3931984843
F	7.392209387	-7.0108882814	0.7235608712				

Table S18. The coordinate of 1/PC₇₁BM (353 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	19.7695705274	-2.2590432876	0.6954624697	H	-29.012437167	-1.6216282293	3.6891482585
C	22.0345550562	-1.2229330824	1.0664714581	C	-28.0210067606	3.2061619151	-0.6011132259
C	20.6404933399	-1.1718272113	0.8809511892	H	-27.7615266963	4.0251660891	-1.2748263659
C	18.315476251	-1.9942559976	0.48136371	H	-27.2218869063	2.454413951	-0.6131407672
C	17.4066311603	-3.0260795214	0.7449512164	H	-28.9574143002	2.7416451191	-0.9341575084
C	16.0444109603	-2.8374685138	0.5751619107	C	-14.4779560804	-0.712622044	2.9575931125
C	15.5361582733	-1.6108182756	0.121609377	S	-15.002328449	1.2073112889	1.3360346183
C	16.4496683771	-0.581326754	-0.1542575933	C	-15.8559512543	-0.4651692743	3.0910323468
C	17.8116779503	-0.7716454255	0.0188643027	H	-13.948810517	-1.47691176	3.5171009958
H	20.1858627481	-0.191638186	0.920556234	C	-16.312273443	0.5547649655	2.2767065785
H	17.7933777174	-3.9814255206	1.084209246	H	-16.5005573743	-1.0122545408	3.7710637155
H	15.3634581492	-3.6598710749	0.7796301914	C	-20.1567475121	1.4455868402	2.4487511075
H	16.0838206014	0.3846209029	-0.4900371403	C	-21.5099300755	1.2857356559	2.9092342507
H	18.4888362816	0.0412526195	-0.2249711096	C	-21.915487181	0.5971281388	4.040163923
C	22.8000565306	0.0582556744	1.1618198201	S	-22.8963003811	1.8764600626	2.0399558412
C	22.3226224718	1.2710736333	0.6507061289	C	-23.3103847022	0.5549543398	4.2048083543
C	24.0601346408	0.0353911331	1.7727117211	H	-21.2139509162	0.1629177927	4.7448129557
C	23.0770169514	2.4337018973	0.7652289464	C	-23.9980226159	1.2132980722	3.2043876351
H	21.3692531906	1.306212486	0.1323603479	H	-23.8032156793	0.0845695951	5.0490820876
C	24.8100721349	1.1986964776	1.8947606682	C	-25.4209696956	1.3954297166	3.0678394423
H	24.4381345807	-0.9122350986	2.1430588955	C	-17.6459562586	1.069879164	2.1580811658
C	24.3195264374	2.4029237575	1.3939886063	C	-18.1375902842	2.1532002662	1.4547877494
H	22.6959642175	3.365399842	0.3558375711	C	-13.8536271159	0.1118335699	2.0430508658
H	25.782333503	1.1657678178	2.3791476762	C	-39.8122312687	0.3077303844	4.8655892411

H	24.9068260693	3.3127336661	1.4856163689	C	-39.4246290634	1.4098403106	4.0406946465
O	20.0841772853	-3.4924811216	0.6901684453	S	-38.8809978844	3.3877367082	2.5187614173
O	22.7407576978	-2.271412955	1.2032096451	S	-37.2193630088	0.10256928	4.7017255372
Ir	22.0205266882	-4.3073722769	1.1838866165	F	-41.0779481466	0.0719381936	5.1785980531
C	23.8575424508	-4.9945969545	1.4847082296	C	-38.7717384076	-0.4622665306	5.2945687771
C	24.4477743477	-5.3242679288	2.7078878243	O	-39.9771630023	-2.012592496	6.558275994
C	24.6362735937	-5.1112584939	0.2981086584	C	-40.0067673266	-3.170915157	7.389770993
C	25.7688575944	-5.7395243549	2.7459553747	H	-41.0577322249	-3.3293078829	7.6309001902
H	23.8953305643	-5.2634452494	3.639619563	H	-39.5989093744	-4.0354359783	6.8593073317
C	25.9650536862	-5.5342224548	0.4010201835	H	-39.4230878181	-3.0061810896	8.2993647418
C	26.5573588193	-5.8526364746	1.6077055073	C	-38.7555968558	-1.6540013051	6.1477513718
H	27.5886947907	-6.1794389832	1.657721162	O	-37.7344379546	-2.2397947316	6.4407638887
C	23.9447124539	-4.7842718754	-0.9403797019	C	-47.2009283119	2.8593895406	5.2200870698
C	24.4593704567	-4.8372882305	-2.2418917909	C	-47.688237139	3.8101270681	4.2835922465
C	23.647239956	-4.5210558894	-3.3191765318	C	-49.8922747595	3.6641249065	5.1956251442
H	25.4888720615	-5.1294392702	-2.3921774352	C	-49.4045252172	2.7182730966	6.1362048247
C	21.8621292495	-4.113344305	-1.794257938	C	-48.0752106453	2.3146305611	6.1708558264
C	22.3211857376	-4.1549429494	-3.099226036	C	-45.8143913662	2.5829402595	5.0228738154
H	24.0477030145	-4.5642581243	-4.3281189334	H	-45.2682316908	1.8531858753	5.6109331698
H	20.8429043517	-3.8440419076	-1.5385032132	C	-51.299118822	3.8953075863	5.3582979483
H	21.6523438151	-3.9066224672	-3.9159874398	S	-50.6775300374	2.1492578407	7.1814653925
C	20.7477082641	-5.4071346143	3.5555013743	H	-51.8725322273	4.5629032982	4.7257792323
C	21.6396336302	-3.276048097	3.9707714822	S	-46.4303532524	4.3425422977	3.2025776368
C	20.2634445187	-5.4581166049	4.8690093298	C	-49.0107467538	4.2285671159	4.2620933098
C	21.1867955965	-3.2789607378	5.2783300667	C	-51.8311804892	3.1656723863	6.37002637
H	22.1988798072	-2.4481517451	3.5499961539	O	-49.4417425516	5.1329463118	3.3318364631
C	20.4820913674	-4.3932819485	5.7281256751	O	-47.6451269878	1.3876213378	7.0775223668
H	19.7252202173	-6.3346049883	5.2004254132	C	-49.4463863058	6.4754196282	3.799703351
H	21.3830621666	-2.4272664051	5.9202849714	H	-49.8049667218	7.0892089321	2.9708942362
H	20.1065705733	-4.4348642792	6.7466344382	H	-50.117048128	6.5936782905	4.6601187326
C	20.6405698906	-6.4397029706	2.5350116266	H	-48.4373461698	6.7993175603	4.0837341104
C	20.0149690266	-7.6804848755	2.6949700459	C	-47.1245439505	1.9546154823	8.2733618833
C	21.2544150483	-6.1346751097	1.2867175015	H	-46.8285447058	1.1166849334	8.9076279783
C	19.9739037734	-8.6318763258	1.6946127012	H	-46.2497744241	2.5836903027	8.0655169083
C	21.2258955831	-7.0973908057	0.2738344606	H	-47.8840839967	2.5536818205	8.7907996875
C	20.593387942	-8.3100625079	0.4932794633	C	-34.399537214	3.6862386982	1.4846697106
H	19.4839146508	-9.5856603077	1.8468156559	S	-34.8231333142	1.9097076517	3.2888809113
H	21.6866129671	-6.92029955	-0.6922550825	C	-35.7949503891	3.641559584	1.6572272595
N	21.4239992274	-4.3011467354	3.1352452986	H	-33.9031349365	4.3472079863	0.781831538
N	22.6478429411	-4.412749231	-0.7511196497	C	-36.201507061	2.7221018102	2.6063079605
F	20.5701551247	-9.2203079121	-0.4884959367	H	-36.4892404011	4.2574337894	1.0951845513
F	19.4171258682	-7.9950949346	3.8602534156	C	-40.0710917407	2.4298346938	3.3448045387
F	26.7296764419	-5.647828587	-0.7020183332	C	-41.4547716677	2.7997607202	3.2107127433
F	26.321885274	-6.0476442393	3.9261726749	C	-42.0106257796	3.5488254716	2.1876439862

C	-0.3753009064	-2.6943835579	0.4750158523	S	-42.665076299	2.4242750232	4.4023970917
C	0.0617656343	-1.4864753784	-0.1536671598	C	-43.3822226111	3.8055186578	2.3579744188
S	0.6956845622	0.6812074475	-1.346105207	H	-41.440897489	3.8746840005	1.323660412
S	2.2255872156	-2.8515947441	0.5240962891	C	-43.9008481533	3.2555582783	3.5133520927
F	-1.6586603567	-2.9809494852	0.6349340574	H	-43.9860950211	4.3520134226	1.6413114401
C	0.6390581748	-3.5052823982	0.8920034764	C	-45.2602022257	3.291672633	3.992444278
O	-0.639798237	-5.2140340758	1.840932105	C	-37.5349294871	2.414372772	3.0373116708
C	-0.7183070487	-6.4578144394	2.534663067	C	-38.0073525832	1.4103663981	3.8609631918
H	-1.7831140007	-6.6575706226	2.6529298707	C	-33.7134535903	2.802602348	2.2933931555
H	-0.2377436884	-7.25138716	1.9565121975	H	-52.8646405336	3.1483887115	6.6928015715
H	-0.2311092182	-6.3832490269	3.5106357822	C	-3.9239108233	1.964622669	10.1081554253
C	0.6054245076	-4.7935035333	1.5902594314	C	-2.957449608	1.6221006325	11.1878635734
O	1.6089888607	-5.3984302849	1.9042506972	C	-1.6679273184	2.1923303604	10.7037737052
C	-7.7620016423	-0.0908009302	0.7316491801	C	-1.9340164901	3.0584209801	9.5878596379
C	-8.2102907769	0.8939812913	-0.1892072301	C	-1.4148262167	-2.7060612021	4.0245682589
C	-10.4565536637	0.6944451794	0.6021819575	C	-2.0051235837	-3.7015078161	4.8901674504
C	-10.0061695395	-0.2849373373	1.5278290222	C	-0.9760294782	-4.1822733735	5.7862238972
C	-8.6800331874	-0.6806908422	1.6153210437	C	0.2494399431	-3.4788461168	5.4743468505
C	-6.3652638515	-0.3446392584	0.5990006793	C	-0.0229293943	-2.5683453533	4.384462502
H	-5.8405979646	-1.0861334138	1.1921466208	C	-3.3207148623	2.920280228	9.2250360958
C	-11.8623766154	0.9126265402	0.7039751773	C	-4.8385847114	1.0615242341	9.5957174471
S	-11.3171576075	-0.8992560347	2.4953738243	C	-2.9035621148	0.0604954913	11.5776931948
H	-12.401834602	1.5999602638	0.0609921145	C	-0.4743144608	1.4920808571	10.7238750507
S	-6.9038386351	1.4809804748	-1.1800671096	C	-0.9775513537	3.2712230375	8.5917431651
C	-9.5337780801	1.3031805819	-0.2633322169	C	-2.1508447776	-1.577970157	3.6672532915
C	-12.4637868206	0.1473497551	1.6668366683	C	-3.3053984484	-3.5288614851	5.3587045539
O	-9.9265307811	2.2408096582	-1.1758189505	C	-1.2919669873	-4.4689396126	7.1115067979
O	-8.2947769448	-1.6397907659	2.5072626807	C	1.1042994503	-3.091434106	6.5028547004
C	-9.9740783526	3.563754872	-0.6547468733	C	0.5725782938	-1.3078439851	4.3729579091
H	-10.2990223871	4.2059164277	-1.4756587039	C	-3.7009563903	3.0026342279	7.8828992778
H	-10.689495753	3.6385172976	0.1736403719	C	-4.7893500388	-0.350753236	9.9586817731
H	-8.9851627639	3.8867675219	-0.3066089212	C	-1.5820440458	-0.5992546451	11.4178162757
C	-7.7661902231	-1.1173548343	3.7211105258	C	0.5038257313	1.683057433	9.6860665002
H	-7.4889391284	-1.9778406559	4.3326288852	C	-1.3722098458	3.3317137527	7.2055064115
H	-6.8778535155	-0.5010188079	3.5355361197	C	-3.4922833618	-1.3998814288	4.1633225107
H	-8.515875937	-0.5170898388	4.2514150694	C	-3.6248394594	-3.8188980796	6.7350714326
C	12.0596926814	-0.5477037579	-0.8202130259	C	-0.4040977129	-4.0604112935	8.173606773
C	11.6086788438	-1.5487558255	0.0807497834	C	1.7101246939	-1.7823541121	6.4888187892
C	9.325578751	-0.9946714662	-0.3587286072	C	-0.1962250052	-0.1447277988	4.0062761137
C	9.776758974	0.0014942438	-1.2661646074	C	-1.5299145546	-0.27689234	3.6598768637
C	11.1218074936	0.2295552485	-1.5174484468	C	-4.0587066012	-2.3546257036	4.9917260751
C	13.4855293029	-0.4911469457	-0.8775363906	C	-2.6397664867	-4.2824551778	7.5930525495
H	14.020736603	0.2022077345	-1.515986183	C	0.767283171	-3.3829033547	7.8749340179
C	7.9022502292	-1.0214246255	-0.2635502781	C	1.4483958224	-0.910070567	5.4464131692

S	8.4408942343	0.8656483957	-1.9765410286	C	-2.705453324	3.200385117	6.8582503656
H	7.3680905916	-1.6895610409	0.4035544189	C	-5.2076981125	1.1183347683	8.2052582983
S	12.9440603572	-2.3751939424	0.8290304287	C	-3.824905211	-0.8211928584	10.8204668474
C	10.2621566987	-1.7917368779	0.3161537596	C	-0.4313360851	0.0795501854	11.0849291045
C	14.1021153715	-1.4013710484	-0.0660895094	C	0.2659596997	2.5662480929	8.644164555
O	9.8655786187	-2.7506200684	1.2045548454	C	-4.6624053204	2.0784520983	7.3651118241
O	11.522543118	1.2040429834	-2.3890921254	C	-5.1420449249	-1.1244289235	8.7927307909
C	9.60673694	-4.014491902	0.6053077543	C	-1.780815443	-1.9140504302	10.8745778545
H	9.3059627972	-4.6827441717	1.4144751561	C	1.1571724864	0.4265191709	9.4212177138
H	8.7972554782	-3.944858435	-0.1320812563	C	-0.3566717101	2.6853563993	6.4087230537
H	10.5056677913	-4.4116271422	0.1177042777	C	-3.6996685838	0.0036485042	4.4379346715
C	11.67561371	0.7427988053	-3.7254155209	C	-4.5824173005	-2.84435133	7.2005104658
H	11.9886874403	1.6064764423	-4.3156884468	C	-1.2007359346	-3.6437253378	9.3016041271
H	12.4408554026	-0.0412873044	-3.7877963929	C	1.7644126616	-1.2851005653	7.8436167247
H	10.7292446251	0.3541067855	-4.1215699816	C	0.2230966091	0.9665322894	4.8303273228
C	7.2853566775	-0.0986336311	-1.0635605503	C	-2.4911011502	0.6980043196	4.1243508913
C	5.8746407333	0.1495051104	-1.2176157421	C	-4.8501603555	-1.9411264001	6.1269226466
C	5.2451120155	1.1614794504	-1.913845943	C	-2.5776687145	-3.781137629	8.9437963067
S	4.7000363129	-0.8989028972	-0.4831116682	C	1.1855592206	-2.2728226473	8.6971700271
C	3.8408684563	1.0951785902	-1.8579180805	C	1.2350671585	0.4926596751	5.7199967528
H	5.7887368396	1.9344380576	-2.4470138515	C	-3.0721478909	2.4158732971	5.703752461
C	3.3706803485	0.0287795774	-1.1141526372	C	-5.4073339421	-0.2230228754	7.7184118539
H	3.1865430383	1.8052533508	-2.3528349765	C	-3.1541093663	-2.0502405639	10.513896472
C	-0.5416729649	-0.3862758078	-0.7594656534	C	0.5785313719	-0.5583556998	10.2760743241
C	-1.9161881612	-0.0082366261	-0.9535399991	C	0.6535996303	2.2089431083	7.2984192449
C	-2.4075943828	0.8411435058	-1.9301010736	C	-4.2796981067	1.7205370958	6.0178978531
S	-3.1986196039	-0.5019704006	0.1120715488	C	-4.5951144821	-2.4076764803	8.5477033757
C	-3.7888758327	1.0799764069	-1.824976428	C	-0.7677182101	-2.6132754138	10.1690735183
H	-1.7834468132	1.2533018845	-2.7160834491	C	1.6394521588	0.0957078556	8.1305829857
C	-4.3784940786	0.41744509	-0.7661094141	C	-0.6811003363	1.9825409599	5.2211153914
H	-4.3470033397	1.6999071765	-2.5186443571	C	-2.0923177739	1.8425217573	4.8547280275
C	-5.7638858244	0.4133601435	-0.3694775521	C	-5.1353697003	-0.5754934909	6.3724960188
C	2.0110425998	-0.3424269685	-0.8451670222	C	-3.5551848443	-2.8898728531	9.4438638158
C	1.4888383894	-1.4509895307	-0.2060814429	C	0.4663145369	-1.9070238147	9.86129381
C	-19.9362415458	3.5385719202	0.882399253	C	1.3718577025	1.0202801414	7.0268085141
C	-19.5410238964	2.3721985306	1.6091126185	C	-4.5440542965	0.4339864335	5.4908679931
S	-18.9677952246	0.2998666556	2.987472224	C	-3.3391902347	1.1264840559	12.5595155465
S	-17.3758278351	3.3453162554	0.4365037596	C	-4.8165269108	1.1551386098	12.8805276386
F	-21.1890007979	3.9703646854	0.8687355377	C	-2.5836777226	1.4653958673	13.8529984726
C	-18.918393075	4.1519858268	0.2134204521	C	-5.5345510737	2.3490538864	12.7878724667
O	-20.1323816914	5.8976763421	-0.7525902994	C	-5.4526074375	0.0205695906	13.3879373579
C	-20.1763469664	7.0660193823	-1.5691359313	H	-3.0236172273	2.410349051	14.2023254296
H	-21.2178235404	7.387084659	-1.5620079668	H	-2.9097334356	0.7118011888	14.584113229
H	-19.5301383548	7.8464761664	-1.1586596561	C	-1.0658410693	1.587606586	13.9231221479

H	-19.8506880477	6.8362454133	-2.5871614925	C	-6.8681286924	2.4051579955	13.1824078534
C	-18.9187866441	5.3470585071	-0.635126125	H	-5.0467218346	3.2393978395	12.3983038682
O	-17.9167238388	5.7772424828	-1.1666597382	C	-6.7860709891	0.0745197529	13.7834077891
C	-27.5107964935	2.1621567717	2.3582509691	H	-4.9010096461	-0.9132365866	13.4672586828
C	-27.8969231575	1.2392928802	3.3672387511	H	-0.5751107721	0.654403206	13.6357117026
C	-30.2074355441	1.7447126541	3.0266140475	H	-0.6969179038	2.3560567348	13.2388248204
C	-29.8220914174	2.6633466154	2.0133437861	C	-0.6403122161	1.9484179998	15.3403202216
C	-28.4977870614	2.8767104529	1.6605611306	C	-7.4977154831	1.2668696436	13.6793069421
C	-26.0933207875	2.2306052577	2.2165328949	H	-7.4160256481	3.3397429841	13.0987434867
H	-25.5994566746	2.9091311866	1.5292282443	H	-7.2697212213	-0.8179377497	14.1710649834
C	-31.6211549309	1.7203664866	3.2111842253	H	-1.0921280126	2.8944770454	15.6674643736
S	-31.2055054697	3.462670339	1.3194678097	H	-0.981094778	1.1964600501	16.0650839103
H	-32.1083873807	1.1034701552	3.9587188791	C	0.8574352039	2.0753976167	15.4741356372
S	-26.5123455396	0.4766376983	4.0971583752	H	-8.5398140768	1.3087161109	13.9839638598
C	-29.2226333205	1.0093656978	3.7047993683	O	1.6594452868	1.8953260515	14.588642876
C	-32.2942910779	2.5719537573	2.3771545184	O	1.199592324	2.4191314615	16.726825185
O	-29.5504200356	0.1255741528	4.6932010926	C	2.600705915	2.5591544007	16.9488329612
O	-28.1657850221	3.7812457318	0.6918203737	H	3.1194508732	1.6178566537	16.7477072177
C	-29.8659594932	-1.1771762307	4.2159104536	H	3.0184551455	3.3351497539	16.3016391372
H	-30.1040189318	-1.7775681099	5.0960239006	H	2.7075043237	2.8377365665	17.9974556526
H	-30.7322589539	-1.1541797198	3.5431296293				

Table S19. The coordinate of 2/PC₇₁BM (353 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	19.2909724002	-3.1269953934	0.7414834218	H	-29.2229814268	4.3535511579	-2.6103629904
C	21.67950675	-2.4166984353	1.1096595924	C	-14.9865417302	-1.6486276105	-0.2635523508
C	20.3010346036	-2.175801984	0.9662450014	S	-15.4405940978	0.8459746254	-0.5272317895
C	17.8680409567	-2.6756063965	0.6615610672	C	-16.3862835008	-1.5108403601	-0.2941134811
C	16.9268720656	-3.5480533645	0.1011267446	C	-16.8232811238	-0.2133426864	-0.4322934146
C	15.5938663935	-3.1866874471	-0.0104227403	C	-20.7116980177	0.4476934145	-0.5253952954
C	15.1440670771	-1.9397680257	0.4484387472	C	-22.1037808116	0.0990600134	-0.5030036042
C	16.0818915107	-1.0776247404	1.0377325106	C	-22.635631458	-1.1718396704	-0.4206206084
C	17.4169942519	-1.4367879073	1.13666583	S	-23.4207498397	1.2468851613	-0.5650513548
H	19.9855461098	-1.1455194408	1.0468669434	C	-24.0396234632	-1.2227540009	-0.4084162426
H	17.2656059869	-4.5180782956	-0.2474585527	C	-24.6418745562	0.0095960627	-0.4806051744
H	14.8921509779	-3.8737226156	-0.4767957696	C	-26.0422423611	0.3343365998	-0.4918352566
H	15.7511190163	-0.1290765765	1.4507480852	C	-18.1691539874	0.2710854672	-0.4880994424
H	18.1026094245	-0.7541368238	1.6287798885	C	-18.6368980228	1.5677456096	-0.5949632581
C	22.5998084857	-1.2549438597	1.3117071306	C	-14.3007600478	-0.4627612597	-0.3788389303
C	22.2769736507	0.0506178672	0.9222295897	C	-40.4824731312	-0.5149189964	0.0875459971
C	23.8503551966	-1.4922075331	1.895684803	C	-40.0315663507	0.8402525614	0.0102994176
C	23.1739377267	1.0931374657	1.1290237814	S	-39.3472160258	3.3085027427	-0.1348575183
H	21.3339426385	0.2548001674	0.4241728729	S	-37.891787947	-0.7203825459	-0.0278552279

C	24.7420038107	-0.4488054717	2.1119569723	F	-41.7676158814	-0.83479201	0.1612195255
H	24.108253895	-2.5101789221	2.1696956367	C	-39.4838520262	-1.4434799796	0.07780519
C	24.4055712914	0.8487985067	1.7317941926	O	-40.7867901651	-3.3775932197	0.2159657604
H	22.9122289204	2.0990124565	0.8117872759	C	-40.8819050669	-4.8000770245	0.2726422762
H	25.7047189914	-0.6488574426	2.5747416846	H	-41.9481011432	-5.0182913797	0.3294460964
H	25.1037121937	1.6652651579	1.8961993802	H	-40.4436552574	-5.2500498925	-0.6220139124
O	19.4565111596	-4.3743837855	0.5524053029	H	-40.3619533015	-5.184879295	1.1538912894
O	22.2511929274	-3.5526282252	1.1271904228	C	-39.5376338231	-2.9074769693	0.1370698559
Ir	21.3171338465	-5.4540038508	0.7079745645	O	-38.5427052911	-3.6010381993	0.1148429872
C	23.0802360764	-6.3629463933	0.7292935097	C	-47.9571538704	1.4522547419	0.523251925
C	23.6796313389	-7.0190320883	1.8079733641	C	-48.3938913917	2.7982505641	0.4003550617
C	23.7930293618	-6.2804284684	-0.5006841052	C	-50.6813017113	2.1258292264	0.5655018739
C	24.9484466081	-7.5573814832	1.6682208101	C	-50.2442669045	0.7796477221	0.6927256014
H	23.1750560643	-7.1195145588	2.7631591957	C	-48.9005369187	0.4271389234	0.6853622134
C	25.0713978934	-6.8418890551	-0.5793308897	C	-46.5371385742	1.3492253422	0.4528316248
C	25.6737227316	-7.4829627532	0.485698622	H	-46.012207756	0.4012995357	0.5060699971
H	26.6647313911	-7.9104721156	0.3958847084	C	-52.1127300656	2.2223464821	0.5871424474
C	23.092157137	-5.6134714779	-1.5882092377	S	-51.5944571966	-0.3136553173	0.8326821628
C	23.5477056138	-5.4160606428	-2.898177637	H	-52.6497153842	3.1576382365	0.480793285
C	22.7353707783	-4.7815534761	-3.824078093	S	-47.0562840838	3.8944279057	0.2020613658
H	24.5322560978	-5.7657234286	-3.1741320005	C	-49.735818606	3.1520251417	0.4300728846
C	21.0663233824	-4.562057477	-2.1379916743	C	-52.7120294016	1.0142440721	0.7279600097
C	21.4674605525	-4.34630515	-3.4445959206	O	-50.1207689491	4.455888893	0.2902501491
H	23.0899280751	-4.6301889621	-4.8397194021	O	-48.5077628702	-0.8767257053	0.7941709272
H	20.0938453339	-4.2563088686	-1.768238818	C	-50.2748583279	5.1428005157	1.5258188355
H	20.799906884	-3.8498696002	-4.1403057711	H	-50.574695174	6.1623768434	1.2756932525
C	20.0524696839	-6.9443942228	2.859007925	H	-51.0497300209	4.6738731697	2.1453506687
C	21.1669980816	-5.042045967	3.6662443813	H	-49.3319784426	5.1674752364	2.0861858718
C	19.6300112076	-7.2464562369	4.1599623739	C	-48.2998961592	-1.3013628119	2.1357242587
C	20.7788028912	-5.2980259356	4.9695599401	H	-48.0040329079	-2.3510151456	2.0838465905
H	21.7820311574	-4.1910794435	3.3948286231	H	-47.5031729898	-0.7186333391	2.6152526131
C	19.9925044819	-6.4220278841	5.2130599341	H	-49.218906763	-1.210110676	2.7276347837
H	19.0248621999	-8.1256591174	4.3292824253	C	-34.7682168204	3.8544109923	-0.3921765877
H	21.0869012708	-4.6305550898	5.7668306398	S	-35.3805686523	1.3853046912	-0.2317039736
H	19.6642849979	-6.6580497146	6.2213567055	C	-36.17282613	3.8073851654	-0.3216346821
C	19.792990313	-7.7061680603	1.6458567875	C	-36.6913478745	2.5360496496	-0.229709691
C	19.0538392887	-8.8908021552	1.5707553827	C	-40.6087175455	2.1143296638	-0.0192020589
C	20.3685632657	-7.1782472564	0.4551633867	C	-41.9760460882	2.5480826181	0.0313241601
C	18.8625869667	-9.5793868233	0.3885465896	C	-42.4329528499	3.848604481	-0.0340705884
C	20.187136345	-7.8747628792	-0.7426882849	S	-43.3542308401	1.4852751073	0.1945297887
C	19.4460587287	-9.0452687914	-0.7534593317	C	-43.8291827088	3.9868498551	0.0453672032
H	18.2864584989	-10.4960215185	0.3599617761	C	-44.4994204511	2.7953043443	0.1760793308
H	20.6138677209	-7.5216084511	-1.6755418782	C	-45.9134689684	2.5574233365	0.2889751179
N	20.8135741626	-5.8347881411	2.645727605	C	-38.0629651998	2.1355371004	-0.1434189196

N	21.8515667705	-5.1710828652	-1.2392232716	C	-38.6068876387	0.8672831979	-0.0598522398
F	19.2769872866	-9.6992249284	-1.9098618633	C	-34.1604228369	2.6220909802	-0.3551861431
F	18.4904619217	-9.4118203123	2.6772772186	H	-53.7747290022	0.8095544413	0.7642287043
F	25.7744028448	-6.7742941766	-1.7260113672	F	5.8531472595	3.4176439845	-0.4159479482
F	25.5116312552	-8.1786743315	2.7124308992	F	3.0441726921	3.3999910714	-0.5184885184
C	-0.6868006505	-1.9247378922	-0.157685162	F	-1.6984685457	3.500085543	-0.7709837291
C	-0.1984491195	-0.5864691324	-0.2855842383	F	-4.4773059648	3.8237014887	-0.8252078581
S	0.5548066793	1.8558292471	-0.5053161927	F	-14.4053613896	-2.8372368534	-0.1314226392
S	1.8985783164	-2.1870957546	-0.0535090162	F	-17.2006865906	-2.5591408729	-0.1935231044
F	-1.9808393327	-2.2143925725	-0.1594034154	F	-21.9032412705	-2.280758768	-0.355357095
C	0.2868231006	-2.8710491949	-0.0298890706	F	-24.6946155604	-2.3772494433	-0.3336082995
O	-1.0715509739	-4.7625408496	0.1547766465	F	-34.1127544645	5.0073747461	-0.486471525
C	-1.2066233359	-6.1736046021	0.3155432862	F	-36.9173327011	4.9107502049	-0.3441352598
H	-2.2793419327	-6.3656703212	0.3100701686	F	-41.6389073111	4.9089609578	-0.1599863427
H	-0.7161179348	-6.7024519884	-0.5058920145	F	-44.415726739	5.1791350208	-0.0034164612
H	-0.7619734866	-6.4965199519	1.2605771546	C	-2.7643645078	2.4451149666	10.1924048958
C	0.1917201169	-4.3248416192	0.132808344	C	-1.6312072341	2.006376867	11.0529990896
O	1.167413356	-5.0381651026	0.2363555029	C	-0.4448435762	2.6745149735	10.4455646148
C	-8.1046453751	0.162017934	-0.357597221	C	-0.9000632445	3.6606551882	9.5040979873
C	-8.5193404548	1.5068458824	-0.5561851405	C	-1.213860168	-1.3638054799	3.2488000545
C	-10.8185710388	0.8578256988	-0.4876836628	C	-1.6427984534	-2.4765138145	4.065962278
C	-10.4027542942	-0.4860956315	-0.2860819091	C	-0.475695773	-3.0278730672	4.7191459076
C	-9.0665869609	-0.8492932457	-0.2072351135	C	0.6731327999	-2.2506713378	4.3082248396
C	-6.6861927869	0.0427536365	-0.344269538	C	0.2159949609	-1.2241657939	3.3990705686
H	-6.1757353375	-0.9068197774	-0.2242549484	C	-2.325056914	3.5206112142	9.3518641779
C	-12.2379920223	0.9683715623	-0.5409642554	C	-3.7382522782	1.5813369266	9.7232513237
S	-11.7592810606	-1.5705065654	-0.1711650621	C	-1.4943378837	0.4118548887	11.2306429704
H	-12.7496518915	1.9094676295	-0.7127459203	C	0.7455020484	2.0172406107	10.1871096624
S	-7.1587853785	2.5809187276	-0.7222042536	C	-0.1211266894	4.0253375601	8.402774897
C	-9.8566567736	1.8731613933	-0.6122898407	C	-2.0138122961	-0.2249658249	3.1586357065
C	-12.8818634944	-0.2306174763	-0.3821583819	C	-2.8517621387	-2.4044669372	4.7539056114
O	-10.2272253482	3.1707881515	-0.8204386751	C	-0.5687016321	-3.4833135417	6.0311209178
O	-8.6977287104	-2.1517670688	-0.025838175	C	1.6787860092	-1.9631158498	5.227159341
C	-10.4032561568	3.917470929	0.3782493254	C	0.7851148036	0.0476002133	3.4504016012
H	-10.6896319708	4.9255197525	0.0726075179	C	-2.9195547056	3.7534398807	8.1089378946
H	-11.1957638081	3.4835028489	1.000739832	C	-3.6117184352	0.1379456591	9.8935542674
H	-9.4729035566	3.9619180727	0.9576360475	C	-0.2081265305	-0.1785937839	10.7793797914
C	-8.5302350037	-2.5142563589	1.3401688649	C	1.5393770418	2.3658875223	9.0388297852
H	-8.2499244228	-3.5693118472	1.3457465666	C	-0.7364670828	4.2403851579	7.1159205954
H	-7.7369583599	-1.921112825	1.812173061	C	-3.2588801149	-0.1533296536	3.8811709153
H	-9.4629433764	-2.3812649293	1.9018971583	C	-2.9400483454	-2.8705142538	6.1160604699
C	11.8129290611	-0.2348268698	0.1419798873	C	0.4742016285	-3.1777707888	6.9810427418
C	11.2504407947	-1.5397772369	0.1240326121	C	2.2572554678	-0.6426712303	5.2812405274
C	9.0423097613	-0.6425332881	-0.0409515011	C	-0.0486894244	1.2207435866	3.3601871962

C	9.6039858736	0.6622654327	-0.0365924287	C	-1.4190197732	1.0873815568	3.2172424879
C	10.9720191986	0.8840060494	0.0420717317	C	-3.6705769288	-1.2199546758	4.6621638154
C	13.2358223007	-0.2745370726	0.2619534641	C	-1.8227757277	-3.4014026233	6.7407385037
H	13.8505727536	0.6179566085	0.2827729716	C	1.5732940536	-2.4310517829	6.5875421892
C	7.6198296588	-0.6060304888	-0.1136202083	C	1.818276254	0.34109294	4.4115148756
S	8.3731228475	1.8915831192	-0.1235457343	C	-2.1066023172	4.1081693118	6.9718500588
H	7.0069811854	-1.5012487681	-0.1064478733	C	-4.3291645579	1.7946366029	8.4275373099
S	12.4807146114	-2.7622447188	0.2617711209	C	-2.5147950856	-0.4019874894	10.5255021084
C	9.8844004845	-1.763050446	0.0263694995	C	0.8647510449	0.5733427062	10.3562193758
C	13.7434453002	-1.5412563352	0.3274470863	C	1.1239002883	3.3611280242	8.1676594581
O	9.3737023243	-3.0297964716	0.0345583407	C	-3.9402170962	2.8679419488	7.6389522867
O	11.4814677771	2.1523062902	0.0608510788	C	-4.1399787104	-0.4991093216	8.7110622972
C	9.1970645517	-3.5855098521	-1.2628418228	C	-0.4748827801	-1.4240453254	10.1150995183
H	8.7882190063	-4.5869448756	-1.1152510636	C	2.1572344064	1.1733009491	8.5175456001
H	8.4953679432	-2.9871515763	-1.8575833094	C	0.1452312451	3.7302022952	6.0930690088
H	10.1529061257	-3.6558604481	-1.7966064611	C	-3.4376041683	1.1981953239	4.3594018401
C	11.7907537731	2.6621514904	-1.2302138479	C	-3.8237427999	-1.9926430656	6.8463108683
H	12.1802784667	3.6706897617	-1.0776915811	C	-0.1345333832	-2.9276078197	8.2644168664
H	12.5510564951	2.0459302875	-1.7266664814	C	2.5240570446	-0.3124591791	6.6617147638
H	10.8959441691	2.7093963033	-1.8631681497	C	0.4844112171	2.2374674322	4.2388453098
C	7.1114693241	0.664443218	-0.1693338308	C	-2.3053811156	1.9656415585	3.9471275397
C	5.7244903914	1.0380427464	-0.2394222356	C	-4.2736911735	-0.974669684	5.9513196291
C	5.1585892923	2.2852373968	-0.3544881767	C	-1.5492546371	-3.0664207046	8.1162840447
S	4.4626344359	-0.1609036763	-0.1914285092	C	2.1039008702	-1.4157307237	7.4655673433
C	3.7517948613	2.2779702128	-0.4061631203	C	1.6331164262	1.6921273338	4.8894319172
C	3.1906050663	1.0239459258	-0.3313939639	C	-2.6454975214	3.4584370986	5.8012559252
C	-0.7402163371	0.6956724816	-0.4287742879	C	-4.5875135278	0.5167629277	7.8139045698
C	-2.0975031163	1.1565102467	-0.5021523207	C	-1.8866044142	-1.5610923814	9.9632943795
C	-2.5217794343	2.4609323409	-0.6569608552	C	1.7378982161	0.0729264037	9.3230213023
S	-3.5036788402	0.1259602743	-0.3927306771	C	1.2934635533	3.1835449027	6.7431482095
C	-3.9171931622	2.6260329273	-0.6843818312	C	-3.7765439652	2.6894999982	6.2137947756
C	-4.6179049243	1.4521874481	-0.5502080596	C	-3.6233086901	-1.7238945882	8.2224955976
C	-6.0390472302	1.2380087399	-0.517959408	C	0.419611727	-1.9972991967	9.1748406227
C	1.806368171	0.6593539906	-0.3464985316	C	2.4288739179	1.0183630367	7.1355586197
C	1.2271889838	-0.5918076007	-0.2418570014	C	-0.3584855916	3.1668786242	4.8937714366
C	-20.4279146985	3.0589494638	-0.7268736422	C	-1.8084421749	3.0255724815	4.7424160428
C	-20.0587708481	1.6816731236	-0.6169972478	C	-4.5332436747	0.3402425481	6.4085056862
S	-19.522290586	-0.8190413275	-0.4163012872	C	-2.4449049277	-2.2762784714	8.8732574613
S	-17.8270547548	3.1055794401	-0.7051368407	C	1.5778987975	-1.2181922314	8.765583436
F	-21.6930340729	3.4554849874	-0.7705424248	C	1.9731334952	2.0608622067	6.2135878738
C	-19.3744015825	3.9231094593	-0.7824394311	C	-4.1062268015	1.4685153271	5.5781603138
O	-20.5613584368	5.9283133835	-0.9456301562	C	-1.7784701062	1.3357633137	12.3951295667
C	-20.572592079	7.3511618347	-1.0513668661	C	-3.1839779934	1.2747066658	12.948986562
H	-21.6250956166	7.6325188836	-1.0780125999	C	-0.8281376691	1.5461256616	13.5830793054

H	-20.0743060431	7.8041885136	-0.1903132339	C	-3.9241194746	2.4454584965	13.1256451401
H	-20.0643844518	7.672277086	-1.9644162155	C	-3.7122063575	0.0649007884	13.4036501169
C	-19.3409031549	5.3848962594	-0.8923447565	H	-1.2086167876	2.4391948964	14.0990469686
O	-18.3055985837	6.0158259908	-0.9287906168	H	-1.032431869	0.7119509766	14.2694135862
C	-28.0248624025	1.5660518787	-0.5537235047	C	0.6815971063	1.6871477807	13.4256621018
C	-28.5342479124	0.2442232937	-0.4401748914	C	-5.1755082867	2.4059950815	13.7337889374
C	-30.7808110397	1.0576717778	-0.4206812153	H	-3.5197384963	3.3933852435	12.7786904119
C	-30.2718415053	2.3792423657	-0.5400020865	C	-4.9631440651	0.0232193128	14.0124107125
C	-28.9138405456	2.6509780592	-0.6186500266	H	-3.141434652	-0.8515547103	13.2738967365
C	-26.6010235508	1.5828572648	-0.5771208938	H	1.1184454463	0.7999757996	12.9602453819
H	-26.0232277073	2.4992302245	-0.635055135	H	0.9378347288	2.5331167541	12.7826332609
C	-32.2030815818	1.0444105382	-0.3432999074	C	1.3288374104	1.8955246725	14.7884910387
S	-31.5492448308	3.5621284128	-0.5527616614	C	-5.6987911985	1.194084059	14.1768759768
H	-32.7780244054	0.1323593105	-0.2230040957	H	-5.7429751072	3.3241264098	13.8590202666
S	-27.2562046457	-0.9348059555	-0.367261637	H	-5.3639936048	-0.9264077465	14.3562135342
C	-29.8932277966	-0.0294013397	-0.3841146827	H	0.9300542075	2.7874714509	15.2902904335
C	-32.7616253204	2.2938642907	-0.4063431838	H	1.1153045503	1.0588041036	15.4673822405
O	-30.349101113	-1.3098182356	-0.2544922387	C	2.8273879952	2.0460063086	14.6932825302
O	-28.4545400428	3.9335624905	-0.7162175576	H	-6.6772079327	1.1621015466	14.6482816764
C	-30.6375498237	-1.946457779	-1.4941695095	O	3.4740796333	2.0023583457	13.6736864629
H	-30.984135815	-2.952153306	-1.2492444894	O	3.3686167772	2.2386911704	15.9076291335
H	-31.4237447781	-1.4105765495	-2.0406341467	C	4.7858428118	2.3913219441	15.9148251764
H	-29.7411823392	-2.0117451543	-2.1230881317	H	5.2721128568	1.5002271685	15.5086046796
C	-28.2764769939	4.3769598653	-2.0565007529	H	5.0838459143	3.2569674332	15.3169295096
H	-27.9171681323	5.405962277	-1.9945780202	H	5.0624777892	2.5350594237	16.959555529
H	-27.5361143495	3.7602430033	-2.5814578029				

Table S20. The coordinate of 3/PC₇₁BM (296 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	14.5390042527	-0.2173356098	0.6941898212	S	-17.7566708962	1.0112647541	0.1117184627
C	16.6059216862	-1.656098683	0.688849674	C	-20.5388556877	0.8401159446	0.0447929713
C	15.2191688887	-1.4431148177	0.5903464575	C	-16.9097422294	-0.1991366443	-0.8540485202
C	13.0543587245	-0.1950618427	0.5307690014	C	-23.9246749594	-0.320192952	-0.8728828303
C	12.3469901924	0.9050292261	1.0304172637	O	-20.6342082104	1.9242152307	0.8695554116
C	10.9673600977	0.9754892835	0.9242345742	O	-20.2037910872	-2.4763071725	-2.5571847703
C	10.2387104297	-0.0445098713	0.2942029679	C	-20.8089042884	1.5890503275	2.2407663137
C	10.9526832109	-1.1293910098	-0.2390697151	H	-20.8625430532	2.5348694839	2.7834607605
C	12.3310474182	-1.2061880264	-0.1157575018	H	-21.7365783494	1.0247199745	2.3964575428
H	14.6101083122	-2.318619204	0.4157773733	H	-19.9607520129	1.0013344227	2.613472402
H	12.9037749037	1.7045902297	1.5080288656	C	-19.9696957594	-3.7170868695	-1.9024713362
H	10.4433931846	1.8264629577	1.3521629037	H	-19.929173627	-4.4750181189	-2.6872330028
H	10.4212116735	-1.9063651119	-0.7807049953	H	-19.0186646993	-3.7054830423	-1.3560699306
H	12.8489351978	-2.0468643591	-0.5673070779	H	-20.7839236811	-3.9544864083	-1.2065482859

C	17.1328160145	-3.0528263604	0.5945164908	S	-26.8993045965	2.2710517106	1.4768809112
C	16.3506454648	-4.1830871588	0.8612284319	C	-28.3249536341	-0.2984323261	-0.9280386659
C	18.4775213143	-3.2330441201	0.247082191	C	-26.1297907998	-1.1357222574	-1.6707026734
C	16.8946253198	-5.4593445395	0.7646790928	C	-27.5392664103	-1.1394596708	-1.6954568981
H	15.3182778806	-4.0707620254	1.178324591	H	-25.6223676385	-1.8397839585	-2.3246158298
C	19.0181265469	-4.5085270046	0.1408190747	H	-28.0196452826	-1.8526746894	-2.3597253732
H	19.0879243167	-2.3535945042	0.0688506703	C	-27.5932922137	0.6038729481	-0.0809607867
C	18.2274846421	-5.6269192806	0.3966521661	C	-26.1416972613	0.6060219108	-0.053449126
H	16.2765942725	-6.3256905414	0.9846692736	C	-25.3761006803	-0.2921347184	-0.8745968287
H	20.0612400155	-4.6309314217	-0.1383881641	N	-25.6410377531	1.5058046613	0.7931246679
H	18.650212952	-6.6250208314	0.3180337413	N	-28.1282159645	1.5056090726	0.7422489932
O	15.055024972	0.9141570461	0.9635754877	C	-32.0380818085	0.0847410748	-0.5535655574
O	17.5010193893	-0.7615062303	0.8164806642	C	-32.1451148663	-0.8916995492	-1.5792967272
Ir	17.1592923959	1.342812427	1.1482708493	C	-34.5309368901	-0.8356124756	-1.4638184106
C	19.097611116	1.6384081652	1.4493483109	C	-34.4254464514	0.1465945788	-0.4433235231
C	20.0462992962	2.0535894753	0.5107552015	C	-33.2029948675	0.6222432914	0.0141294326
C	19.5320717007	1.345644134	2.7736056029	C	-30.6778293877	0.3779793416	-0.2349055798
C	21.3784700409	2.1574456771	0.8761497733	H	-30.3783655121	1.0763343193	0.5348812834
H	19.7672963835	2.2989170613	-0.5083852792	C	-35.899509495	-1.1627786214	-1.743596566
C	20.8906591889	1.4679299226	3.0817242658	S	-35.9960076191	0.6337208683	0.1340733093
C	21.8345233792	1.8687458561	2.1563148451	H	-36.1989141814	-1.9061136693	-2.4731861909
H	22.880526481	1.9561211764	2.4231354636	S	-30.5777202388	-1.4141592061	-2.1227652197
C	18.4843714045	0.9557014149	3.7056726865	C	-33.3664378855	-1.3525183367	-2.0497411152
C	18.6289702766	0.6372584735	5.0621547787	C	-29.7754482547	-0.3300404546	-0.9824223354
C	17.5138679778	0.3179861794	5.8198042998	O	-33.4285673381	-2.3077215694	-3.0262343231
H	19.6143589616	0.6472863971	5.5055853299	O	-33.1501944081	1.5523952582	1.0120615361
C	16.1651597902	0.6356080881	3.8816555695	C	-33.5334972574	-1.7743027673	-4.3396681201
C	16.2537013774	0.3196724388	5.2260316298	H	-33.567731427	-2.6294059355	-5.0178914429
H	17.6281600986	0.0720552683	6.8717804459	H	-34.4485344432	-1.1792773158	-4.4539562557
H	15.2201026239	0.6634463793	3.3505542092	H	-32.6656771189	-1.1492552122	-4.5845195682
H	15.3558028411	0.0815018183	5.7856607293	C	-32.9747518198	2.8855358183	0.5493004201
C	16.8065505168	3.1216125221	-1.1236174424	H	-32.9572803994	3.5190776278	1.4382897716
C	17.3894490286	0.9533367562	-1.8102021578	H	-32.0300606518	2.995898327	0.0028227314
C	16.7231479785	3.5212708027	-2.4637146759	H	-33.8054531334	3.1893321878	-0.0998447405
C	17.3247861132	1.2987601228	-3.1486035673	C	-36.7681757209	-0.4579149849	-0.9765741569
H	17.6551503401	-0.0438796266	-1.4769593052	H	-37.8491288233	-0.5219961245	-0.9838624177
C	16.9805485755	2.6088380888	-3.4742207409	C	1.8967935135	3.1073785761	9.9603888986
H	16.4603502102	4.5433843811	-2.6961923807	C	3.1804651905	2.4903137688	10.395484456
H	17.5386937031	0.5564359622	-3.9097253299	C	4.0718331569	2.6523711288	9.2118693589
H	16.9157979674	2.9206475588	-4.512827253	C	3.4526051672	3.5610292342	8.2865022471
C	16.6011763574	3.9459970679	0.0584413114	C	-0.6753365534	-2.0825106166	4.3401120834
C	16.2706503634	5.3047551896	0.0558284945	C	-0.9053239993	-2.8592312188	5.537177028
C	16.7746440554	3.2830264845	1.3065844819	C	0.2904130636	-3.6263836483	5.8094820463
C	16.1110324867	6.038252453	1.2154619292	C	1.260490803	-3.3179078972	4.7815006588

C	16.6247315245	4.0215856095	2.4836266421	C	0.6618602432	-2.3651762803	3.8735661807
C	16.2980897537	5.3662036537	2.4166773212	C	2.1179806469	3.8420919895	8.7487403898
H	15.8555401362	7.0901988372	1.1832947453	C	0.662890527	2.517981848	10.1713196986
H	16.7570408985	3.5678271625	3.4601550681	C	3.0532362248	0.981981957	10.9466773244
N	17.1345470975	1.8319295328	-0.8311903576	C	4.8544557728	1.628736266	8.7061122544
N	17.2427415253	0.9374407118	3.144563284	C	3.7061289391	3.4832374806	6.9144492776
F	16.1529856519	6.0591830277	3.5536183654	C	-1.1776888444	-0.7852890063	4.2525447795
F	16.0929185217	5.9590486425	-1.1075092709	C	-1.629446543	-2.308509941	6.591588339
F	21.3339494086	1.1922159089	4.3233883034	C	0.7098217505	-3.8095892415	7.1239489031
F	22.2760033095	2.5518390036	-0.0362283666	C	2.6086846472	-3.2066576232	5.113638845
C	6.5446711602	-0.6324600905	-0.0278062593	C	1.4391889147	-1.3386482686	3.3399248722
C	6.4028740253	0.7740215054	0.1125193712	C	1.0874766631	4.0377359184	7.825574434
C	4.0261767285	0.6117508517	-0.0726576421	C	0.5543324695	1.1540206391	10.6772949048
C	4.1677986333	-0.7953709916	-0.2104919471	C	3.84567169	-0.0399971222	10.2153614842
C	5.4001527166	-1.4316644732	-0.1735861711	C	5.0960209573	1.5235007727	7.2914680882
C	7.9149510035	-1.0313275802	0.0201721099	C	2.6340673792	3.6624965119	5.966006098
H	8.2301125969	-2.0657238905	-0.0552777617	C	-1.9172080829	-0.2175152205	5.35155429
C	2.6603953712	1.0183873736	-0.1359028499	C	-1.1850026338	-2.4947567497	7.9512071978
S	2.624205957	-1.5710847067	-0.4154425513	C	2.107040349	-3.6857970295	7.4637300805
H	2.335353472	2.0474119979	-0.0641564281	C	3.4059629707	-2.1370065664	4.5631144562
S	7.9476370458	1.5548830044	0.2848152549	C	0.914582728	0.0010312771	3.2566545169
C	5.1688472975	1.4086905063	0.1032657201	C	-0.3673119991	0.2722657061	3.7015952999
C	8.7822970221	0.0113960052	0.1906267177	C	-2.1401426752	-0.9625951404	6.4971697014
C	1.7872929897	-0.0218563975	-0.3099405732	C	-0.0414670655	-3.2326606176	8.2128642594
O	5.0917561796	2.7653788415	0.2249665811	C	3.0358750649	-3.3881152599	6.4793468267
O	5.492608885	-2.7897561001	-0.3012642484	C	2.8314396797	-1.2225765649	3.6957715161
C	4.7443688062	3.2129242314	1.5309072763	C	1.3519449714	3.9330290385	6.4117274055
H	4.7568739015	4.3039141408	1.4929541378	C	-0.392730598	2.6860078991	9.2061804138
H	3.743965734	2.8686368548	1.8184890999	C	1.6822868362	0.4163787924	10.954879967
H	5.4726322922	2.8638202673	2.2730898748	C	4.7391554871	0.2665928957	9.2137704357
C	5.5088954203	-3.474060887	0.9460200516	C	4.5447301456	2.4404889239	6.4094731399
H	5.5410214805	-4.5402006611	0.7122499957	C	-0.1919265791	3.4426032611	8.0607507447
H	6.393387819	-3.200914669	1.5354575406	C	-0.5690265164	0.5237998604	10.026404931
H	4.6074500881	-3.2537497136	1.5312631298	C	3.0593982719	-1.2354916382	10.0883351358
S	-1.1955858328	3.2863713929	0.760982393	C	5.1526155837	0.1301907199	6.9287966093
C	-2.6006935858	0.0262719404	-0.5872243309	C	2.832230591	2.7451467417	4.8688995803
C	-0.4034976873	-1.0549997383	-0.8634657976	C	-1.5802649253	1.1830839529	5.4604689857
C	-1.8110323505	-1.0507092849	-0.9486776302	C	-1.4421380736	-1.2806656816	6.8887477059
H	0.1124957677	-1.95646698	-1.1828829423	C	2.2103474447	-3.054454566	8.7566015965
H	-2.2873499539	-1.9558690984	-1.3156619859	C	4.3287072516	-1.6814463415	5.5769719664
C	-1.8781276898	1.1722100344	-0.1056105189	C	1.9825682161	0.9347241425	3.5332779056
C	-0.4297214289	1.1695582832	-0.0225047468	C	-0.627111483	1.4875805081	4.44106256
C	0.3398090345	0.0196375088	-0.4105553986	C	-2.0301588784	-0.3358304107	7.7936322035
N	0.065693123	2.3116827122	0.4547560078	C	0.88664552	-2.7752130807	9.2176272071

N	-2.418218627	2.3195797684	0.3064489055	C	4.1012123524	-2.4542587617	6.7561572494
C	-6.311624226	0.5569407042	-0.5031708327	C	3.1640160322	0.1795417224	3.8063374994
C	-6.4098939505	-0.7008907817	-1.1560359143	C	0.2216665858	3.2971915885	5.7780798606
C	-8.7965936649	-0.5796144061	-1.1520442894	C	-1.1553438226	1.4656036282	9.1286732303
C	-8.6974573512	0.6815584963	-0.5060315518	C	1.7367602426	-0.9554021785	10.5435517462
C	-7.481514053	1.2667082251	-0.1862756375	C	4.9274781204	-0.6403522838	8.1083271066
C	-4.9569058681	0.921370081	-0.2481972455	C	4.0119962407	1.9877661754	5.1443020396
H	-4.6636959389	1.8292651985	0.2612644633	C	-0.7302947737	2.9900326416	6.7979746877
C	-10.1532827134	-0.9689481873	-1.3557238753	C	-0.591250797	-0.8631426406	9.740912265
S	-10.2673537012	1.3511735115	-0.1749054193	C	3.2933863553	-2.2020111634	9.0764536823
H	-10.4482635247	-1.904825113	-1.8108476016	C	4.7317333213	-0.3262913572	5.6552403366
S	-4.8394095984	-1.3909516314	-1.4427562663	C	1.7368763852	2.1722818905	4.1737635241
C	-7.6257987754	-1.275743706	-1.4955971542	C	0.380515644	2.4603842222	4.6450293783
C	-4.048661078	-0.0049086283	-0.688627985	C	-1.7801868732	1.0517275865	7.9256573924
C	-11.0608678519	-0.0517374786	-0.8942800297	C	0.6130828276	-1.6345337821	10.0076480033
O	-7.673775551	-2.4961383644	-2.10630397	C	4.273026212	-1.8937681786	8.0457474818
O	-7.438001827	2.4719180776	0.4537474516	C	4.133266119	0.6388383656	4.7308139051
C	-7.8141444129	-2.425788762	-3.5198050355	C	-1.5538120695	1.8419804636	6.7138832588
H	-7.8329688445	-3.4569406207	-3.8780669057	C	3.5225538694	2.1266087722	11.8180381045
H	-8.7477623535	-1.9234282971	-3.8014769545	C	2.5402314608	2.595515286	12.8677248802
H	-6.9670359875	-1.8964276626	-3.9735153281	C	4.9270926858	2.2245638867	12.4312049707
C	-7.1978515462	3.5757124054	-0.4104376274	C	2.2245457241	3.9511813062	12.9789498321
H	-7.1917321987	4.4650706237	0.2227663663	C	2.0303555777	1.7022701622	13.8118953068
H	-6.2297086424	3.4812823018	-0.9172507777	H	5.0111750524	3.2604245239	12.7893729797
H	-7.9921181597	3.6669528744	-1.161796129	H	4.8886315379	1.6101005467	13.3420830886
S	-13.923434383	-3.1140743288	-2.770633565	C	6.1969285764	1.8760579787	11.663148385
C	-15.4588356027	-0.1911508729	-0.8950085947	C	1.4036593979	4.404527655	14.0072540885
C	-13.3006772932	0.836091947	-0.2977443973	H	2.6199642778	4.6552615928	12.2506588904
C	-14.7095249427	0.8020880143	-0.2903036724	C	1.2092702897	2.153539308	14.8412368681
H	-12.823929476	1.6640180716	0.2198838798	H	2.2729825222	0.6449592468	13.7359945234
H	-15.2206406005	1.6122302946	0.2227349092	H	6.1871373865	0.837355666	11.3237044481
C	-14.6890905475	-1.2106993715	-1.5545869447	H	6.3020893073	2.4948363248	10.7680848194
C	-13.2375484234	-1.1747746069	-1.5637557209	C	7.4148391048	2.089315434	12.552511481
C	-12.510682205	-0.1188349877	-0.9125262578	C	0.8921391969	3.5058505443	14.9399272377
N	-12.6981721961	-2.1994050797	-2.2241098073	H	1.1615110427	5.4614448614	14.0774666016
N	-15.1854892923	-2.2636312602	-2.2041076036	H	0.8147757001	1.4459718248	15.5653929124
C	-19.1522041695	-0.7523662799	-1.2250335373	H	7.4847551452	3.1291130987	12.8985394916
C	-19.3002715752	0.3601980331	-0.3542632577	H	7.3542678878	1.4815415111	13.4659039264
C	-21.6816660193	0.1980063817	-0.4594857031	C	8.7053058321	1.7409436176	11.8524044594
C	-21.5339614476	-0.9186900593	-1.3247893989	H	0.2478379329	3.8581257278	15.7407323959
C	-20.2952679002	-1.411231295	-1.7077639244	O	8.7994454044	1.2840777308	10.7378329381
C	-17.7815872395	-1.0416135905	-1.4923560294	O	9.7627056576	2.002188682	12.6388697194
H	-17.4511323264	-1.8362128039	-2.147620141	C	11.0295750773	1.6965140628	12.0620116055
C	-23.0521310346	0.5146979354	-0.2257768538	H	11.0970874416	0.632243114	11.8201466605

S	-23.0784168839	-1.5470531161	-1.8187076701	H	11.1868827347	2.2749952904	11.1475621637
H	-23.3813803823	1.3428938903	0.3870573919	H	11.7701897009	1.9646680147	12.8158301015

Table S21. The coordinate of 4/PC₇₁BM (338 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	17.7729904407	8.5385260378	0.8165491885	S	-29.178231736	0.9613201414	0.3031195834
C	20.2817052593	8.4880214058	0.5851818981	C	-26.9371391987	2.5979362678	0.0051243141
C	19.0066496017	7.8947345698	0.6165451593	C	-30.7128540875	1.8174902933	0.3945228809
C	16.5162885067	7.7329777446	0.7502737966	O	-26.1236034708	1.5006141285	-0.0301233882
C	15.3503184329	8.2658076842	1.3135575854	O	-29.4860880579	5.9703679163	0.0594324786
C	14.1555588235	7.5640089984	1.2811644855	C	-25.5792477858	1.1520659216	1.2368514079
C	14.0754465074	6.3048660021	0.6679215599	H	-24.9606231241	0.2674419065	1.0730783257
C	15.2374325321	5.7853136071	0.0763076803	H	-24.9595841224	1.963510469	1.6388221454
C	16.4340287043	6.4827758866	0.1227965079	H	-26.3724481253	0.9146964969	1.9566130804
H	18.9731546469	6.8256706421	0.462483566	C	-29.7579184689	6.4720330918	1.3623053047
H	15.4016530677	9.2446990615	1.7788978331	H	-30.4089816831	7.33827403	1.228810867
H	13.2734003523	7.9900425175	1.7526371626	H	-30.2687060724	5.7205849963	1.9774618427
H	15.1901913517	4.8385967317	-0.4539039989	H	-28.8348715311	6.7833390833	1.8668879412
H	17.3008690098	6.0619446881	-0.3770769722	C	-24.9045517148	5.6494610507	-0.4420265362
C	21.4814298081	7.6141056256	0.4014467384	C	-21.2918863258	7.111333986	-0.8992776688
C	21.4849135308	6.2493092705	0.7140340012	C	-22.1975677017	8.1421564282	-1.0593813359
C	22.6595843761	8.1959384973	-0.0829031547	C	-23.5399574165	7.7391310453	-0.9180599378
C	22.6310815291	5.4837454575	0.5288371903	C	-23.6887209258	6.3953145757	-0.6458810356
H	20.5992601853	5.7833323322	1.1354645744	S	-22.1366303444	5.6238109293	-0.5536938627
C	23.8013747145	7.4286301813	-0.2779812011	H	-21.8849691695	9.1549032559	-1.2757798686
H	22.6610304032	9.259975204	-0.2966157359	H	-24.382591355	8.4144847098	-1.0251165593
C	23.7903260277	6.0685666067	0.0246754907	S	-37.2711402685	-3.1281590875	1.2748839126
H	22.6203141262	4.4278999647	0.7857405463	C	-38.6785970439	0.3905521974	1.5109463495
H	24.7047450102	7.8937931986	-0.6634117222	C	-36.5073805643	1.5095512345	1.1838536651
H	24.684043882	5.4682050769	-0.1232565415	C	-37.8984216236	1.5292623513	1.3995234384
O	17.596807905	9.7680371797	1.0939191341	H	-36.0062827705	2.4709268092	1.1067809275
O	20.538742787	9.7315543475	0.6552036477	H	-38.3711760107	2.5042762325	1.4836903636
Ir	19.118662138	11.2978797687	1.0910808081	C	-37.9553608519	-0.8463358926	1.3931506995
C	20.5851755495	12.6287140833	1.2094048207	C	-36.5202054715	-0.8666046584	1.1732898607
C	21.048531126	13.467039548	0.1916746222	C	-35.7609749297	0.3492505297	1.0646568887
C	21.232254935	12.6727083649	2.4770412268	N	-36.0262483701	-2.1021612916	1.0911913068
C	22.1252869352	14.3063247541	0.4265933448	N	-38.485261432	-2.0674739262	1.4662340377
H	20.5856315878	13.4789800372	-0.7893743663	C	-34.3276215891	0.3607831583	0.8506476741
C	22.314920324	13.540171804	2.6526320712	C	-33.4619860026	-0.6940151602	0.6351282524
C	22.7832716287	14.3652382228	1.6486826409	C	-32.1227069188	-0.2957449188	0.4560925367
H	23.6233755127	15.0285141607	1.8136459921	C	-31.9361485252	1.0686662969	0.5318111109
C	20.6779382612	11.7918203244	3.494475457	S	-33.4461514711	1.8669386144	0.8410973912
C	21.1059129374	11.6499218537	4.8208084843	H	-33.8016563568	-1.7206607064	0.6059876153

C	20.4450196413	10.7776413522	5.6705354436	H	-31.311794316	-0.9905352631	0.2629960301
H	21.9501480472	12.2275056642	5.1694081445	C	-47.9150521072	4.192749898	2.7681657483
C	18.9762330622	10.2206871596	3.8790976351	C	-47.0036334906	5.2819494118	2.7580954014
C	19.356393473	10.0476919445	5.1983635141	C	-45.1510083869	3.801505051	2.4537638629
H	20.777504053	10.6698388487	6.6991237004	C	-46.064018165	2.7129257496	2.4595536853
H	18.1386897025	9.6912981029	3.4382924955	C	-47.4330806353	2.8862410294	2.6024709347
H	18.8107745025	9.3575666319	5.832503985	C	-49.2658291476	4.6341289427	2.9675103244
C	17.6164155082	12.5262048668	-1.0732264035	H	-50.1116953294	3.9595310564	3.0306414162
C	19.2224241036	11.0178635894	-1.8848194869	C	-43.8006960497	3.3600140201	2.3111309364
C	17.1936341451	12.7784011264	-2.3846580071	S	-45.2401689084	1.1890543153	2.2791941021
C	18.8450433377	11.2348952496	-3.1983320906	H	-42.9530972543	4.0366883214	2.3234335335
H	20.022272741	10.3390042831	-1.6102843417	S	-47.8276456853	6.7996949752	2.9922878635
C	17.8076894107	12.131511788	-3.4450678641	C	-45.634457848	5.1098949386	2.593469878
H	16.3903821901	13.4806547239	-2.556072442	O	-44.7843070252	6.1797110943	2.6056535219
H	19.3533297226	10.7117311626	-4.000851752	O	-48.2773409896	1.8108436007	2.6187239929
H	17.4788159019	12.3288270977	-4.461447353	C	-44.5119444027	6.7071851179	1.3135929871
C	17.1094846819	13.1298195761	0.1505100348	H	-43.835033698	7.5509916613	1.461816314
C	16.0861801542	14.0798944234	0.226019384	H	-44.0292404802	5.9576985784	0.6736796083
C	17.7423617157	12.7034591379	1.352808116	H	-45.4308157084	7.0575531557	0.8272578107
C	15.6640437984	14.6314308888	1.4201015898	C	-48.824365484	1.4965547676	1.3448126072
C	17.3265094302	13.264391299	2.5634401171	H	-49.4675064781	0.626448534	1.4916927392
C	16.3079699816	14.2034535689	2.5741895271	H	-49.4200704498	2.3304583893	0.9523865895
H	14.8696227933	15.3669683975	1.4486715105	H	-48.0347202458	1.248956088	0.6244190548
H	17.7824185947	12.9831703269	3.5068444	C	-43.6807020703	2.0016546495	2.2038789081
N	18.6275592496	11.6389454784	-0.8575063926	C	-40.1107581135	0.4426312961	1.7267975998
N	19.6153855438	11.0611951886	3.0542632354	C	-41.0065720009	-0.5877523941	1.9359423794
F	15.9179091903	14.7286004203	3.7428146986	C	-42.3333401267	-0.1515097277	2.1212724462
F	15.463314207	14.4984603365	-0.8921009651	C	-42.4795983177	1.2181175595	2.0567962638
F	22.9526373218	13.6003960288	3.8372775721	S	-40.9477981136	1.9739701964	1.7495272185
F	22.5606800994	15.1001211534	-0.560228289	H	-40.6973018512	-1.6241595813	1.9567255468
C	11.3120649592	3.769771375	0.5116413615	H	-43.1640051733	-0.8233457508	2.3114659542
C	10.4182872537	4.8697405428	0.6071493293	C	-49.3581388373	5.9810557898	3.0944043815
C	8.5268419898	3.4137935581	0.4717527997	H	-50.2552591431	6.564042265	3.2611225033
C	9.4217299593	2.3126997126	0.3910024836	C	-2.2063360513	2.848213309	9.897714282
C	10.7999409474	2.4665036148	0.4204835697	C	-1.217587781	2.247156424	10.8346695625
C	12.6757116913	4.1933334644	0.5259140417	C	0.0997388587	2.563699024	10.2125132468
H	13.5085215402	3.5016329051	0.4713161117	C	-0.101424063	3.5313318192	9.1689918396
C	7.1642706587	2.9950609171	0.408428084	C	-1.4852466324	-1.869382052	3.3897676475
S	8.5640442459	0.8053420379	0.2328321666	C	-2.171134006	-2.769406185	4.2894945303
H	6.3306486175	3.6880615247	0.4426870849	C	-1.1726178684	-3.5069216447	5.0319723671
S	11.279950556	6.3787725206	0.7048724895	C	0.1302892554	-3.0580013059	4.592616498
C	9.0386026094	4.7140488626	0.5979639505	C	-0.0636221372	-2.0482442768	3.5760307163
C	12.8267124707	5.5470598354	0.6309895198	C	-1.5179206723	3.707781392	8.9789777299
O	8.2073033508	5.7960088469	0.6710256244	C	-3.346898354	2.1891767104	9.4746969814

O	11.6326128298	1.3862152965	0.3248307903	C	-1.455959509	0.6882536176	11.1617108565
C	7.8007655165	6.1161985105	1.9958373462	C	1.1089717658	1.6288021636	10.0576670029
H	7.1510473025	6.9899673836	1.9155605098	C	0.7563838215	3.5995067791	8.0677823722
H	7.2451807876	5.2866771754	2.4511778812	C	-1.9978487899	-0.5922207855	3.1693037236
H	8.6643935557	6.3603252369	2.6267707743	C	-3.3400508177	-2.3558855476	4.9243665294
C	11.9982986021	0.8370405679	1.5844100807	C	-1.3864426722	-3.8000682571	6.3758930922
H	12.6493146921	-0.0135909871	1.3724833891	C	1.1626234111	-2.9210569444	5.5173849936
H	12.5405056547	1.5712645315	2.1936555912	C	0.783568044	-0.9409665798	3.533516791
H	11.1160202255	0.4919514212	2.1376022119	C	-2.02498234	3.947930512	7.6994845778
S	0.4698706363	-3.3885697919	0.0365219908	C	-3.5604671607	0.7788031084	9.7797836686
C	-0.9777395484	0.0930850882	-0.404749362	C	-0.3351430265	-0.2219690722	10.8131570247
C	1.199511756	1.2427482828	-0.3051910273	C	1.9782387826	1.6731544104	8.9117845739
C	-0.2016725011	1.2395997797	-0.4389388404	C	0.2251829829	3.8241001481	6.7452640962
H	1.6971604355	2.2079978247	-0.3479747436	C	-3.2023041502	-0.1674050081	3.8365710502
H	-0.6866092098	2.2027376927	-0.5747682638	C	-3.5518825771	-2.6547194294	6.3194043315
C	-0.2386123928	-1.1273611816	-0.2309248165	C	-0.3145517144	-3.6508605575	7.3309275365
C	1.2070289049	-1.1248342705	-0.0958529015	C	2.0302185412	-1.7695648876	5.4714974629
C	1.9606941843	0.0991354128	-0.1285910314	C	0.2458305297	0.3773636424	3.3070666496
N	1.7147301486	-2.3476344081	0.0579754011	C	-1.1161186901	0.5474812814	3.1302524147
N	-0.761708431	-2.352374795	-0.1721670149	C	-3.8606890105	-1.029880503	4.6960823019
C	7.0154870161	1.6399225784	0.2904573508	C	-2.597113961	-3.3650840246	7.0296641478
C	3.4027893112	0.1332190674	0.0095889579	C	0.9328794387	-3.2182236185	6.9101983633
C	4.2984166494	-0.9116818354	0.1303901436	C	1.8438555818	-0.8006089758	4.500182945
C	5.6393015961	-0.4939662699	0.2357945172	C	-1.1363326257	3.9949263556	6.5647058551
C	5.7969135932	0.8757444226	0.200968657	C	-3.854319535	2.4053140362	8.1445589773
S	4.2560651124	1.6555109397	0.0282941746	C	-2.6274054973	0.0659256575	10.4973392813
H	3.9790786674	-1.9451094893	0.1435619676	C	0.888340386	0.2194723166	10.3618286002
H	6.473337087	-1.1795164714	0.3451174574	C	1.8165460545	2.6476230401	7.9386721002
C	-10.3240380282	3.7720036645	-1.0496740706	C	-3.2161037222	3.2787200395	7.2759615445
C	-9.426315138	4.8723647949	-1.0976353834	C	-4.2058967764	0.1678210475	8.6426371507
C	-7.5396241517	3.4102301402	-0.9735193971	C	-0.873652453	-1.4318690319	10.2564498226
C	-8.4372388764	2.3092239193	-0.9343666967	C	2.3107356894	0.3259722705	8.52372913
C	-9.8147962186	2.4656104619	-0.9824244832	C	0.9782025198	3.0278930071	5.8056633413
C	-11.6848290141	4.1970298634	-1.0723949264	C	-3.0697984505	1.2290990812	4.1829568633
H	-12.5200939438	3.5069679794	-1.0217416383	C	-4.2181645659	-1.531416406	6.9347519604
C	-6.1797567421	2.9884486323	-0.8947881104	C	-0.8658986901	-3.1460245055	8.5643579899
S	-7.584232396	0.7970472798	-0.7999617307	C	2.3477794917	-1.3771916286	6.8247014887
H	-5.3453582931	3.6813714514	-0.8884063553	C	0.9875623398	1.3241522074	4.1089012443
S	-10.2797508663	6.3885508601	-1.1681350458	C	-1.7849549193	1.6726455719	3.7433802402
C	-8.0485300451	4.7148953818	-1.0729866804	C	-4.4078681137	-0.5291093666	5.9352710934
C	-11.8305062814	5.5566377283	-1.1395462121	C	-2.2720930847	-2.9699987821	8.3781664618
O	-7.2176484629	5.7992641424	-1.1036473144	C	1.6721941561	-2.2710520885	7.7100675531
O	-10.6499911559	1.3853631653	-0.9264933905	C	1.9706149399	0.5963861345	4.8463990724
C	-6.7668009532	6.1371549391	-2.4095691945	C	-1.7950059604	3.3769968277	5.4390223046

H	-6.1209821928	7.0100937216	-2.2956923665	C	-4.3937337187	1.1674450721	7.641219327
H	-6.195294662	5.3143014491	-2.8571605219	C	-2.2764428484	-1.2551230895	10.0664332259
H	-7.6089475959	6.3890458018	-3.0660238364	C	1.6359902352	-0.5654823715	9.4102128916
C	-11.0056539467	0.8726918209	-2.2045633319	C	1.9598659038	2.2986927958	6.5433281075
H	-11.6626639388	0.0199412683	-2.0221693371	C	-3.0784723745	2.9305699452	5.8798585984
H	-11.5384224493	1.6258615552	-2.7986872188	C	-3.9800091416	-1.1842665085	8.2871723017
H	-10.1192562319	0.5386062345	-2.7578839484	C	-0.1234313697	-2.2831494693	9.4048177888
C	-6.0340426825	1.6301725802	-0.8051549172	C	2.557677865	-0.0205380756	7.171884474
C	-2.4221270703	0.1237440325	-0.5183622628	C	0.3745806068	2.4815671171	4.6451353003
C	-3.3232211548	-0.9224833773	-0.5669752579	C	-1.0664852491	2.6625843898	4.4549810284
C	-4.6643151297	-0.5052818559	-0.6731288315	C	-4.3627394816	0.8481602735	6.2606513961
C	-4.8174666385	0.8651504025	-0.7043042249	C	-2.9706746184	-1.9263394725	9.0279536403
S	-3.2711172059	1.6462504262	-0.5955439467	C	1.1892545496	-1.8332631292	8.9674120216
H	-3.0081959025	-1.9564776249	-0.525495396	C	2.3686469917	1.0040852232	6.1428520232
H	-5.5021864997	-1.1927212039	-0.7282175693	C	-3.6740972512	1.7626248126	5.3469237304
S	-18.3683524879	10.6018786748	-1.4320233458	C	-1.5360553519	1.7614733122	12.2255805865
C	-19.8450018083	7.1334824564	-0.9779644752	C	-2.9252448423	2.0794305858	12.7308143318
C	-17.668584734	5.9781314844	-0.9492479626	C	-0.5809608843	1.8638178862	13.4238104317
C	-19.0749590134	5.985855816	-0.8897917434	C	-3.3759548556	3.4003194339	12.7720276457
H	-17.1766378235	5.0127735597	-0.8637533131	C	-3.727442381	1.0734991314	13.2731574226
H	-19.5692571135	5.0253343739	-0.7700040166	H	-0.7408700159	2.8722613018	13.8315674877
C	-19.0949778243	8.3479072805	-1.1483482423	H	-0.9934315386	1.1818192089	14.180970777
C	-17.6443361481	8.339906711	-1.2111324634	C	0.9197809655	1.617480468	13.3178780866
C	-16.8959534978	7.116760817	-1.106444573	C	-4.6117458598	3.7089458368	13.3333402873
N	-17.1264344233	9.5579265526	-1.3703621977	H	-2.7571136773	4.1914099109	12.3552951556
N	-19.6115949072	9.5716649722	-1.2615640453	C	-4.9634108507	1.379836757	13.8349029608
C	-15.4483436012	7.0772807345	-1.1584020054	H	-3.3837864184	0.0420833695	13.2490320254
C	-14.5436110944	8.1144276237	-1.2782464908	H	1.1334044807	0.6060202091	12.9628629564
C	-13.2000953068	7.6916347318	-1.2839637775	H	1.3880282915	2.3021899365	12.605974971
C	-13.0485445473	6.3253908321	-1.1697091437	C	1.5711598968	1.8067932827	14.681569584
S	-14.6000669422	5.5555998065	-1.0523897794	C	-5.4095444292	2.6986621451	13.8640485742
H	-14.8579482881	9.1464085679	-1.3583093667	H	-4.9522852695	4.7406069507	13.3525759901
H	-12.3590374071	8.3717726302	-1.3712686813	H	-5.5796315188	0.5857256052	14.2476245542
C	-29.1913724755	3.5775212721	0.1718910546	H	1.3999527646	2.8192989645	15.071274029
C	-28.310365764	2.4629103701	0.146972551	H	1.1387142853	1.1292697985	15.4303602604
C	-26.4174156171	3.8939701437	-0.1394672808	C	3.0605715194	1.5677106489	14.6453292664
C	-27.2981441442	5.0088301555	-0.1108509283	H	-6.3763334669	2.9381846655	14.2981990334
C	-28.6690776454	4.8750503086	0.0527677104	O	3.6984655769	1.251978806	13.6690464543
C	-30.5523804458	3.1743011421	0.3092781424	O	3.6053786019	1.751611783	15.8597050066
H	-31.3798307681	3.8755448683	0.3101357191	C	5.0140785308	1.5441733569	15.9222936312
C	-25.0624610235	4.2939439409	-0.3346051985	H	5.2665484524	0.5196243074	15.6356168847
S	-26.4352424374	6.5076913205	-0.3133565228	H	5.5361792402	2.2341845153	15.2537846131
H	-24.2440969968	3.5877527356	-0.4237876386	H	5.2947574549	1.7309203911	16.9591455681

Table S22. The coordinate of 5/PC₇₁BM (338 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	16.6719037434	8.3300225701	2.992036974	H	-26.111105432	7.6154491215	1.7434400236
C	19.0978228176	8.8286460005	2.5197402673	H	-26.3330162945	7.612942935	-0.0310117226
C	17.8863575384	8.1454855923	2.3081513564	H	-27.7129744594	7.9839086939	1.0440930549
C	15.4735560735	7.5461021883	2.5654699935	C	-31.1390236968	5.0387708778	-3.7140461669
C	14.394257159	7.4391312831	3.451206903	H	-31.8050216662	4.520479289	-4.4066164072
C	13.2529566773	6.7326117534	3.1057086234	H	-31.695884559	5.8237967329	-3.186968829
C	13.138940441	6.1169011384	1.8504041666	H	-30.3144101516	5.496004367	-4.274495782
C	14.2104042955	6.2469797147	0.9532323425	C	-26.0529064384	4.4100021572	-2.8618537945
C	15.3559762398	6.9420571842	1.3066179421	C	-22.4529101218	4.0900805351	-4.4383007757
H	17.8902628363	7.3991298639	1.5265197045	C	-23.3597909402	3.5500807154	-5.3135889875
H	14.4690858931	7.9246183084	4.418754105	C	-24.6953115445	3.6087856136	-4.8536246765
H	12.4420242079	6.6437454863	3.8244018131	C	-24.8474835246	4.1838553685	-3.616719103
H	14.1261296568	5.8272662191	-0.044929845	S	-23.2876468827	4.6793745429	-3.0274514111
H	16.1460739989	7.0505530185	0.570183271	S	-38.3816584807	8.6818573274	4.5690172827
C	20.2952033875	8.4426019629	1.711247989	C	-39.6464400958	5.525674325	2.9102361373
C	20.4364538599	7.1846033199	1.1130563982	C	-37.4270660904	4.7054843535	2.2484990094
C	21.330230578	9.3751259786	1.5685030168	C	-38.8350059974	4.5853456127	2.3058836639
C	21.5742606566	6.8751647402	0.3757306084	H	-36.8651437364	3.9086162584	1.768808481
H	19.6705139224	6.4268235234	1.24812307	H	-39.2933880738	3.7172800129	1.8399213443
C	22.4622439535	9.0694336034	0.8231017876	C	-38.978811737	6.6521328135	3.4916084656
H	21.2295987877	10.3387560369	2.0575730132	C	-37.5410831633	6.7845779735	3.4156178669
C	22.586967137	7.8188626339	0.2213171663	C	-36.7411516066	5.7777865091	2.7844426684
H	21.6730123242	5.8907982361	-0.0739186842	N	-37.0850149458	7.9040598745	3.9771569912
H	23.2522723744	9.8077036813	0.7143202014	N	-39.5664660599	7.6587665919	4.1381222368
H	23.4738371137	7.5771370478	-0.3584283307	C	-35.2956476802	5.8975924735	2.6858185177
O	16.4745648873	9.0911532176	3.9928645863	C	-34.3809113362	6.3328506545	3.6099183575
O	19.289293777	9.8007372999	3.317350598	C	-33.0430913548	6.2682461301	3.1567930924
Ir	17.8732106782	10.5405906984	4.7658450739	C	-32.8953700891	5.776871804	1.883869414
C	19.2491936084	11.753466809	5.5218257353	S	-34.4661128362	5.4067656982	1.2348007446
C	19.4616000835	13.0963622367	5.1984580339	C	-48.5792622288	0.9313214325	3.653277518
C	20.1158987857	11.1330734829	6.4660536045	C	-47.5633274168	-0.0561812675	3.7603554567
C	20.5093972015	13.7882949357	5.783774588	C	-45.8560451558	1.6029527948	3.5499608097
H	18.8233820973	13.6184691314	4.4932726995	C	-46.8711603831	2.5906751815	3.4470145702
C	21.157161686	11.8833911965	7.0212368322	C	-48.2228687222	2.2789891897	3.5062909307
C	21.3788440288	13.2082217908	6.6990237508	C	-49.890380622	0.3505077983	3.7078906908
H	22.1925365276	13.765951803	7.1459988806	H	-50.803140824	0.9282784648	3.6213933029
C	19.8125027004	9.7438645429	6.7776033066	C	-44.552660102	2.1726561998	3.4434798939
C	20.4859314417	8.9079736023	7.6777038337	S	-46.2010079942	4.18183876	3.2228756808
C	20.0451232003	7.6095895258	7.8771452768	H	-43.645677277	1.578050296	3.4702023558
H	21.3452464257	9.2883423095	8.2112970303	S	-48.2455185484	-1.6518160157	3.9222579264
C	18.3038329369	8.0090291256	6.3005484344	C	-46.210547009	0.2573636277	3.7225700763

C	18.9312136624	7.1453001805	7.1810425058	O	-45.2560443547	-0.7164239171	3.8116237237
H	20.5681244885	6.9629960157	8.5761100231	O	-49.1742148463	3.252954967	3.3849934625
H	17.4297538682	7.7233639641	5.7254205792	C	-44.8193244728	-0.9688639464	5.1413474672
H	18.5525245634	6.1375926012	7.3123503557	H	-44.072339661	-1.7624095217	5.07464957
C	15.9212870845	12.5457718726	3.981349284	H	-44.365160841	-0.0738057256	5.5851256375
C	17.4468917757	12.1069723955	2.251561495	H	-45.6501966291	-1.3024905345	5.7752152817
C	15.2444762167	13.4496916637	3.1525020292	C	-49.5915430598	3.8019679163	4.628458125
C	16.8165180216	12.9921721071	1.3948440878	H	-50.3378174198	4.563583487	4.3937204832
H	18.3286220706	11.5448776131	1.963703423	H	-50.0410394651	3.0329204204	5.2693944621
C	15.6921751574	13.6705839614	1.8599601425	H	-48.7511671142	4.2666256237	5.158963894
H	14.3766957083	13.9690637834	3.5332907071	C	-44.5665454135	3.5303921837	3.2739197322
H	17.2006884037	13.1401339768	0.3915442718	C	-41.0898639799	5.3692638267	2.9801894576
H	15.166195966	14.3720652439	1.2185812466	C	-42.0865962412	6.298665294	2.8288181692
C	15.6103446599	12.2126879835	5.3640014432	C	-43.3884100069	5.753925381	2.9193481489
C	14.5584840052	12.7481500164	6.1138650419	C	-43.4257622332	4.3988414893	3.1323417502
C	16.4808814465	11.2680771882	5.9780847451	S	-41.7969743166	3.7988245626	3.2433942562
C	14.3297303601	12.4056421838	7.4324923767	C	-49.855138913	-0.9970998335	3.8528592427
C	16.2613148742	10.9242914882	7.3147775772	H	-50.6992885591	-1.6727526777	3.9113056078
C	15.2029848878	11.490423651	8.0066022615	C	-0.0308613352	2.8495995879	9.2308002348
H	13.5077077582	12.8376312121	7.9898068885	C	1.267011982	2.5371907524	9.890251449
H	16.9019465364	10.2177218718	7.8320359936	C	2.2820029776	3.134524554	8.976475462
N	17.0132043982	11.8877168786	3.5003240783	C	1.6119222998	3.9869233853	8.0330237288
N	18.7309719143	9.2634459629	6.1022314317	C	0.2351493084	-1.8014864348	2.6395421811
F	15.0020886692	11.1475397465	9.2857321038	C	0.0201972997	-2.8044219553	3.6590168767
F	13.7131764505	13.6385050728	5.5605475551	C	1.313731157	-3.2541255423	4.1246848362
F	21.9988368466	11.3238912128	7.911473934	C	2.3274786294	-2.5243107253	3.3956445108
F	20.7034939352	15.0733552273	5.4605819364	C	1.6602766419	-1.6282417647	2.4783551667
C	10.5221911621	3.8543692989	0.3943120769	C	0.1913911509	3.813275086	8.1921259422
C	9.5989206901	4.5282073788	1.2386999557	C	-1.0461695037	1.9220066206	9.079148889
C	7.7876800355	3.228041499	0.3807159193	C	1.4952674482	0.9798342845	10.2323471711
C	8.7124375659	2.5413900263	-0.4505130455	C	3.4201649886	2.4626078314	8.5652411674
C	10.0705104923	2.8286198717	-0.4492647835	C	2.1411300355	4.2160197378	6.7600336481
C	11.8479572	4.3623376746	0.5493616155	C	-0.6087338959	-0.6930266346	2.5739023548
H	12.6960217725	3.9737031904	-0.0027438389	C	-1.0276992808	-2.6578387168	4.5640376666
C	6.4543231136	2.7656255477	0.1805205677	C	1.5028305759	-3.5392116399	5.4739025647
S	7.9218568944	1.3494778012	-1.4445271343	C	3.4864890065	-2.1107280401	4.0482787995
H	5.6013909966	3.1716921269	0.7139755206	C	2.1808999983	-0.3539816444	2.2588057314
S	10.3865959507	5.7571484792	2.1862491937	C	-0.648073978	3.8777606046	7.0770426517
C	8.2443962025	4.2269899363	1.2545400777	C	-0.8352237181	0.513828023	9.396626326
C	11.9427525157	5.3708819046	1.4658311262	C	2.6860366847	0.3505883191	9.6050878384
O	7.3825424951	4.9135706825	2.0611000584	C	3.9547733214	2.6696853674	7.2454352159
O	10.9330670959	2.1610529247	-1.2734727929	C	1.2729515115	4.2578428238	5.6089245213
C	7.0968947418	4.2583394722	3.2917511203	C	-1.6865849087	-0.5432528791	3.5196908394
H	6.4060831009	4.9076463999	3.8331591209	C	-0.8236519442	-2.9462329566	5.9625304019

H	6.6224374413	3.2834643505	3.12383131	C	2.7027365971	-3.1025713889	6.1469245173
H	8.0090493645	4.1185418332	3.8848218343	C	4.0149674992	-0.7877231681	3.8210230442
C	11.5117058579	1.0072345683	-0.6764454415	C	1.3036415973	0.787603606	2.1958633017
H	12.1637267986	0.5637478419	-1.4316785847	C	-0.0620812599	0.6220034874	2.3500154923
H	12.1032693492	1.2747438531	0.2083099273	C	-1.8912209448	-1.5041112761	4.4949932601
H	10.7412573218	0.2812965253	-0.3885080777	C	0.4142826509	-3.3811033636	6.4080532392
S	0.0482439884	-3.2692214939	-0.9283970887	C	3.6728027134	-2.4011695307	5.4487813762
C	-1.5904902246	0.1321417476	-1.1433030563	C	3.3746071903	0.0713850579	2.9442886555
C	0.4986768761	1.3784749219	-1.4772467331	C	-0.0925166283	4.0922425463	5.7636803818
C	-0.907904181	1.3159479233	-1.3407682595	C	-1.8920823404	1.9607864964	7.9145904189
H	0.9555389417	2.3519238065	-1.6335524425	C	0.3847838844	0.0717636098	9.8546901608
H	-1.4678571969	2.2466112593	-1.37374247	C	3.6239492851	1.0540027652	8.8831498038
C	-0.7931672051	-1.0567065387	-1.0973400973	C	3.3374705744	3.5411296998	6.3607562783
C	0.6451858334	-0.9911453742	-1.2239998844	C	-1.7088766502	2.9281205232	6.9372485982
C	1.309475727	0.2621799195	-1.421193297	C	-1.5657901174	-0.2752506298	8.4338965671
N	1.2367439772	-2.182149303	-1.1306358845	C	2.3372720478	-0.9727162737	9.1679214795
N	-1.2525836583	-2.2981327551	-0.9420359785	C	4.4999740385	1.4272515348	6.7606999403
C	6.3600726377	1.7684835711	-0.7520672403	C	1.949488935	3.6304826037	4.4991000676
C	2.7589723648	0.3556980232	-1.4890279177	C	-1.8136319245	0.8564517118	3.8557537104
C	3.6707853071	-0.43796244	-2.1356717897	C	-1.5745036326	-1.9913626317	6.7427641969
C	5.0102822609	-0.0180315193	-1.9618304845	C	2.3548518144	-2.6975662035	7.4869137706
C	5.1574167492	1.1003120729	-1.1797133619	C	4.5411061992	-0.2804575371	5.0665374061
S	3.5899636969	1.6409845482	-0.6613179927	C	1.9643979522	1.9147160801	2.8146553104
C	-11.2490241014	2.3704070359	-2.8918801069	C	-0.8151541537	1.5767296779	3.1313684923
C	-10.4430893324	3.2390697611	-3.6758102219	C	-2.2321908757	-1.1020902455	5.839569668
C	-8.4478261021	2.2439572631	-2.8168819692	C	0.9451366074	-2.8695824391	7.6475432961
C	-9.2532405179	1.3737495036	-2.033917503	C	4.3309745655	-1.2759579429	6.0689063135
C	-10.6401672153	1.4142602369	-2.0642165941	C	3.2410165559	1.4707532931	3.2784151394
C	-12.6382775683	2.6304561471	-3.0768925496	C	-0.830922036	3.2919838383	4.8164036738
H	-13.4151312919	2.0903484534	-2.5462688514	C	-2.2217025581	0.6120149364	7.5288643144
C	-7.0580496549	2.0138144897	-2.6009104966	C	0.9296314023	-1.1430070219	9.3240224533
S	-8.2845601062	0.3064604149	-1.0572568166	C	4.2902469068	0.434431126	7.7640614775
H	-6.2815678631	2.5964545336	-3.0849650689	C	3.2247422628	3.1847825624	4.9643431523
S	-11.4082566681	4.3469595145	-4.6085507743	C	-1.8270662501	2.5698100236	5.5419200562
C	-9.0567612262	3.1858244131	-3.6601759642	C	-1.1130322406	-1.546772292	8.0057160346
C	-12.8870586817	3.6437950424	-3.9633528011	C	3.0458690177	-1.6526382398	8.1441436325
O	-8.3092816908	4.0473285113	-4.4119014019	C	4.4950953763	1.0992404094	5.3820935756
O	-11.3898416255	0.577472585	-1.2870648744	C	1.2364776723	2.9116328095	3.5067153208
C	-7.9711985129	3.5411633559	-5.6979628365	C	-0.2083217617	2.7356425263	3.6713074369
H	-7.3854067227	4.3198355694	-6.1902791471	C	-2.444162768	0.2572377014	6.1746308273
H	-7.3712749428	2.6258839489	-5.6174679146	C	0.190896695	-1.9982298398	8.4671713276
H	-8.870212419	3.3317214544	-6.2905487807	C	4.0692736259	-0.9192565942	7.4144433951
C	-11.7264502801	-0.6490604604	-1.924739295	C	3.8260953047	2.0106156249	4.4499254896
H	-12.3097951166	-1.2216615035	-1.2010686406	C	-2.2332259986	1.274127765	5.1423660297

H	-12.328355771	-0.4735488924	-2.8253480397	C	1.4166048681	2.0429258388	11.3064180103
H	-10.8269988507	-1.2146962399	-2.197089682	C	0.1533407007	2.041751532	12.1372519986
C	-6.8070622577	1.0115562009	-1.7028247681	C	2.5773091552	2.4165077386	12.2403947167
C	-3.0382844625	0.0843641021	-1.0189560689	C	-0.5759817806	3.2197041764	12.3107038595
C	-3.8242598183	-0.6489173683	-0.1682109982	C	-0.2323717786	0.897395019	12.8379569088
C	-5.2082722295	-0.402217437	-0.3218639126	H	2.2796560471	3.3704555266	12.6986332848
C	-5.5170880158	0.5284163315	-1.2822922227	H	2.5383606571	1.6832025832	13.0585438304
S	-4.0461962824	1.0879108179	-2.0227412179	C	4.020892696	2.5382681508	11.7661948819
S	-19.7936323579	5.1099960391	-7.9999731411	C	-1.6785829791	3.2506099797	13.1595464155
C	-21.0059442132	4.1893484988	-4.5369570026	H	-0.2813112492	4.1174514182	11.772385986
C	-18.7702985099	4.1035619335	-3.5222023238	C	-1.3344968278	0.9261577015	13.6875164834
C	-20.1778711529	3.9835687978	-3.4508991324	H	0.3312801684	-0.0239999427	12.7120819349
H	-18.1964870889	3.9421209032	-2.6136405399	H	4.3849842851	1.5962024635	11.3484774214
H	-20.6199555076	3.7050063312	-2.4981058245	H	4.1182001617	3.2868068051	10.9755989237
C	-20.3579722846	4.5395043521	-5.7656010629	C	4.9176202097	2.9371735835	12.9309377268
C	-18.9182783435	4.64318951	-5.8430248869	C	-2.0615226824	2.1028481138	13.8487137771
C	-18.1012624793	4.4293335331	-4.6858043999	H	-2.2402650948	4.1728951405	13.2800522638
N	-18.4772587909	4.9450350512	-7.0640986118	H	-1.626568018	0.026360359	14.2220504701
N	-20.9674777916	4.7992114766	-6.9221990352	H	4.6030339645	3.8922065464	13.3723584105
C	-16.6516277706	4.5182906663	-4.7465900033	H	4.8620219769	2.2053287813	13.7484411792
C	-15.8508872833	5.4165057812	-5.4041774388	C	6.3646094828	3.065177709	12.52215581
C	-14.4690026798	5.199822152	-5.1990866912	H	-2.9244215709	2.1249797806	14.5085848573
C	-14.1738152252	4.1422878008	-4.3754843467	O	6.8051261689	2.8429478057	11.4191613456
S	-15.6574183505	3.3904745772	-3.8663604517	O	7.1220377565	3.4629441748	13.5575623652
C	-30.2541640968	5.0102562316	-0.6312888745	C	8.509788431	3.6075830503	13.2656189883
C	-29.326914215	5.4990990755	0.327804043	H	8.936652955	2.6556485841	12.9381122713
C	-27.4957095657	5.0429706166	-1.1383215915	H	8.6631535839	4.3505443805	12.4782232628
C	-28.4234269377	4.5580471631	-2.0989725299	H	8.9750164873	3.9349828048	14.1956543858
C	-29.7922333839	4.542678812	-1.8712345885	F	-44.4690122773	6.5183643479	2.7852222969
C	-31.5934641431	5.0689630294	-0.1478184302	F	-41.9061489713	7.5820248874	2.5587609426
H	-32.443408241	4.7180947356	-0.7232827019	F	-34.6615315919	6.7275196757	4.8419133481
C	-26.1523850991	4.9402812395	-1.6035429142	F	-32.030347121	6.6450498348	3.9328747297
S	-27.6232482392	3.9906493519	-3.5369969412	F	-25.6990397871	3.121783221	-5.5782625875
H	-25.296958418	5.2339841203	-1.0045693906	F	-23.0628128694	2.9630162849	-6.4622646552
S	-30.1224072968	6.013398715	1.7882581921	F	-16.2773178418	6.4425728565	-6.1235900318
C	-27.9599167191	5.5329939462	0.0922345312	F	-13.5541717303	5.9861387621	-5.7599330789
C	-31.6918016448	5.5839200273	1.1168993328	F	-6.1118910092	-1.0251034856	0.4299514459
O	-27.0908995996	5.9914348813	1.0412620442	F	-3.3791525954	-1.4748143381	0.7669159207
O	-30.6598587794	4.053519797	-2.8061698369	F	3.3753887287	-1.4784423091	-2.8998725423
C	-26.8035673299	7.3807457252	0.9327257928	F	6.0224292575	-0.6739365666	-2.524164666

Table S23. The coordinate of 6/PC₇₁BM (296 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	14.7719156545	-0.2692975145	0.9254780422	O	-20.390883121	3.2180194932	1.134954442
C	16.8447985584	-1.699538214	0.9273946901	O	-20.101087838	-2.2088102451	-0.1922898934
C	15.4555379652	-1.4943966688	0.8441066881	C	-20.4787636913	3.4817037624	2.5297662722
C	13.2845712844	-0.2531104211	0.777121583	H	-20.5133545156	4.5677770527	2.6352340236
C	12.587539893	0.8785506599	1.217985334	H	-21.3882308641	3.0429318195	2.9588673318
C	11.2070992309	0.9501627398	1.1229504057	H	-19.6022874556	3.0908983356	3.0613326581
C	10.4673014538	-0.1042584278	0.5675793288	C	-19.8778706944	-3.077524335	0.9113766219
C	11.1689852198	-1.2243746629	0.0952842508	H	-19.8613126011	-4.0909972156	0.505705949
C	12.5489061669	-1.2989412456	0.2038084792	H	-18.9188922299	-2.8629869309	1.3987870061
H	14.8497366141	-2.3764792745	0.6945320041	H	-20.6854884149	-2.9921709841	1.649042182
H	13.1540084335	1.7017653833	1.6407210298	S	-26.6315559595	3.9814683488	1.4766282355
H	10.6912386168	1.828401411	1.502985853	C	-28.1697575982	0.632527392	0.5421289989
H	10.6261583492	-2.0309414247	-0.3889560304	C	-25.9776154224	-0.4967714061	0.2241902243
H	13.0557388232	-2.169222826	-0.2014462859	C	-27.3840646422	-0.4620794261	0.2344676603
C	17.3764319061	-3.0955344026	0.8498162851	C	-27.3883625478	1.7996029072	0.8662491813
C	16.6027270274	-4.2246117616	1.1448193455	C	-25.9345328758	1.7858164641	0.8649387806
C	18.717476142	-3.2758110423	0.4885078187	C	-25.1955897842	0.5970160641	0.5316162628
C	17.1510664499	-5.4999671573	1.0622654934	N	-25.4020112147	2.9597465841	1.1957177678
H	15.5739535609	-4.1117613538	1.4732188568	N	-27.8870231673	2.9899704145	1.1954985249
C	19.2623404795	-4.5505493088	0.3962462384	C	-31.8417973057	1.3369901994	0.7612819988
H	19.3217319216	-2.396884547	0.2881906272	C	-32.0429159881	-0.0099967182	0.362190688
C	18.4799067521	-5.6679185782	0.6801646065	C	-34.4157497202	0.2507593794	0.4939240092
H	16.5396971707	-6.3652104367	1.3040984315	C	-34.213910385	1.6014241054	0.8872377375
H	20.3023840741	-4.6730978654	0.1059218479	C	-32.9500912203	2.1607734181	1.0149741092
H	18.9059805385	-6.6653803269	0.6123980608	C	-30.457560123	1.6616080477	0.8580185401
O	15.2873032918	0.8700261914	1.1605025548	H	-30.0922073593	2.629734097	1.1704656395
O	17.7373048169	-0.7991705291	1.0271453427	C	-35.810591267	-0.0826124258	0.4435358813
Ir	17.3903905395	1.3082869772	1.3366000659	S	-35.7302126904	2.4108885546	1.1796522276
C	19.3283817778	1.6130983707	1.6305077998	H	-36.1788406697	-1.0685817942	0.185265988
C	20.2735034078	2.0226136636	0.6858903873	S	-30.5348672527	-0.836037372	0.1175323567
C	19.7667811377	1.3337721864	2.9563208838	C	-33.3093488038	-0.5624298288	0.2159495796
C	21.6062812325	2.1336167742	1.0471128166	C	-29.6228424738	0.6200068869	0.5406421318
H	19.9914371976	2.2579063024	-0.3347722205	O	-33.4734798889	-1.8695336404	-0.1522361025
C	21.1258149184	1.4625147494	3.2599727171	O	-32.8012204708	3.4593107827	1.4119556463
C	22.0662560543	1.8576397876	2.3286532921	C	-33.5451496579	-2.059924819	-1.5588098286
H	23.1126593997	1.9503368396	2.5920929329	H	-33.6631171407	-3.1335993611	-1.7192645953
C	18.7223627848	0.9505141052	3.8947891078	H	-34.4054587828	-1.5286800074	-1.9858676326
C	18.871155201	0.64633248	5.2541085165	H	-32.62818145	-1.7166274263	-2.0537620669
C	17.7586802475	0.333068745	6.0180657221	C	-32.6019658492	4.3683733399	0.3373362176
H	19.857690251	0.6629474009	5.6947505733	H	-32.5092123461	5.3593947093	0.7861979532
C	16.4042697618	0.6281973594	4.0803422946	H	-31.6866366694	4.1318744963	-0.2192165639

C	16.4969168483	0.3265587935	5.4276732267	H	-33.4563141438	4.3573684133	-0.3510004976
H	17.8761191126	0.0985800593	7.0722916492	C	-36.6063242175	0.9636601278	0.7765225044
H	15.4576025724	0.6492073194	3.5518640303	H	-37.6880694405	0.9744749383	0.8250429551
H	15.6009434372	0.0932138193	5.992382756	F	-2.1828679836	-2.354389094	-0.3409857767
C	17.0306597849	3.0625125314	-0.9531914766	F	-14.9354864682	2.6607873743	0.8134721684
C	17.6176020913	0.8884178565	-1.6176339766	F	-27.9720411018	-1.6217191968	-0.0913397613
C	16.9462927858	3.4482670828	-2.2972914631	H	0.2598872345	-2.1508550267	-0.2756065186
C	17.5518293827	1.2198924943	-2.959502123	H	-12.5128750087	2.3507918887	0.6591777518
H	17.8852816432	-0.1047179214	-1.273917269	H	-25.5313091181	-1.4486616257	-0.0465389006
C	17.2052675265	2.5259871544	-3.2984498962	C	1.2674233129	2.8205813832	10.8843501621
H	16.6817661731	4.4675081797	-2.5402051982	C	2.5218185904	2.148598664	11.3220166927
H	17.7669473783	0.4702171867	-3.7130358768	C	3.5231487321	2.5656901773	10.2997455388
H	17.1399880898	2.8270688265	-4.3401811642	C	2.9684088347	3.6354285411	9.516579728
C	16.8236077346	3.898354949	0.2205196662	C	-0.5148890213	-1.1413186386	4.0834323099
C	16.4889369221	5.2560063062	0.204136336	C	-0.8367635125	-2.1520437747	5.0655346906
C	16.9997418169	3.2487560908	1.4753252493	C	0.3535854284	-2.938469754	5.3051197185
C	16.3274576751	6.0007981353	1.356290792	C	1.4113903137	-2.4089840632	4.4728223178
C	16.8478933098	3.998770244	2.6448369416	C	0.873376088	-1.3000047007	3.718032121
C	16.5170196432	5.3416553625	2.5642692081	C	1.5834954418	3.7928782855	9.8783591467
H	16.068949022	7.0516361776	1.3135432693	C	0.0416828508	2.1807259947	10.8371631664
H	16.9821877021	3.5555253326	3.6259080257	C	2.3972891813	0.5575047806	11.5392982556
N	17.3614356998	1.7765965283	-0.6476863999	C	4.3926380593	1.6812440065	9.6846610665
N	17.4793418672	0.923987397	3.3371073014	C	3.3641190985	3.8459539561	8.1929436497
F	16.3700866364	6.0456777526	3.6940252487	C	-1.0554804349	0.1378047813	4.2064263766
F	16.3085531229	5.8977011834	-0.9657712234	C	-1.6848685687	-1.841688713	6.1254879185
F	21.5728409116	1.1991589078	4.5028904478	C	0.6428032634	-3.381726224	6.5922723424
F	22.5003292225	2.5224028304	0.1290319258	C	2.713644407	-2.346997354	4.9639255367
C	6.7656940157	-0.6949622931	0.3639897609	C	1.6616923873	-0.1727647049	3.4928657202
C	6.6354022784	0.7199593985	0.3453014092	C	0.6463549274	4.1581243928	8.9086611953
C	4.2563195405	0.5536297881	0.2066700956	C	-0.065607884	0.7403635179	11.0408508218
C	4.3859465835	-0.8609593945	0.2328819842	C	3.2985748281	-0.278565505	10.7050227987
C	5.6148566466	-1.4978537785	0.3261388442	C	4.7819666921	1.8734080045	8.3128324993
C	8.1338899167	-1.0973136082	0.4378501778	C	2.3886086739	4.1990761478	7.1902733311
H	8.4426185634	-2.1357003127	0.4763381692	C	-1.9244196627	0.4548197579	5.3119124172
C	2.8942731583	0.963048171	0.113707138	C	-1.3748034378	-2.2960528535	7.458948308
S	2.8347101623	-1.6420088657	0.138759409	C	1.992347532	-3.3086745822	7.0993827786
H	2.5799518753	1.9968404117	0.0684327573	C	3.5209884689	-1.1733915258	4.7325385414
S	8.1878825543	1.502175003	0.4088139604	C	1.0980195049	1.1466305862	3.6243157944
C	5.4051416849	1.3580115624	0.2769812182	C	-0.2329436867	1.299524148	3.9736738687
C	9.0097109274	-0.0487734635	0.4785488755	C	-2.2338562173	-0.5136731243	6.2516448645
C	2.0107967005	-0.0835324907	0.0777530132	C	-0.2376383291	-3.0537587443	7.6879838802
O	5.3291909583	2.7196027676	0.2444960728	C	3.0054152077	-2.7993466529	6.3023123726
O	5.6995028782	-2.8615743272	0.3535853072	C	3.0045632829	-0.1098960968	4.0113298369
C	5.0670906993	3.3155020647	1.5107624075	C	1.0581366739	4.3518672622	7.5400876857

H	5.0615395157	4.3944551786	1.3449002137	C	-0.9143402017	2.5263888681	9.8173663062
H	4.0943360469	2.9998609237	1.9066384681	C	1.0548557896	-0.0203644728	11.2843933873
H	5.8502675727	3.0601597146	2.2352064594	C	4.2778680251	0.2421014988	9.8896882028
C	5.7160843099	-3.4009469227	1.6704792919	C	4.2894339363	2.9431712233	7.5808205467
H	5.7561304612	-4.486234874	1.5579596432	C	-0.6266689531	3.5062109674	8.8783716039
H	6.5967450588	-3.0566362045	2.2272543434	C	-1.0912149573	0.239250707	10.1577666283
H	4.8109566727	-3.1233571749	2.2249431506	C	2.5758974356	-1.435423933	10.2542675979
S	-0.9180338567	3.4231865404	0.4756542524	C	4.9290499182	0.5855794117	7.683263523
C	-2.4090921011	-0.0391754628	-0.0160009495	C	2.7332015459	3.5307547752	5.9579530081
C	-0.201803932	-1.1767711158	-0.1467106776	C	-1.6539152737	1.8083524654	5.7386403629
C	-1.6089073199	-1.1564261878	-0.1643296059	C	-1.7529626299	-1.2647713604	8.39543691
C	-1.6454435506	1.1710577873	0.1551036729	C	1.9383141197	-2.9557215301	8.4971264315
C	-0.1926575456	1.1750844153	0.1662242492	C	4.3169737897	-0.9217733186	5.9110277457
C	0.5626900914	-0.0406635926	0.0193640687	C	2.0957035732	2.021520362	4.197621586
N	0.3239633065	2.3892023152	0.3392738487	C	-0.6131668415	2.3318642801	4.9118069619
N	-2.1602014975	2.3886007344	0.3190090988	C	-2.2810864622	-0.1654994766	7.6523438637
C	-6.0852936381	0.6542877155	0.0958927921	C	0.5644612583	-2.798667774	8.8591654901
C	-6.2744545835	-0.728639427	-0.1635044942	C	3.9995247557	-1.924800984	6.8769932037
C	-8.6499950982	-0.4688441572	-0.079822604	C	3.2707004408	1.2443329	4.4393744605
C	-8.4575191797	0.9169336171	0.1710480528	C	0.024009457	3.8411402823	6.6722050918
C	-7.2011090147	1.4951518187	0.2513026375	C	-1.6183489624	1.3360909764	9.4120726297
C	-4.7061053794	0.9963876451	0.1715130851	C	1.2039451817	-1.2769604043	10.6111820481
H	-4.3484917543	1.9937093747	0.3848995873	C	4.6128786418	-0.4148851885	8.6503069911
C	-10.0318512987	-0.8187901398	-0.1043835367	C	3.9058862898	2.7518549216	6.2005434809
S	-9.9739518514	1.7456815893	0.3648562678	C	-1.0149501552	3.3149064442	7.4992446541
H	-10.3932670551	-1.8265152467	-0.2596130123	C	-1.0310097673	-1.0594501056	9.5963510879
S	-4.7590292871	-1.5654587212	-0.3063321975	C	2.9490647348	-2.1690362794	9.098589506
C	-7.5352212761	-1.3024388873	-0.2628577463	C	4.658707048	0.394549776	6.3056988161
C	-3.8617651741	-0.067627646	-0.0286104555	C	1.7381306759	3.0962738648	5.0463972799
C	-10.8681705301	0.2454056673	0.1110852154	C	0.3305916809	3.2574196555	5.4174648494
O	-7.6831627308	-2.6401449129	-0.4923826603	C	-2.0996871915	1.1688670422	8.0894661398
O	-7.0655014858	2.8279208464	0.5146492436	C	0.1681423734	-1.8496561656	9.8299140336
C	-7.8238027071	-2.9739763189	-1.8677431361	C	4.0165582643	-1.6390562616	8.264197644
H	-7.9249300529	-4.0601347073	-1.9113797538	C	4.121370264	1.5196927454	5.5377130458
H	-8.7172093236	-2.5050243489	-2.2987143434	C	-1.7811649446	2.1953993897	7.095024024
H	-6.9406532879	-2.6661335573	-2.4411115815	C	2.7304955426	1.5064488079	12.6699522741
C	-6.827665556	3.6230861274	-0.6403115412	C	1.628600227	1.7302846062	13.6810464648
H	-6.7451375946	4.6541091384	-0.2908986764	C	4.0608065892	1.507178092	13.437421886
H	-5.8960424049	3.3306542849	-1.139897167	C	1.2464066135	3.026334007	14.0324574799
H	-7.6596835666	3.5433718706	-1.3509912951	C	1.0656519474	0.6501405465	14.3636482729
S	-13.9771305477	-3.0748108727	-0.5408780346	H	4.0823726251	2.4674724721	13.9722833178
C	-15.2847796549	0.3943870789	0.3022032879	H	3.9418218017	0.7466509297	14.2221874654
C	-13.0224994123	1.4139249097	0.4566745789	C	5.4114189615	1.2973846917	12.7625286
C	-14.4270824141	1.4570427591	0.516389109	C	0.3092243941	3.2389420005	15.0394321745

C	-14.5850139375	-0.8284417476	-0.002043401	H	1.6820325596	3.8744906585	13.5096666648
C	-13.1344349815	-0.8953042847	-0.0720940921	C	0.1283440055	0.8604087986	15.3707540295
C	-12.3168641359	0.2645977492	0.166443056	H	1.3592549694	-0.3631302946	14.0996132282
N	-12.6825310998	-2.1108192459	-0.3705376517	H	5.456122799	0.331195783	12.2534643508
N	-15.1624116625	-2.0032355066	-0.2476948687	H	5.5997436086	2.0587800443	12.0012516509
C	-18.9939900594	-0.1140070742	0.3016129704	C	6.5247549203	1.3558051707	13.799996074
C	-19.1008468475	1.259422419	0.6443229077	C	-0.2535791145	2.1559808975	15.7097483572
C	-21.4874842889	1.1245448558	0.6470622171	H	0.0170089239	4.2530035421	15.2981461563
C	-21.3786901961	-0.2527902592	0.313380694	H	-0.3056371573	0.0098490498	15.8892627682
C	-20.1580564586	-0.8874979684	0.1476753248	H	6.5381825245	2.3219138858	14.3223023146
C	-17.6376909881	-0.5189381686	0.150757184	H	6.3811212208	0.6017274874	14.5858656334
H	-17.3403895449	-1.5187009064	-0.132829434	C	7.8880769642	1.1363996354	13.1915115604
C	-22.8462594558	1.5428834781	0.7511531391	H	-0.9881388323	2.3210381179	16.4931235812
S	-22.9449297008	-0.9902175604	0.1420412044	O	8.1101686687	0.9215349757	12.0234199727
H	-23.1461860419	2.5575131446	0.9757655777	O	8.8482078582	1.2085816701	14.1282819271
S	-17.5408927513	2.0104687304	0.7741629572	C	10.1743352711	1.0105698318	13.644924853
C	-20.3245161386	1.8893253	0.8277353478	H	10.2752858178	0.0219748417	13.188714044
C	-16.732714992	0.4890982414	0.3756937343	H	10.43091472	1.7687453245	12.8999728277
C	-23.746687329	0.5370160993	0.5172946085	H	10.8229117601	1.0971070092	14.5169864026

Table S24. The coordinate of 7/PC₇₁BM (338 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	17.9099729055	8.3265204919	0.2398048023	C	-30.8513447547	1.5831618556	-4.5356580326
C	20.4144084139	8.1815157353	-0.0026402319	O	-26.2416259402	1.3642499134	-4.4324615147
C	19.1182769032	7.6363437611	0.0406805241	O	-29.7244495057	5.6019108147	-3.3348977741
C	16.6251286559	7.5646078778	0.1933710856	C	-25.8224722117	0.6356131994	-3.2849840791
C	15.4840567016	8.1444745851	0.7612300471	H	-25.1599336428	-0.153143911	-3.6467513034
C	14.2665745979	7.4820326596	0.7539737882	H	-25.2770230838	1.2792246236	-2.5835506735
C	14.1385829014	6.2164473973	0.1627476629	H	-26.6792422319	0.1851302808	-2.7686074219
C	15.2750193322	5.6505360326	-0.435815712	C	-30.1770431826	5.6536652465	-1.9874047706
C	16.4941349135	6.3090973331	-0.4148543278	H	-30.8307545638	6.5251788867	-1.9157103128
H	19.0449011574	6.5678357338	-0.1030539815	H	-30.7406187772	4.7497862705	-1.723841216
H	15.5732975696	9.1278420387	1.2111571521	H	-29.3365723275	5.769228243	-1.2919494694
H	13.4046209566	7.9435059396	1.2294560852	C	-25.1086390269	5.4064949594	-3.3057751889
H	15.1901603074	4.6978902791	-0.9505129779	C	-21.5185049788	6.8921835303	-2.7718123088
H	17.3405774319	5.8528233591	-0.9185562981	C	-22.4245244215	7.9391762701	-2.7833126786
C	21.5791759607	7.2620441459	-0.1890399692	C	-23.7575227968	7.5300642336	-2.964775275
C	21.5341279014	5.900192507	0.132970647	C	-23.8997904246	6.1643708419	-3.098793922
C	22.7743545807	7.7961171683	-0.6865051711	S	-22.362267233	5.3760182279	-2.9842281279
C	22.6493536181	5.0910315056	-0.0558606287	H	-22.1164413043	8.9691170598	-2.6680969715
H	20.6351655766	5.4703858971	0.564566036	H	-24.593838559	8.2197882083	-3.013475497
C	23.8850508055	6.9853107165	-0.8852403959	S	-37.3226187502	-3.2556135109	-6.2685996939
H	22.8138221725	8.8578911242	-0.9076790144	C	-38.8652495543	-0.0444731405	-4.944191695

C	23.8255242894	5.6286553184	-0.5731440929	C	-36.6780057634	1.0816773726	-4.5857827157
H	22.6012386577	4.0380722476	0.2084753035	C	-38.0811099764	1.025964759	-4.5539233103
H	24.802055685	7.4137368413	-1.2809159297	H	-36.2343254275	2.0111668737	-4.2421564451
H	24.6949165696	4.9942639777	-0.7239460927	C	-38.0826027261	-1.1590805024	-5.4140527754
O	17.7791031988	9.5647207311	0.5028301986	C	-36.6298540504	-1.1246983673	-5.4549916967
O	20.7185504433	9.4147700974	0.0586851089	C	-35.8927944826	0.033839311	-5.025102054
Ir	19.3591466679	11.0345300277	0.4938013262	N	-36.0955318685	-2.2521780669	-5.9188595741
C	20.875245058	12.3089959394	0.6095393417	N	-38.5793136626	-2.3150209744	-5.8511248566
C	21.3677320478	13.1297956245	-0.4087417635	C	-34.4466706618	0.1008797853	-5.0460968028
C	21.5254794444	12.3283732195	1.8761342746	C	-33.5301448804	-0.8318172915	-5.4919195736
C	22.475943833	13.9276591911	-0.175612674	C	-32.1921906357	-0.4127359947	-5.3590289264
H	20.9031572008	13.1600931999	-1.3885979311	C	-32.0585830471	0.8461376219	-4.8105356271
C	22.6406107627	13.1540977854	2.0498797275	S	-33.6180902979	1.5133223758	-4.4442523282
C	23.1380996545	13.9609953341	1.0451884993	H	-33.8325622577	-1.7850524961	-5.9043851887
H	24.0030064247	14.5919667641	1.2086958516	H	-31.3426040229	-1.0122343013	-5.6691619646
C	20.9384582702	11.4708981352	2.8952421141	C	-48.3884002186	2.8332877185	-3.3127786456
C	21.3622517495	11.3141668254	4.221294939	C	-47.5453722111	3.8309987218	-2.7553157657
C	20.6679304408	10.4707795206	5.0735362711	C	-45.5881566445	2.6348659106	-3.4303034431
H	22.2294662726	11.8580602845	4.567736034	C	-46.4322742199	1.6397705853	-3.9922805673
C	19.1754883862	9.97031927	3.2849402307	C	-47.816532785	1.7246546423	-3.9534988462
C	19.550041958	9.7846522892	4.6040603646	C	-49.7758549362	3.1381885874	-3.1096454312
H	20.9971820986	10.3515113744	6.1018915399	H	-50.5833706514	2.4938689121	-3.4373539712
H	18.3163839736	9.4743429008	2.8467823878	C	-44.2069867423	2.3077786637	-3.5847451116
H	18.977649015	9.1184511011	5.2401931105	S	-45.5068075968	0.3442467448	-4.6982509767
C	17.9018516637	12.3109218581	-1.673056289	H	-43.4060729053	2.9232263807	-3.1894914736
C	19.4542542429	10.7457601065	-2.4815467943	S	-48.4754953012	5.100738009	-2.006804722
C	17.4881177397	12.575130476	-2.9850080861	C	-46.1588878302	3.7559682839	-2.8118345261
C	19.084710753	10.9733260975	-3.7955045811	O	-45.3796394062	4.7269998016	-2.248578511
H	20.2304484874	10.0404138222	-2.2056586757	O	-48.5936778118	0.7364914961	-4.4920006932
C	18.0791978479	11.9050152179	-4.0440724114	C	-44.9893822847	5.7463575065	-3.1598388635
H	16.7102490702	13.3050399818	-3.1579599293	H	-44.3824962153	6.4529369828	-2.5900945679
H	19.5747157853	10.4314921829	-4.5970054606	H	-44.39451059	5.3341346654	-3.9846361388
H	17.7575449063	12.1117929535	-5.0608829699	H	-45.8641427127	6.2652836661	-3.5712105583
C	17.4178376719	12.9357166237	-0.4506542439	C	-48.9932879947	0.9922166194	-5.8318466108
C	16.4286547713	13.9214350107	-0.3769659257	H	-49.5934978575	0.1349090069	-6.1435510447
C	18.0370468815	12.491523533	0.7522790208	H	-49.5975386115	1.9059095775	-5.898149856
C	16.0288468716	14.4923528965	0.8156996209	H	-48.1233578666	1.0882541666	-6.4934913419
C	17.644491974	13.0721790276	1.9613428804	C	-43.9972588761	1.1254234307	-4.2399266452
C	16.659915303	14.0468361803	1.9702706223	C	-40.3130113644	-0.0553817081	-4.8900270052
H	15.2608906537	15.2555383103	0.8428084	C	-41.1691107975	-1.0767831473	-5.2646826677
H	18.0925780978	12.7786921962	2.9047629473	C	-42.5289847085	-0.7696685745	-5.0803097598
N	18.8810030257	11.3888739345	-1.45551787	C	-42.7427775656	0.4900544367	-4.5601150412
N	19.8469812938	10.7825622046	2.4574628927	S	-41.2379314835	1.3083346668	-4.305634201
F	16.2913453059	14.5903808418	3.1374170569	H	-40.8073073316	-2.0174395605	-5.6561196192

F	15.8183366928	14.356924408	-1.4955106777	H	-43.3343918715	-1.4590890782	-5.31157903
F	23.2820677713	13.190037849	3.2334317655	C	-49.9586736175	4.3040230991	-2.4415911031
F	22.9390118226	14.7049718781	-1.1628923052	H	-50.9005117138	4.754633569	-2.1545615384
C	11.3015429864	3.7605172647	0.103089035	F	-38.6792941624	2.1366120878	-4.0960902887
C	10.440186035	4.8878549302	0.1772269383	F	-19.7796589808	4.6394854397	-2.7379696118
C	8.5078456693	3.4820988946	0.1009435752	F	-0.8207615785	2.6876965793	-0.8889510666
C	9.3707251066	2.3544577138	0.0415136728	C	-2.4151148247	3.2374274509	9.6013855601
C	10.7527821314	2.470077575	0.0529386342	C	-1.4270819863	2.6419305617	10.5426644686
C	12.6766947551	4.1447637853	0.0912112666	C	-0.109220332	2.9566647158	9.9206905863
H	13.4888611883	3.4282481187	0.0479194293	C	-0.309878714	3.919156641	8.8723498959
C	7.1335864323	3.1001141331	0.063589088	C	-1.6798947033	-1.5105372165	3.117250946
S	8.4707917557	0.867945895	-0.0671406127	C	-2.3661732738	-2.4071044107	4.0202077665
H	6.3200438639	3.8169598005	0.089783625	C	-1.3679649706	-3.14002951	4.7676115416
S	11.3460756622	6.3734831069	0.2235049214	C	-0.0648739109	-2.6918263073	4.3280571812
C	9.0564453572	4.7707748304	0.1859692234	C	-0.2584044196	-1.6870855221	3.3064873617
C	12.8673764738	5.4958425986	0.1572500191	C	-1.7262575275	4.0932757074	8.6794761804
O	8.2532521357	5.8746560809	0.2359678489	C	-3.5543307576	2.5751482972	9.1798693747
O	11.5533667184	1.3644457361	-0.0224589037	C	-1.6641661503	1.0842814185	10.8766122313
C	7.9027618334	6.2689290998	1.5569852393	C	0.9012416789	2.0221378301	9.7717977569
H	7.2708143241	7.1534883762	1.4563216572	C	0.5493882106	3.9829964485	7.7720241954
H	7.3450959933	5.4761542612	2.0713930352	C	-2.1936026276	-0.2350506652	2.8897668452
H	8.7938222161	6.5221800013	2.1445717804	C	-3.5362661754	-1.9915831545	4.6514411211
C	11.9234446606	0.842050272	1.2473505019	C	-1.5833691767	-3.4268867675	6.1126014627
H	12.5474407403	-0.0321723903	1.0508515529	C	0.9660166742	-2.5493203025	5.2535759061
H	12.4950330274	1.5781700085	1.826649019	C	0.5879779202	-0.5791713933	3.2596005672
H	11.0407157654	0.5378799649	1.8233568002	C	-2.2317558133	4.3267966857	7.39813637
S	0.2892655563	-3.1331669455	-0.1764551298	C	-3.7667960664	1.1660004464	9.4913518049
C	-1.1009082659	0.3672463212	-0.6790489545	C	-0.5419787992	0.1735193124	10.5341213618
C	1.1236283175	1.4719784889	-0.5716177875	C	1.7720036197	2.0619446008	8.6269596202
C	-0.2740150345	1.4753863852	-0.7116017694	C	0.0198743245	4.2008179665	6.4477224704
H	1.6063560432	2.4431461978	-0.6234488791	C	-3.3994427246	0.1918348793	3.5531529507
C	-0.3727702714	-0.8595215515	-0.4809734917	C	-3.749848769	-2.2839833133	6.0475527937
C	1.0729137814	-0.8881569567	-0.3336321786	C	-0.5129327748	-3.2719100127	7.0684220192
C	1.8571359799	0.3176276719	-0.3784533494	C	1.832507179	-1.3971421339	5.2034184513
N	1.5536360497	-2.1168717986	-0.1593322444	C	0.0490631119	0.7376334629	3.0261414111
N	-0.917825071	-2.0729142089	-0.4107678431	C	-1.3130383055	0.9055581614	2.8466277428
C	6.9469216678	1.7468582579	-0.0157951534	C	-4.0579381068	-0.6671651567	4.4160065604
C	3.2980072146	0.323629089	-0.2377374339	C	-2.795418309	-2.9900580693	6.7625491198
C	4.1659020375	-0.7380253261	-0.0686339601	C	0.7347185768	-2.8401645444	6.6474516588
C	5.5160418953	-0.3500030621	0.0227129152	C	1.6466898522	-0.4330056651	4.2271452625
C	5.7078878313	1.012912848	-0.0725678075	C	-1.3415514106	4.3692493571	6.2644055815
S	4.1886345946	1.823088394	-0.2867477372	C	-4.060073889	2.7843834133	7.8479791313
H	3.820200849	-1.7614003279	-0.0115288752	C	-2.8339643949	0.4575738204	10.2135694037
H	6.3323967075	-1.0501497224	0.1664939723	C	0.6817425961	0.6140583878	10.0825206113

C	-10.4855282687	3.901666198	-1.7223631762	C	1.6107282256	3.0316510553	7.6490157974
C	-9.6298607281	5.0256452617	-1.5700337012	C	-3.4215607425	3.6542895727	6.9761345589
C	-7.7112402894	3.6115518824	-1.3880777158	C	-4.4099672245	0.5489357604	8.3562293746
C	-8.5668783757	2.4876916789	-1.5469481175	C	-1.0784138026	-1.039625921	9.9824689952
C	-9.937154615	2.60950989	-1.7245957383	C	2.1065518133	0.7132761625	8.2458864993
C	-11.8515511065	4.2890102244	-1.8483043953	C	0.7749552086	3.4007866525	5.5130439592
H	-12.6611788314	3.573756106	-1.9458876849	C	-3.2687916546	1.5901296001	3.8930317269
C	-6.3523566639	3.2205055081	-1.2007678929	C	-4.4181122161	-1.1584131674	6.6565029461
S	-7.6759033805	0.9938538283	-1.4734579734	C	-1.0665371686	-2.7618621595	8.2986437164
H	-5.5511043893	3.9290753284	-1.0211831453	C	2.1478195734	-0.9979996987	6.5551255326
S	-10.5271962928	6.5178174155	-1.5899849924	C	0.7886802461	1.6891057656	3.8245141348
C	-8.2568102309	4.9051507442	-1.4151361399	C	-1.983933706	2.0330642175	3.4531522718
C	-12.0402228238	5.644219995	-1.8011721844	C	-4.6074659864	-0.1611002242	5.6519574461
O	-7.4730543263	6.0125579261	-1.25445207	C	-2.472651578	-2.5881490616	8.1095826094
O	-10.7325006244	1.5065968636	-1.8593418044	C	1.4718900345	-1.8883408698	7.4437903406
C	-6.8683547375	6.4659629218	-2.4594100394	C	1.7713935527	0.9657865761	4.566838737
H	-6.2803831954	7.3472519877	-2.1956452077	C	-1.9979582734	3.7452649355	5.1407435457
H	-6.2087900794	5.6998445405	-2.8856512013	C	-4.5974423075	1.5435569957	7.3497954671
H	-7.6272149095	6.7413281861	-3.2023353037	C	-2.4810702572	-0.8651611595	9.7895036247
C	-10.9323789925	1.1087271015	-3.2102462561	C	1.4314903618	-0.1746547253	9.1356587102
H	-11.5698276594	0.2228741285	-3.1790095936	C	1.7563038431	2.6760973162	6.2556067814
H	-11.4305422732	1.8992699208	-3.7855877924	C	-3.2815328156	3.2995722578	5.5819078311
H	-9.9805195022	0.8566526387	-3.6938539496	C	-4.1822311106	-0.8046106675	8.0075595494
C	-6.1670838291	1.8642284879	-1.2241735292	C	-0.3261275485	-1.8942272902	9.1360032783
C	-2.5426529744	0.4227196343	-0.8111539132	C	2.3557779802	0.3605467757	6.8960908067
C	-3.4373209768	-0.6339159939	-0.7853828209	C	0.1735120412	2.8483596989	4.3543312211
C	-4.7792215601	-0.2401396713	-0.9279479897	C	-1.2674116299	3.0269797787	4.1611227894
C	-4.9412024291	1.1233994491	-1.0631847202	C	-4.5641743603	1.2177481038	5.9708112146
S	-3.4074384529	1.927033758	-1.0218898199	C	-3.1731920115	-1.54208622	8.7533062624
H	-3.1156025149	-1.6584207302	-0.6604930961	C	0.9867101853	-1.4450526612	8.6983097075
H	-5.6106582819	-0.9374099707	-0.9191865501	C	2.1671269646	1.3800448371	5.8619261993
S	-18.7214759511	10.4907443752	-2.211817501	C	-3.8752448383	2.1285287878	5.0536590755
C	-20.0805459532	6.9636910547	-2.6083865878	C	-1.7469592923	2.1623220996	11.9353989
C	-17.8493277429	5.8807824143	-2.4355676521	C	-3.1373765651	2.480068678	12.437354524
C	-19.2448545223	5.8617397353	-2.5931569961	C	-0.7937386822	2.2696555721	13.1346800717
H	-17.3594581808	4.9118939478	-2.4461428015	C	-3.5908322153	3.8002334616	12.4715754185
C	-19.3638585866	8.2021053963	-2.4419030868	C	-3.9380532796	1.4751572658	12.9837840187
C	-17.9201114039	8.2466029892	-2.2779308165	H	-0.9642843569	3.2747860191	13.5461737573
C	-17.1262329017	7.0463834709	-2.2729918538	H	-1.1996149608	1.5805342768	13.8889870277
N	-17.4501781712	9.4842579752	-2.1399750917	C	0.7097726567	2.0408288916	13.0285801728
N	-19.9186574619	9.4127494107	-2.4197709366	C	-4.827893	4.1090123457	13.0299656152
C	-15.6879193283	7.0531536735	-2.1103534637	H	-2.9731234758	4.590593117	12.0517843225
C	-14.8295232293	8.1193610882	-1.9224260554	C	-5.1752550233	1.7816845935	13.542724343
C	-13.4797520701	7.7384947817	-1.7975715959	H	-3.5922545406	0.4443402412	12.9651563852

C	-13.2779367511	6.3763344392	-1.8872189638	H	0.935826333	1.0329789457	12.6711499424
S	-14.7885935029	5.5582719573	-2.1337597276	H	1.1698865829	2.7330107791	12.3185528487
H	-15.1813210676	9.1413481517	-1.8768000209	C	1.3585070973	2.2346979847	14.3929101541
H	-12.670507726	8.4441236903	-1.6408286905	C	-5.6241579477	3.099693942	13.5648298389
C	-29.3711377583	3.300862276	-3.9714931141	H	-5.1706051945	5.1400361706	13.0437575329
C	-28.4594852607	2.2449607516	-4.2418467404	H	-5.7902320786	0.9883631473	13.9587874116
C	-26.5914619044	3.6664248729	-3.7911234549	H	1.1744171944	3.2438889794	14.7852950686
C	-27.5035087696	4.7216568583	-3.5180319908	H	0.9345521267	1.5497137622	15.1397655315
C	-28.8792101891	4.5591982732	-3.5903994944	C	2.8508078966	2.0143932807	14.3561835621
C	-30.7248974197	2.8913215979	-4.1528123826	H	-6.5918934316	3.3393542035	13.9967720324
H	-31.5673315888	3.5638599471	-4.0322163531	O	3.4923167826	1.7074047593	13.3794525313
C	-25.2357469362	4.0920250927	-3.6661653421	O	3.3935039974	2.2041809251	15.5705254357
S	-26.6694643596	6.1931761525	-3.1049851268	C	4.8047131469	2.0143817152	15.6328128254
H	-24.3900608309	3.4461681646	-3.8759827891	H	5.0699011347	0.9930364568	15.3461788768
S	-29.2918365688	0.7852534021	-4.6989933477	H	5.3179643026	2.7108331082	14.964137124
C	-27.0843814254	2.4012195282	-4.1478407519	H	5.0832497052	2.2046823373	16.6695891088

Table S25. The coordinate of 8/PC₇₁BM (338 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	16.9277976335	7.5398221138	2.5423125952	H	-28.1913802811	2.916057951	1.2170319955
C	19.432773773	7.7872628589	2.4243873505	C	-30.2289820414	5.2253180743	-4.5735110397
C	18.2220897192	7.1040283229	2.2093058805	H	-30.6797153395	5.5181543231	-5.5237313642
C	15.7587011877	6.6882281383	2.1670679836	H	-30.9748322657	5.3060332832	-3.7725899409
C	14.5382184278	6.9030081715	2.8187695155	H	-29.3863015043	5.8907994279	-4.3495497698
C	13.4197026662	6.1450728051	2.5096018405	C	-25.3535955646	3.8578667384	-3.4540256441
C	13.4734774171	5.1512043302	1.521062047	C	-21.5145843674	4.6615255752	-3.8354825472
C	14.6894077259	4.9570891568	0.8473727422	C	-22.1742670644	5.1521445571	-4.9341953525
C	15.8101460531	5.705961848	1.169084862	C	-23.5684073994	4.9289384112	-4.9063589181
H	18.297083984	6.1393825079	1.7279034517	C	-24.0118664698	4.2557702223	-3.7956740868
H	14.4856125855	7.6795792895	3.5748024437	S	-22.6580458634	3.8948065262	-2.7677112237
H	12.4933560407	6.3147422132	3.0528351248	S	-38.6324531696	-2.598145176	-0.7327329509
H	14.7438736666	4.2330777137	0.0396757489	C	-39.7622605071	0.5784422883	-2.4497388919
H	16.7214703791	5.5490920199	0.6005014693	C	-37.5714732917	1.7146822385	-2.2678930047
C	20.7156168347	7.1256664958	2.0331290371	C	-38.9276387313	1.6568958024	-2.6513615517
C	20.8502786474	5.7374016634	1.9109809944	H	-37.039261311	2.6374515804	-2.4770183391
C	21.8365293327	7.9330300852	1.8031115084	C	-39.1439929978	-0.5254673737	-1.7755242077
C	22.0695177311	5.1738149119	1.5504645865	C	-37.7510186185	-0.4940046684	-1.3855428797
H	20.0093554586	5.0859837972	2.1293902624	C	-36.9433145289	0.6638361674	-1.633596418
C	23.0515719026	7.3704642857	1.4321239821	N	-37.3409178173	-1.6178349632	-0.8009445278
H	21.7350615673	9.006481067	1.926891954	N	-39.7540586408	-1.6616181503	-1.4432612815
C	23.1716885271	5.9883628516	1.3018390579	C	-35.5381890579	0.7196728711	-1.2700086703
H	22.1604345531	4.0939186311	1.4700015344	C	-34.8961796468	0.2603924804	-0.1481338713
H	23.9094127432	8.0117507651	1.2481356832	C	-33.510871878	0.5426113457	-0.134013633

H	24.1226882132	5.5467250469	1.0161870412	C	-33.0572445991	1.2279464601	-1.2334354602
O	16.6255184877	8.5980120541	3.1813480715	S	-34.3890029511	1.5073586265	-2.316197437
O	19.5648121947	8.962579751	2.8914616748	C	-49.2857630871	3.5049342422	-4.0214391537
Ir	17.9885619779	10.1817628535	3.7220867538	C	-48.565833299	4.6195000264	-3.5133921035
C	19.3124007909	11.5387041923	4.3066604843	C	-46.5494957163	3.3398703178	-3.4162639822
C	19.6971184214	12.6925673214	3.6186260528	C	-47.268043448	2.2269301238	-3.9279548446
C	19.939182132	11.2440476433	5.5505666171	C	-48.6185191886	2.2922973231	-4.2431566357
C	20.6820187942	13.5122028961	4.1451282848	C	-50.6702476938	3.8192042393	-4.2309870046
H	19.2426906305	12.9682698738	2.6729408198	H	-51.3972126217	3.1011395661	-4.5920781071
C	20.9281866618	12.1090919384	6.0295386936	C	-45.1829413326	3.0159990122	-3.1660965155
C	21.3203656518	13.2460834654	5.3499807462	S	-46.2522228709	0.8222413142	-4.0866990982
H	22.088312422	13.8992940268	5.7456089645	H	-44.4746306406	3.7269068747	-2.7541140294
C	19.4629791169	10.0442104027	6.2231228993	S	-49.6043067668	6.0047689882	-3.3108743989
C	19.888989354	9.5367933064	7.4572343503	C	-47.2095437187	4.5609744143	-3.2180628843
C	19.3079042426	8.3882343077	7.9698807804	O	-46.5468529102	5.6457700488	-2.7165320327
H	20.669095485	10.0513933749	7.9998050971	O	-49.2811492892	1.1950328463	-4.718198321
C	17.9182412169	8.2860377689	6.0370203772	C	-45.9699648463	6.4756486117	-3.7168400605
C	18.30016346	7.746793947	7.2529087436	H	-45.4856746176	7.3007761536	-3.1907185492
H	19.6389729363	7.9964200128	8.9275078564	H	-45.2231455882	5.9262325396	-4.3040149712
H	17.1402067349	7.8475736353	5.4217848019	H	-46.7368566852	6.8741141872	-4.3925489787
H	17.8178052549	6.8480843436	7.6213593854	C	-49.319060361	1.1208682628	-6.137500624
C	16.3955918902	11.8727644215	1.9757970894	H	-49.8630050294	0.2067274424	-6.383672578
C	18.1576256883	10.8493095273	0.8096175828	H	-49.8421824188	1.985551715	-6.5652654833
C	15.9625343164	12.4760303352	0.7881037101	H	-48.3075411444	1.06761202	-6.5589757306
C	17.7735531386	11.4247216882	-0.3888709711	C	-44.8673945298	1.7211683051	-3.4759249222
H	19.0213373698	10.1991707662	0.8951209992	C	-41.1528634942	0.5509507428	-2.8690914502
C	16.6512189837	12.2500459453	-0.3927600098	C	-41.8543279738	-0.4928604052	-3.4184226544
H	15.0926125851	13.1168061445	0.8067098311	C	-43.2113451497	-0.1944204777	-3.673241182
H	18.3420799225	11.2264028316	-1.2908323352	C	-43.5831687058	1.0824090626	-3.3354021648
H	16.3142561019	12.7191395602	-1.3128214916	S	-42.2091148664	1.925061607	-2.6869136434
C	15.8162777749	12.0200281291	3.3031314885	C	-50.9669525538	5.1007345565	-3.9025602986
C	14.7015457456	12.801538297	3.6227254177	H	-51.933862559	5.5850353236	-3.9579256814
C	16.47622387	11.3057360319	4.3431921314	F	-39.4093850668	2.7538173076	-3.2480011609
C	14.2142722168	12.9186382246	4.9100349939	F	-19.9832765324	2.5703784401	-2.6845841722
C	15.9949071931	11.4281240136	5.6495018351	F	-0.656744566	0.8354591302	-3.1349026753
C	14.8869663436	12.2197490066	5.9043933604	C	-0.8907831473	5.4313567813	6.6826744349
H	13.349502375	13.5328488076	5.1288158742	C	0.1581875984	5.1913774695	7.7118985095
H	16.4686479655	10.9151663707	6.4797554102	C	1.4340907133	5.2889167076	6.9474537219
N	17.4904376884	11.0620444502	1.9519143109	C	1.1570547879	5.8456189805	5.6515798178
N	18.4811410124	9.3944736456	5.5371840804	C	-0.363425587	-1.2034288029	2.1173985255
F	14.4347508384	12.3232794769	7.1608753719	C	-0.9807002911	-1.7519789588	3.3045436239
F	14.0505853427	13.4832710872	2.6610058913	C	0.0720387653	-2.1862168436	4.1965729133
F	21.5457533208	11.8548708395	7.1991124237	C	1.3394509237	-1.9009784893	3.5612436537
F	21.0437728375	14.6120594951	3.4722026308	C	1.0695325427	-1.2953657432	2.2766628298

C	10.9755476011	2.5776013985	0.4145718765	C	-0.2711220537	5.9353770191	5.4912761701
C	9.976344561	3.5006474795	0.8264043974	C	-2.0324047245	4.6583618625	6.569585098
C	8.243557899	2.0149069641	0.1216302122	C	-0.02371437	3.8322297454	8.5589890145
C	9.2413243265	1.0852294625	-0.2757764388	C	2.4591419666	4.3658995045	7.0626800027
C	10.5976486081	1.3400571042	-0.1270182033	C	1.9583565496	5.544850334	4.5466526982
C	12.2906207318	3.0904283929	0.6315656214	C	-0.9213351088	-0.0808300007	1.5060232536
H	13.1876313907	2.532058815	0.3897356559	C	-2.1273343144	-1.1583083298	3.8260213564
C	6.9314112631	1.5283230915	-0.1488393151	C	-0.0679415548	-2.0097502557	5.5700119774
S	8.5425565486	-0.3545153654	-0.9622690217	C	2.4120440761	-1.4516593363	4.3272783522
H	6.0332338472	2.0934734096	0.0767883166	C	1.8837154636	-0.2606764116	1.8179959451
S	10.6840914915	4.960238203	1.4570480587	C	-0.846396338	5.7246609855	4.2356751213
C	8.6195349731	3.2373190274	0.6998112212	C	-2.1936527654	3.4325451344	7.3434253752
C	12.3058905874	4.3400138352	1.1831956198	C	1.1024907458	2.8674295653	8.4755029169
O	7.6831957119	4.1538774847	1.0844708709	C	3.2699092075	4.0274923779	5.923005776
O	11.5344458652	0.43188088	-0.5343028271	C	1.3573145334	5.3044493147	3.2574820128
C	7.2053559929	3.9660961574	2.4118724489	C	-2.1029615782	0.534525878	2.0567671209
H	6.4691817097	4.7526305758	2.5887718064	C	-2.2633818079	-0.969472805	5.2496952112
H	6.7243826101	2.9865919314	2.5260321831	C	1.0451376616	-1.5375610231	6.3587892547
H	8.0204589397	4.0558798292	3.1404251403	C	3.2463433288	-0.3759165728	3.8484387873
C	11.9295575084	-0.4762760117	0.4865431855	C	1.3004824797	0.8979880851	1.1900691513
H	12.6665634137	-1.1440704237	0.0360189404	C	-0.0729754039	0.9864383288	1.0371373855
H	12.3833919367	0.0541457701	1.3332227219	C	-2.6936706885	0.0079052996	3.1926539415
H	11.0762494818	-1.0646815675	0.8457951429	C	-1.2565117344	-1.3893326037	6.104078796
S	0.3291541692	-4.3500111002	-0.3663823572	C	2.258781009	-1.2622929545	5.7490143604
C	-0.9431675934	-1.2882691923	-2.1875305191	C	2.9862136467	0.2065124188	2.6194764319
C	1.2818197121	-0.2270457388	-2.4048218847	C	-0.0155406556	5.3924328405	3.1050253196
C	-0.1199417921	-0.2477560248	-2.5614583843	C	-2.6098400364	4.4079029393	5.274389414
H	1.8070162589	0.6471864475	-2.7767247551	C	-1.2086385427	3.0124255475	8.20741851
C	-0.2628713166	-2.3791229485	-1.5528798177	C	2.2906811871	3.1406245556	7.8357267429
C	1.1734657551	-2.3800238003	-1.3830790472	C	3.0361510441	4.6150154391	4.6886594148
C	1.9693712686	-1.2774841797	-1.8363048681	C	-2.038995629	4.9419904935	4.1284352056
N	1.627144458	-3.4444579981	-0.7242929461	C	-2.8765796683	2.4677186383	6.5158794751
N	-0.8537264032	-3.4451521026	-1.0166590447	C	0.5698883297	1.5361521201	8.3892532916
C	6.921935537	0.2847748833	-0.7201268523	C	3.6179147393	2.6311860221	5.994504265
C	3.4056756075	-1.2338551925	-1.628192121	C	2.0841216887	4.2439670178	2.6016395341
C	4.3464544515	-2.2228363712	-1.7618794306	C	-1.9900823234	1.9672257343	1.904810713
C	5.6632480824	-1.79150559	-1.4809422534	C	-2.927996359	0.2906462494	5.4850003213
C	5.7624705217	-0.4698216767	-1.122894	C	0.5407525406	-0.6497741626	7.3777949494
S	4.1814350719	0.2492049096	-1.1522999633	C	3.6183568385	0.4535970971	4.9702870647
C	-10.4875244651	1.9409584235	-2.6103399984	C	2.0557675007	2.0666845947	1.5816333323
C	-9.6758573576	3.0380113624	-2.2151800069	C	-0.7401850984	2.2468562273	1.2720711438
C	-7.7125397486	1.6787609807	-2.3022632334	C	-3.1928437692	0.8938326429	4.2181874128
C	-8.5243723907	0.5813493751	-2.69721475	C	-0.8770521019	-0.5590233888	7.2205110069
C	-9.8975441625	0.6932920542	-2.8650614006	C	3.0105203037	-0.0939072156	6.1408666823

C	-11.8632792485	2.3036249508	-2.6879932067	C	3.0939369765	1.6391066599	2.4656755428
H	-12.6443682151	1.5976135779	-2.9492981549	C	-0.7115840869	4.4240602866	2.2921384948
C	-6.3400253953	1.309263697	-2.1966838343	C	-3.139882893	3.0680691082	5.2483213082
S	-7.5834579092	-0.8659875652	-2.9206565106	C	-0.8445846402	1.6262725252	8.2286029325
H	-5.5647708703	2.002147818	-1.8874942982	C	3.0110186854	2.086264523	7.1651916434
S	-10.6212340253	4.4746727124	-1.9462335957	C	3.1206318749	3.8158887513	3.4868908115
C	-8.300335499	2.9313851399	-2.0670925967	C	-1.9601363055	4.1425605445	2.9268094054
C	-12.0963942549	3.6161678042	-2.3757935913	C	-2.633115002	1.0769127124	6.6256264609
O	-7.5482665519	4.0008400763	-1.6720013215	C	1.2997402395	0.4529889717	7.8355912171
O	-10.6605565771	-0.378696489	-3.2315391711	C	3.8085532065	1.8496795747	4.8277584379
C	-7.0330917089	4.769861268	-2.7526876071	C	1.438707685	3.3315344218	1.7296337384
H	-6.4659075215	5.5879379492	-2.3045578943	C	-0.0139215244	3.4250317082	1.5685182748
H	-6.3699041548	4.1671546286	-3.3858846655	C	-3.1683377279	2.3004267212	4.0572849623
H	-7.8431481652	5.1810935133	-3.3674729996	C	-1.5700781175	0.6375608093	7.5164143276
C	-10.7692290674	-0.5517236019	-4.6397541182	C	2.5771796158	0.7394013714	7.2010101186
H	-11.3853180514	-1.4397723798	-4.7932980945	C	3.5436250724	2.4650337528	3.5251508828
H	-11.2519642153	0.3158912293	-5.107115362	C	-2.5499100503	2.8579476916	2.8527714889
H	-9.7850791334	-0.7074627232	-5.0981978125	C	-0.0780150704	5.2015920017	9.2005918859
C	-6.1066730915	-0.0047530245	-2.5019106183	C	-1.4489464943	5.6621207203	9.6424437846
C	-2.3820874667	-1.282813348	-2.3828453961	C	0.9317845091	5.7098467535	10.239898213
C	-3.1907074087	-2.3302353311	-2.7471549049	C	-1.9280931588	6.9159882696	9.2577835433
C	-4.5606776049	-1.9943193133	-2.8106743933	C	-2.2002184839	4.8948696935	10.5347866889
C	-4.8370619938	-0.6851222657	-2.504858411	H	0.7617010597	6.7944180442	10.2972397326
S	-3.3546848365	0.1402784937	-2.1302875811	H	0.5788873248	5.3148558267	11.2031863402
S	-18.5838991238	8.1137385039	-4.38173991	C	2.4320363513	5.4619645208	10.1333344843
C	-20.0978536285	4.7537285247	-3.5265493942	C	-3.1429864587	7.3888347845	9.7453011592
C	-17.9887816034	3.7717116174	-2.6836207903	H	-1.3484330437	7.5234920548	8.5667618638
C	-19.3677907082	3.7213495883	-2.9777862693	C	-3.4153719127	5.3659337038	11.0235607762
H	-17.5469189303	2.8852843989	-2.2391524722	H	-1.833578631	3.9186869621	10.8433625603
C	-19.3410969635	5.9466222563	-3.7692972601	H	2.6615668076	4.3933361477	10.1275117027
C	-17.9235110833	6.016362174	-3.4893758486	H	2.8383855415	5.8721976674	9.2052431793
C	-17.2288022278	4.8969146331	-2.9238389499	C	3.1498741487	6.109628522	11.3101384088
N	-17.379143993	7.1882018785	-3.8107217857	C	-3.8906991654	6.6134744125	10.6277005095
N	-19.8332517087	7.0814397096	-4.2626586136	H	-3.5065586094	8.3637667412	9.432344747
C	-15.8019892923	4.9308279084	-2.6556055137	H	-3.9923127262	4.7552059825	11.7125961269
C	-15.0219290599	5.9384553856	-2.1472967546	H	2.9637917367	7.1912216025	11.3497299385
C	-13.6622461263	5.5813682764	-1.9996284256	H	2.7848462758	5.7155515205	12.2684613793
C	-13.3660782392	4.2956289887	-2.3787207864	C	4.6426908579	5.8944528304	11.2596337484
S	-14.8159459555	3.5250483161	-2.9511577825	H	-4.8412426314	6.9800996581	11.0052613421
C	-29.9274884044	2.6615264815	-2.6597813906	O	5.2324607513	5.256821204	10.4195774387
C	-29.2688963158	2.1196570291	-1.5234086744	O	5.2506433479	6.5105340125	12.2865618092
C	-27.1585010866	2.9275303538	-2.3008926079	C	6.6676943299	6.3599662705	12.3234103284
C	-27.8180353841	3.4722614177	-3.4355847405	H	6.9417243406	5.3049798915	12.4102424425
C	-29.1881066204	3.3613094142	-3.6256592721	H	7.1226412983	6.767428611	11.4165036674

C	-31.3254347598	2.3864601916	-2.6404094306	H	7.0012310747	6.9147128026	13.2006720058
H	-31.9984059006	2.7003919961	-3.431209727	F	6.6989195293	-2.6220909886	-1.5651799796
C	-25.7532674051	3.1626606904	-2.3443809408	F	4.1033186161	-3.4617364555	-2.1589019677
S	-26.6994669271	4.2507475116	-4.5180044921	F	-5.4796899136	-2.8897494884	-3.1637350532
H	-25.071253169	2.8033208857	-1.5812247506	F	-2.7714648442	-3.5451925953	-3.064856456
S	-30.3796317413	1.2901935982	-0.4703532646	F	-12.7698856156	6.4405534352	-1.5154540879
C	-27.9022340279	2.2508950657	-1.3215336728	F	-15.4564263441	7.1256815262	-1.7574739121
C	-31.7222495371	1.6711270195	-1.542545209	F	-21.6006368071	5.7438657278	-5.9702829063
O	-27.2951484131	1.7047161844	-0.2266287655	F	-24.3557403235	5.3346408195	-5.8994496751
O	-29.7946622378	3.8800683991	-4.7341757637	F	-32.740649456	0.176146197	0.886484009
C	-27.1984733025	2.5948262338	0.8790484233	F	-35.4762494698	-0.3357267894	0.8805594206
H	-26.7050072295	2.0389400785	1.6785855049	F	-44.0288370551	-1.0932772555	-4.2162723786
H	-26.6009616266	3.4790482646	0.623643502	F	-41.3444443281	-1.670540442	-3.7440040582

Table S26. The coordinate of 9/PC₇₁BM (296 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	14.7543961269	0.4364064197	0.2897098434	O	-20.6535052912	2.6414763214	0.4340049143
C	16.8810190614	-0.9160186452	0.2735494112	O	-20.0175994198	-2.7841891025	-0.7728438479
C	15.4828313678	-0.7656360385	0.3174168713	C	-20.8061180061	2.9246740107	1.8194334093
C	13.2621917837	0.3743980142	0.2835103556	H	-20.9076700004	4.0085404305	1.9019893044
C	12.5410931726	1.5051335443	0.6849328357	H	-21.7029705104	2.440515019	2.2255697444
C	11.1551811262	1.5040082359	0.6881082011	H	-19.9277718443	2.595983405	2.3886304597
C	10.4333491657	0.3768533393	0.2672691197	C	-19.850817954	-3.6267681883	0.3607390149
C	11.1582498197	-0.7458837147	-0.1624304596	H	-19.7533105341	-4.6436616554	-0.0243442045
C	12.5437775837	-0.749101579	-0.1463695297	H	-18.9475428776	-3.3598847133	0.9233773378
H	14.9050268922	-1.6770950771	0.3806870393	H	-20.7213742486	-3.5701338812	1.025917909
H	13.0914484199	2.3879580404	0.9936435917	S	-26.8078548193	3.1904266401	0.5223306499
H	10.6226644594	2.3867893822	1.0332238564	C	-28.285283374	-0.2051224735	-0.3319527845
H	10.6271506737	-1.6125480737	-0.5448160756	C	-26.0719249675	-1.2995128833	-0.5522024851
H	13.0683093669	-1.6232900404	-0.5196101555	C	-27.4893997636	-1.3009342801	-0.5820747011
C	17.4627142175	-2.2892136153	0.3822891241	C	-27.5213306121	0.9805763849	-0.0300530616
C	16.7869146669	-3.3548703604	0.9887409904	C	-26.0673003158	0.9814368401	0.0033015124
C	18.7498982806	-2.5088942366	-0.1235871523	C	-25.2892373853	-0.2020377475	-0.2693750479
C	17.3763849825	-4.6118655831	1.070181845	N	-25.5607843162	2.1731005048	0.3060614791
H	15.807286984	-3.1985308928	1.430471155	N	-28.0424144821	2.1727181013	0.2450803468
C	19.3340127753	-3.7675818607	-0.0520856552	C	-31.9672788843	0.4590818355	-0.2233582625
H	19.2814793263	-1.6729590752	-0.5669927689	C	-32.1426003707	-0.9024238541	-0.5833893276
C	18.6479015938	-4.8244644543	0.5428971083	C	-34.5202871879	-0.6675763848	-0.514595006
H	16.8431470279	-5.4262290591	1.5532758086	C	-34.3441934656	0.6977422726	-0.1605054419
H	20.3299355767	-3.9242613947	-0.4578300808	C	-33.0906389918	1.2770823479	-0.0218190847
H	19.105814725	-5.8082074171	0.6033830885	C	-30.5903452927	0.8045481301	-0.1047539971
O	15.2342988054	1.6150846202	0.305961106	H	-30.2443298763	1.787049334	0.1839126589
O	17.7363146468	0.0095297553	0.1034557088	C	-35.9092924301	-1.0207850474	-0.5837900486

Ir	17.3178925537	2.1286378068	0.0582453612	S	-35.8762773376	1.4958880717	0.0732861472
C	19.2580499567	2.535142993	-0.0256251849	H	-36.2599739615	-2.0192687877	-0.8171019383
C	20.022938615	2.7753219361	-1.1701641741	S	-30.6200516608	-1.7175192649	-0.7659510218
C	19.9071381255	2.5363992718	1.2419052354	C	-33.3982476869	-1.47555117	-0.7413242825
C	21.38615869	2.9934027036	-1.0548185652	C	-29.7370690217	-0.2369964148	-0.3684852869
H	19.5751811188	2.7954772164	-2.1580373186	O	-33.5352580723	-2.7956787177	-1.0697146986
C	21.2863510221	2.7607831275	1.2936327156	O	-32.964270349	2.5883738869	0.3371587939
C	22.0499951965	2.9899238271	0.1655664056	C	-33.6008239956	-3.031314267	-2.4701272222
H	23.1168251306	3.1627998878	0.2357037216	H	-33.6981458607	-4.1114621349	-2.5967023961
C	19.0412882305	2.3132432146	2.3905521679	H	-34.4700706777	-2.530093772	-2.9147813948
C	19.4099481567	2.2819063248	3.7415576457	H	-32.6893965905	-2.686274494	-2.9739776424
C	18.4453254712	2.0846807311	4.716561933	C	-32.7683056771	3.4688607743	-0.762064735
H	20.4481220823	2.4148962386	4.0106891027	H	-32.6941640738	4.4735971685	-0.3413375035
C	16.8009106886	1.9560982772	2.9975140223	H	-31.8443740765	3.2294931294	-1.3029994182
C	17.1125195425	1.9214729017	4.3453988261	H	-33.6157405711	3.4253476838	-1.45748396
H	18.7332893215	2.061528459	5.763820393	C	-36.7248334264	0.0252643082	-0.3016031389
H	15.7880034191	1.8410625302	2.6271790317	H	-37.8074276135	0.0232774222	-0.2762933022
H	16.3278089084	1.7699272111	5.0784623175	F	0.3155958635	-2.362378093	-0.2519335341
C	16.5111577858	3.3958377375	-2.4305594155	F	-2.1995946723	-2.3892435635	-0.3026375967
C	17.0912243097	1.144690068	-2.7584371068	F	-12.6420976712	2.40332123	0.2929983268
C	16.192777715	3.5096924319	-3.7898882527	F	-15.1530880697	2.3820796435	0.3060283405
C	16.7944846003	1.2058948719	-4.1086178525	F	-25.5177385565	-2.4806992202	-0.8271867709
H	17.457779799	0.2432004305	-2.2802178544	F	-28.0290850431	-2.4832691872	-0.8806557082
C	16.3336202475	2.414293705	-4.6266646493	C	1.1772467201	2.9212341648	10.7715146528
H	15.8408272877	4.4568642702	-4.1728778637	C	2.4306806563	2.2503556557	11.2137151043
H	16.921984379	0.327014609	-4.7310118964	C	3.4353442649	2.6683790298	10.1950439977
H	16.0864801381	2.5044990128	-5.6806512204	C	2.882397268	3.7375568308	9.4097994311
C	16.4511617229	4.4405192694	-1.4187173533	C	-0.5768293377	-1.0428965015	3.9648117203
C	16.0530813377	5.7631545205	-1.6373419865	C	-0.901328697	-2.0539483332	4.9457291027
C	16.8536434133	4.0507521315	-0.1097550031	C	0.28888342	-2.8392266793	5.1895155876
C	16.0396983236	6.7152622974	-0.6365835692	C	1.349211269	-2.3089172034	4.3610468474
C	16.8520673659	5.0114586089	0.9051959006	C	0.8129498646	-1.2003707906	3.6044243207
C	16.4486771829	6.3072558639	0.626772316	C	1.4960515368	3.8937560712	9.7666546288
H	15.7276809641	7.7332725238	-0.8346459084	C	-0.0477492786	2.2802404351	10.720011241
H	17.1607633349	4.7698301711	1.916792615	C	2.3068363451	0.6592453044	11.4305818447
N	16.9514348012	2.2009763119	-1.9463113718	C	4.3077699859	1.7846982746	9.5830871058
N	17.7325997639	2.1409313682	2.0526555232	C	3.2826084284	3.9483009214	8.0875623187
F	16.4482230056	7.2155412538	1.6109792252	C	-1.119146007	0.235880697	4.0856096547
F	15.6605713712	6.1613025023	-2.8624794454	C	-1.7535888312	-1.7442053076	6.0025382102
F	21.9310235942	2.7614151043	2.4760053771	C	0.5738121673	-3.2821150688	6.4777339278
F	22.1065960151	3.2179059548	-2.1611792024	C	2.6493858844	-2.2453871322	4.85679755
C	6.7597400497	-0.3951133187	0.2345512801	C	1.6009257675	-0.0722918512	3.3820257188
C	6.5581227619	1.0111752216	0.1792312196	C	0.5620383674	4.2580509443	8.793537187
C	4.1890693615	0.7183507912	0.0907546519	C	-0.1544548774	0.8397976793	10.9234296095

C	4.3888782988	-0.6857790575	0.151646588	C	3.2118989888	-0.1760988492	10.5996446139
C	5.6523877514	-1.2553974608	0.2399543123	C	4.7018270434	1.9771213721	8.2126272524
C	8.1476049049	-0.7274839163	0.2783227649	C	2.3103798614	4.3004340174	7.0813631017
H	8.5052850424	-1.7491637518	0.332663771	C	-1.9924226374	0.5521455079	5.1879182588
C	2.809165968	1.0544366497	-0.0033392646	C	-1.447990844	-2.1982169676	7.3371045728
S	2.8848680615	-1.5505129878	0.075373257	C	1.9214292548	-3.2077744777	6.9896480672
H	2.4456740493	2.0700412717	-0.0699057705	C	3.4564516421	-1.0710297977	4.6281549987
S	8.0721331477	1.8696717996	0.1724065705	C	1.0355750813	1.2466628002	3.5109648998
C	5.2963304031	1.5831462581	0.1210097504	C	-0.2967923476	1.3983375122	3.855648965
C	8.9722781966	0.3619765899	0.2549439603	C	-2.3041983326	-0.4166335972	6.1266119056
C	1.976454765	-0.0367781465	-0.0117230636	C	-0.3108447538	-2.9547499707	7.5702370516
O	5.1478196431	2.9380815416	0.0530268877	C	2.9367574602	-2.6973735825	6.1961595021
O	5.8136119293	-2.6116860025	0.294835563	C	2.9419743651	-0.0080385358	3.904887942
C	4.879246906	3.5525935187	1.3084091075	C	0.9785508051	4.4520905278	7.4264542567
H	4.8047625519	4.6243632939	1.1143655974	C	-1.0004486858	2.6249637358	9.6967854217
H	3.9363972735	3.1908239896	1.7363791793	C	0.9658644578	0.0801050589	11.1709382316
H	5.6926845392	3.3651672315	2.0202732552	C	4.1935814549	0.3454474475	9.7877580829
C	5.8156428379	-3.1284714691	1.6204326399	C	4.2109425383	3.0463519467	7.4787802258
H	5.920679144	-4.2114027069	1.528529886	C	-0.7102859225	3.6049932718	8.7587391423
H	6.6564451362	-2.7254464175	2.1992746555	C	-1.1764268029	0.3376698935	10.0367076266
H	4.8780806139	-2.8951134586	2.1403032156	C	2.4918993022	-1.3336438059	10.1464224548
S	-1.0139393221	3.4371289081	0.240831988	C	4.8523296573	0.6894088408	7.5836674749
C	-2.4686859117	-0.0568394293	-0.0979629049	C	2.6600931555	3.6324953663	5.8502670849
C	-0.2484976368	-1.1573152077	-0.1629113194	C	-1.7246420566	1.905954004	5.6154464527
C	-1.6660611689	-1.172824953	-0.1853395201	C	-1.8304057912	-1.1671347414	8.2721208075
C	-1.7138205232	1.1661674416	0.0213541768	C	1.8620488256	-2.8546496039	8.3871397909
C	-0.2602958263	1.1828654383	0.0347783129	C	4.2480071835	-0.818598692	5.8094260723
C	0.5253532256	-0.0229170091	-0.0570260469	C	2.0305466404	2.1226583153	4.0875406422
N	0.2390780496	2.4095066993	0.1533674357	C	-0.6814058902	2.4303777659	4.792326434
N	-2.2427136947	2.3816637144	0.1284223881	C	-2.356942438	-0.0683945513	7.5270908708
C	-6.1517403109	0.5995694884	-0.0593929877	C	0.4867553039	-2.698854606	8.7442857358
C	-6.321667393	-0.7902939034	-0.2981400686	C	3.9280168286	-1.8218653102	6.7743255695
C	-8.699329267	-0.5479153897	-0.2808072046	C	3.2053515078	1.3464979629	4.3335600735
C	-8.5284996632	0.8427590014	-0.0485406022	C	-0.0519111589	3.9402700706	6.554886786
C	-7.2771089859	1.4322085906	0.0551361961	C	-1.7019118612	1.433980962	9.2890575821
C	-4.7776201362	0.957587079	0.0364096047	C	1.1185218351	-1.1764289203	10.4984499146
H	-4.4352850134	1.9637446333	0.2329272813	C	4.5336255909	-0.3112672812	8.5496265493
C	-10.0745223625	-0.9109590369	-0.3367752346	C	3.8324990738	2.8545953941	6.0971430035
S	-10.0527161429	1.6617217385	0.0964546454	C	-1.0933859089	3.4131593029	7.3782288845
H	-10.4178134902	-1.9250439742	-0.4858809344	C	-1.112953704	-0.9610264021	9.4755856479
S	-4.7956215565	-1.6153183929	-0.3912218413	C	2.8699130361	-2.0669989359	8.992151662
C	-7.5733711618	-1.3765511516	-0.4196586749	C	4.5870686245	0.4980812418	6.2051526361
C	-3.9202569335	-0.1017009248	-0.1269552328	C	1.6687661132	3.197012675	4.935095747
C	-10.9305455197	0.1483215924	-0.1622862634	C	0.2597412432	3.3567604458	5.3012776305

O	-7.7027943113	-2.7195137862	-0.6301313542	C	-2.178307765	1.2661911791	7.9647327007
O	-7.1526300914	2.769593618	0.2998474707	C	0.0860755999	-1.7500951036	9.7134881975
C	-7.8258512694	-3.075653351	-2.0015229125	C	3.939875442	-1.5360571266	8.1615176566
H	-7.9125701207	-4.1635853004	-2.029806527	C	4.0515170287	1.6226502871	5.4350983334
H	-8.7207701993	-2.6248692017	-2.4484371867	C	-1.8571359707	2.2929507171	6.9713692183
H	-6.9410662441	-2.7650646871	-2.5709017653	C	2.6350446356	1.6084342744	12.5624485995
C	-6.9551469281	3.5534830772	-0.8702822698	C	1.5292727949	1.8311121442	13.5695544603
H	-6.8795314196	4.5899925725	-0.5359096499	C	3.9625101992	1.610135023	13.3348428234
H	-6.0312170211	3.2674982318	-1.3880839994	C	1.1443726735	3.1267182615	13.9196337961
H	-7.8025085276	3.453214487	-1.5598563636	C	0.9649663262	0.7503359576	14.250033535
S	-13.8553503325	-3.3314312758	-0.8433691287	H	3.981328067	2.5702600797	13.8701289885
C	-15.3787439395	0.0807263266	-0.1517066315	H	3.8413282328	0.849200855	14.1188883567
C	-13.1799227223	1.2060192895	0.0583141309	C	5.315680034	1.4017602777	12.6646864208
C	-14.5973467088	1.1942266378	0.0649044971	C	0.2032601859	3.3382530045	14.9231672397
C	-14.5989889724	-1.1084930123	-0.3929372694	H	1.5809612522	3.9753465912	13.3984210539
C	-13.1446548916	-1.0960094006	-0.4017838503	C	0.0237269189	0.9595168035	15.253690893
C	-12.3821998621	0.1053487522	-0.1648744446	H	1.2606050208	-0.262593477	13.9869688482
N	-12.6218800587	-2.2936896386	-0.6475009757	H	5.3626302697	0.4361065831	12.1547956217
N	-15.104168463	-2.3158377315	-0.6282916835	H	5.5064282389	2.1639643016	11.9048405251
C	-19.0515348531	-0.6249827962	-0.2814954736	C	6.425333131	1.4595713283	13.7061264565
C	-19.2435453643	0.7479315441	0.0278719982	C	-0.3608447286	2.2546521733	15.5913558945
C	-21.6167603282	0.4805895215	-0.0486523564	H	-0.0910367834	4.3519856033	15.1808256175
C	-21.4250679427	-0.8939129505	-0.3506542208	H	-0.4112601875	0.1084382802	15.7705117295
C	-20.1646214221	-1.4629823861	-0.4612938525	H	6.4357906621	2.4249363676	14.2299780538
C	-17.6710360896	-0.9601496447	-0.3721472106	H	6.280054624	0.7041093645	14.490304471
H	-17.3120808866	-1.9493517871	-0.6191764854	C	7.7909542298	1.2433582032	13.1016361743
C	-22.9967028093	0.8260963688	-0.0007235984	H	-1.0984913033	2.4188667433	16.3720112769
S	-22.9375403327	-1.7198364725	-0.566798924	O	8.0177036134	1.0387738094	11.9326221709
H	-23.3541275235	1.8274788263	0.1937870338	O	8.7472833682	1.3058563226	14.0430405424
S	-17.731383662	1.5849051523	0.1971777292	C	10.0751128225	1.1104449382	13.5632174769
C	-20.5041574324	1.3129397675	0.1562636911	H	10.1768654073	0.1255177962	13.0993366486
C	-16.8309288383	0.0997430178	-0.1363828891	H	10.3353148087	1.8743348216	12.825402686
C	-23.8371355197	-0.2310738793	-0.2466643816	H	10.7203886985	1.1891708507	14.4384674696

Table S27. The coordinate of **10/PC₇₁BM** (338 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	17.4773663442	8.4995309132	-1.4306572581	O	-30.165705247	6.229272519	-2.0780086194
C	19.7977295978	8.4775181519	-2.4123939925	C	-26.7538343738	1.0232212498	-1.0163308771
C	18.5568412539	7.8946423877	-2.0974155603	H	-26.0853370102	0.1788864031	-1.1957511385
C	16.2054565472	7.7338389654	-1.2556082428	H	-26.3428553428	1.652829859	-0.2171809176
C	15.2674144062	8.2062347552	-0.3290556644	H	-27.7392507156	0.6503632917	-0.7106256384
C	14.0674171248	7.543894869	-0.1239658344	C	-30.87334278	6.3907874324	-0.8547691044
C	13.7515889722	6.3853495528	-0.8487605706	H	-31.4700823681	7.2987013219	-0.9623381962

C	14.6803536537	5.9266609052	-1.7957146772	H	-31.5359831262	5.5372057345	-0.6643817378
C	15.8840895026	6.5851039195	-1.9910193003	H	-30.1823010443	6.5056320471	-0.0104777362
H	18.4160674605	6.8729300618	-2.419622613	C	-25.6698258388	5.7638340822	-1.1142796963
H	15.5010576167	9.1076691202	0.2277911555	C	-22.1131791879	7.0754177017	-0.1127413333
H	13.3699950677	7.9193408627	0.6207874989	C	-23.0151638692	8.1149608854	0.0364844543
H	14.4369403898	5.0636443816	-2.408703021	C	-24.3361183994	7.7661448044	-0.2954668753
H	16.5574348482	6.2165155766	-2.7583668454	C	-24.4730831261	6.4551139668	-0.7042693935
C	20.8318704496	7.6431890045	-3.0986339647	S	-22.9424799803	5.64568096	-0.6811273184
C	20.8551375283	6.2455120604	-3.0201680924	H	-22.7138943936	9.0955915166	0.3780497198
C	21.8345026396	8.2926866693	-3.8292416066	H	-25.1704280843	8.4569947592	-0.2321201133
C	21.8446099089	5.5166278626	-3.6711212332	S	-37.4748504695	-2.4512750898	-6.1146543633
H	20.1173444062	5.7205121752	-2.4207786782	C	-39.1042509613	0.9464629343	-5.6263897707
C	22.8163349122	7.5637277733	-4.4889295317	C	-37.0283495688	2.0116598105	-4.7937825631
H	21.829477271	9.3774600733	-3.8634511989	C	-38.3978996274	2.0293198451	-5.1476845733
C	22.823279443	6.1723183575	-4.4142902505	C	-38.2956514565	-0.242452971	-5.7347222544
H	21.8550530538	4.4328746585	-3.591743382	C	-36.8878731491	-0.2605765706	-5.370896089
H	23.5817831701	8.0826430124	-5.0597360036	C	-36.2046619719	0.9093429122	-4.8775607748
H	23.5934868176	5.6011937519	-4.9258135974	N	-36.3268242668	-1.4536558683	-5.5450326274
O	17.4685864681	9.6594251409	-0.907364801	N	-38.7305103889	-1.4226332691	-6.1667513742
O	20.1399458564	9.6860118564	-2.2125371418	C	-34.8029207262	0.9209439276	-4.5137071125
Ir	19.0172205362	11.1501972659	-1.0896418436	C	-33.9044202666	-0.1306796766	-4.5691723092
C	20.5345147206	12.425698202	-1.179705793	C	-32.6085413304	0.2133363786	-4.1476330217
C	20.7260796781	13.4448570003	-2.1162783998	C	-32.4866630791	1.5328311362	-3.7618690135
C	21.5305327438	12.2183432335	-0.1835786841	S	-34.0015493228	2.3570832073	-3.9207597417
C	21.8754955078	14.2166601391	-2.0699438795	H	-34.1900023794	-1.1162618793	-4.9096546227
H	19.9926303755	13.6514953984	-2.8881586105	H	-31.7803842802	-0.4875211777	-4.1310955491
C	22.6697598189	13.029377925	-0.188781513	C	-48.462502005	4.3429928324	-7.206251295
C	22.8699565138	14.0321129676	-1.1175765661	C	-47.7576093846	5.3659863008	-6.5179303762
H	23.7618843834	14.6461021894	-1.0970128353	C	-45.7775416858	4.0282135428	-6.4424446055
C	21.2465192004	11.1614648336	0.7760495694	C	-46.4823640312	3.0071934641	-7.1348630258
C	22.0369614702	10.7644685671	1.8621425515	C	-47.8046071888	3.1477613761	-7.5304370891
C	21.6008142546	9.751074059	2.7002650998	C	-49.8222955123	4.7198772424	-7.4669004477
H	22.982544939	11.2576382135	2.0365784244	H	-50.5378013619	4.0724603777	-7.9603064924
C	19.6339811023	9.5612526129	1.3690745391	C	-44.4398576901	3.6344429394	-6.1358091225
C	20.3751171461	9.1351972545	2.4572388578	S	-45.4818375642	1.606130939	-7.3958235098
H	22.214758718	9.4451361561	3.5426784164	H	-43.7528282972	4.260705037	-5.577000475
H	18.6688707003	9.1363035268	1.1164542548	S	-48.7785798953	6.7459162157	-6.2162766461
H	19.9964294854	8.3419079731	3.0923571489	C	-46.4267339756	5.2334486087	-6.1401473818
C	17.0096358037	12.7658448362	-2.4324494549	O	-45.785003322	6.230946516	-5.4621249146
C	18.2150389231	11.4475999623	-3.9563824946	O	-48.4508897563	2.1345142597	-8.1826577433
C	16.2256218488	13.2598346826	-3.482872577	C	-45.0883723298	7.1401068226	-6.3050937239
C	17.4719125158	11.9079280097	-5.0290746945	H	-44.6366574853	7.8852079236	-5.64719081
H	19.0235774262	10.733456361	-4.0681924539	H	-44.301757522	6.6291259291	-6.8745495654
C	16.4567588967	12.828882416	-4.7793675035	H	-45.7735192855	7.6368227902	-7.0032047833

H	15.4467700804	13.9778311022	-3.2691977211	C	-48.4187527631	2.2565228429	-9.5986511455
H	17.6870705156	11.5496748045	-6.0297928112	H	-48.9581862457	1.3936854773	-9.9946550372
H	15.8480041526	13.2132618903	-5.5928591036	H	-48.911636658	3.1797748475	-9.9286521032
C	16.9296786737	13.1269559927	-1.0243440603	H	-47.3878312944	2.2459695313	-9.9739123899
C	16.0304410889	14.0424824469	-0.468731764	C	-44.1281666674	2.3778432111	-6.5773193035
C	17.8728952323	12.4857319356	-0.1717497132	C	-40.50665995	0.9932492601	-5.9848247002
C	16.0229774907	14.3618658072	0.8752589256	C	-41.2930624055	-0.0394597974	-6.4656277683
C	17.8784976273	12.8126587753	1.1869823331	C	-42.6233615837	0.3371633734	-6.7201411409
C	16.9644877259	13.7305965609	1.6783427707	C	-42.8832771787	1.662769449	-6.4388515753
H	15.3160107619	15.076501349	1.2783032057	S	-41.4570436761	2.4552981545	-5.8597464743
H	18.584759941	12.362210901	1.8765575144	H	-40.9043382221	-1.0363105149	-6.6208869525
N	17.9893900833	11.8580844874	-2.7011414673	H	-43.3790437025	-0.3486426993	-7.0887660933
N	20.0556873304	10.5375221551	0.5539680319	C	-50.1149186184	5.9602115646	-7.0033347873
F	16.9785037671	14.0297549815	2.9836866898	H	-51.0657299029	6.4749755862	-7.0625216241
F	15.1197606513	14.6582872769	-1.2464448146	F	-38.9985009032	3.2110119806	-4.9865959072
F	23.6333884964	12.8541445513	0.7356854235	F	-20.3636738495	4.8419365376	-0.4758262036
F	22.0471609232	15.186193835	-2.9776923832	F	-1.2940626651	2.9592541671	0.6182094914
C	10.9019891698	3.9598760552	-0.5614166626	F	1.2296674809	2.9536371343	0.4741052526
C	10.1207666679	5.0662251617	-0.1328732583	F	-17.8703203616	4.8283141314	-0.0814793393
C	8.1727095617	3.6918792926	0.0480852869	F	-36.5527585292	3.1792189929	-4.3538121008
C	8.9604180998	2.5814337423	-0.3599205016	C	-0.8795005942	2.1194358943	11.4018550745
C	10.311219404	2.6905931162	-0.6547623174	C	0.2947181196	1.4387442685	12.0143325136
C	12.2481529523	4.3418758596	-0.8474418617	C	1.4444257505	1.8976752399	11.1837967641
H	13.0032359409	3.6396827944	-1.1819629958	C	1.0122010875	2.9914375909	10.3578567976
C	6.8122008394	3.3226970547	0.271860027	C	-1.4878456197	-1.6072958074	4.2696338146
S	8.0080703244	1.1277146149	-0.4632199488	C	-1.9536293948	-2.6542266717	5.1510623967
H	6.0495940464	4.0286805345	0.5823375999	C	-0.8095575648	-3.4428866894	5.5531847969
S	11.0622027729	6.5297829889	-0.0968315376	C	0.3637293723	-2.8785459	4.922825039
C	8.7727769766	4.9532655618	0.18085906	C	-0.0567159551	-1.7460434905	4.1283249331
C	12.4939150648	5.6700438504	-0.6438770321	C	-0.4146697145	3.1288561881	10.4950294999
O	8.0474264063	6.045030828	0.565909425	C	-2.0741061378	1.4748033705	11.1337104004
O	11.0295623126	1.6014414566	-1.0637914278	C	0.1545789733	-0.1595693922	12.1525228464
C	7.9809792657	6.2198897777	1.9757653141	C	2.4116828752	1.0404010275	10.6881386452
H	7.3859911444	7.1192178297	2.1464639962	C	1.6155715557	3.2513572667	9.124405271
H	7.496015083	5.3624136563	2.4590081985	C	-2.0552139499	-0.3365194762	4.347588878
H	8.9813689134	6.3568156168	2.4048539001	C	-2.9666414879	-2.3865267852	6.0684956931
C	11.7108174594	0.9395559467	-0.0058443005	C	-0.7280349576	-3.9295069171	6.8547787597
H	12.2357198376	0.0953555515	-0.4576686947	C	1.5667674002	-2.8248174728	5.6223963633
H	12.4361967322	1.6065315854	0.4770530621	C	0.7459840516	-0.6064773797	4.0718022563
H	11.0054982056	0.5691742826	0.7485025382	C	-1.1852126711	3.5219296022	9.3979367281
S	-0.0444282177	-2.8781767102	0.5712626596	C	-2.1970363363	0.0271585571	11.2677869681
C	-1.5313070146	0.6164218957	0.6426817892	C	1.1889070535	-0.96142555	11.4499578023
C	0.6716175117	1.7413652373	0.5119872921	C	3.0167765803	1.2832637538	9.4053635056
C	-0.7407641486	1.7445118056	0.5929678948	C	0.812343731	3.6339095628	7.9887301256

C	-0.7653762743	-0.604067863	0.604959804	C	-3.0959997771	-0.0638698045	5.3063510075
C	0.6860116158	-0.6075863976	0.5186235462	C	-2.8729237185	-2.8865309617	7.4181395401
C	1.457298408	0.6094795173	0.4677228712	C	0.5200786238	-3.8663341801	7.5771163613
N	1.19664625	-1.8349599301	0.489606469	C	2.3874906867	-1.6397468724	5.5655078261
N	-1.2816747016	-1.8292976132	0.6379829224	C	0.1525729225	0.7053179509	4.1561070327
C	6.5662918528	1.9949220193	0.0517338341	C	-1.2186120912	0.8366516326	4.2929155266
C	2.9020968242	0.633929059	0.3685667521	C	-3.5439194991	-1.0667570851	6.1489514674
C	3.7647204116	-0.447694648	0.3188170461	C	-1.7784801825	-3.6450324409	7.8024375767
C	5.1175961005	-0.0836561757	0.2044335532	C	1.6431708393	-3.3233857011	6.9739613992
C	5.318298185	1.2808975502	0.1673946828	C	1.9850403138	-0.5542265809	4.8061376751
S	3.8097528006	2.1242313058	0.2652670618	C	-0.5587779675	3.7667907143	8.1223861589
H	3.4126120029	-1.4687118334	0.3672073906	C	-2.8553548811	1.8510190049	9.9843147503
H	5.9298853034	-0.8018844812	0.1649587346	C	-1.1218595697	-0.7355545504	11.6632690626
C	-11.0286569477	3.9841482997	0.8140831496	C	2.2821844782	-0.4062036048	10.8233627457
C	-10.1857642648	5.1164601217	0.9776747259	C	2.6383142754	2.3759511568	8.6401301281
C	-8.2321402167	3.7400357207	0.9173883425	C	-2.42925267	2.8650246949	9.1388329867
C	-9.0760134458	2.6082952629	0.752991213	C	-3.0598532769	-0.4476516225	10.2127535531
C	-10.4578852362	2.7079447263	0.6896047059	C	0.5620734195	-2.1046590436	10.8467173614
C	-12.4078248289	4.3458258041	0.8082155938	C	3.2788667488	0.0198646374	8.7645859485
H	-13.2097215893	3.6192770755	0.7339896195	C	1.3601587896	3.0116858871	6.8071324011
C	-6.8545619137	3.3716009282	0.9593172622	C	-2.9129313942	1.2749986565	5.8177613392
S	-8.1543413663	1.1356227151	0.6456805679	C	-3.4093596866	-1.8909963344	8.3154114529
H	-6.0543882792	4.0865631537	1.1172743171	C	0.2354958923	-3.563156397	8.95812115
S	-11.1121192019	6.5855692009	1.1086564615	C	2.9796520155	-1.426150865	6.8653093503
C	-8.80240772	5.0188097536	1.0214272695	C	1.0338905201	1.5641004826	4.9150584818
C	-12.6184824159	5.6909031412	0.948971023	C	-1.7579549383	1.8335087383	5.1899763542
O	-8.0255509138	6.1295007323	1.1929128153	C	-3.8221770329	-0.768835345	7.5344915755
O	-11.2365570585	1.5947762164	0.5437119644	C	-1.1804426258	-3.4270077997	9.0964614856
C	-7.5686976725	6.7021739195	-0.0264355763	C	2.5218277727	-2.4647576411	7.7320098553
H	-6.9710727379	7.5736430453	0.2480434216	C	2.161298277	0.7851555489	5.3181565606
H	-6.9471874518	5.9939825306	-0.5885510224	C	-1.4324924518	3.2821572689	7.0809187503
H	-8.4108310473	7.0193603883	-0.6539160462	C	-3.4705124692	0.6721641579	9.429067948
C	-11.5751367418	1.3062402571	-0.8074734097	C	-0.8513576671	-1.9663270521	10.9805858843
H	-12.1871258587	0.4023984277	-0.7847684617	C	2.8224132735	-1.0162639661	9.6329460411
H	-12.1494609472	2.1265113748	-1.2560729918	C	2.4868392467	2.2317927366	7.2097817975
H	-10.6765644644	1.1241517779	-1.4098608563	C	-2.5864576113	2.7213172499	7.7091386579
C	-6.6469913847	2.0253800416	0.8235371888	C	-2.8944465648	-1.7251543529	9.6243126842
C	-2.9769033171	0.6480222637	0.7257757263	C	1.1268140291	-2.7940388561	9.7426988056
C	-3.8421363259	-0.4278206019	0.8287145569	C	3.2377625716	-0.12299709	7.3552947401
C	-5.197209028	-0.057591386	0.8757995117	C	0.5316427218	2.6058775496	5.7308658018
C	-5.3974263765	1.3062125795	0.8111205352	C	-0.9193456685	2.7458141833	5.8734124968
S	-3.8852821278	2.1405743296	0.6867185576	C	-3.7291203853	0.5501239214	8.0408642846
H	-3.4899781568	-1.4491485082	0.8686585485	C	-1.7402213477	-2.5163084767	10.0221503501
H	-6.0094681981	-0.7711090136	0.9676214906	C	2.3102491251	-2.2288702532	9.1126103622

S	-19.3430713926	10.4369706127	1.3423379737	C	2.8198206203	1.0255121271	6.5484654308
C	-20.6861007574	7.0946317468	0.1331830156	C	-3.2636348389	1.612980268	7.1472570676
C	-18.4655814669	5.9970167756	0.1692103624	C	0.2878717007	0.7494281081	13.3547724125
C	-19.8623917519	6.0048359826	-0.0524982648	C	-0.9659762301	0.9286185033	14.1807009987
C	-19.9728578144	8.2596856319	0.5943979505	C	1.4750752847	0.7221334193	14.3286452084
C	-18.5365334582	8.2515809779	0.8226770336	C	-1.4152703673	2.2090586968	14.5098912861
C	-17.7281717935	7.0779790049	0.6032882728	C	-1.619624454	-0.1786507148	14.7247580405
N	-18.0760545038	9.4254046906	1.245267084	H	1.3712181945	1.6353452591	14.9317216532
N	-20.5287936542	9.4391519568	0.8556625499	H	1.2613678544	-0.1032402038	15.0228521179
C	-16.2955185498	7.0426649098	0.8119524158	C	2.9255351808	0.6117039871	13.8722578654
C	-15.4741952975	8.070093773	1.2439110376	C	-2.5060116333	2.3799959155	15.3573935328
C	-14.1186434058	7.7074710019	1.334651105	H	-0.9104333721	3.077824781	14.094108541
C	-13.8753796311	6.3969164634	0.9773303178	C	-2.71046026	-0.0099870203	15.5726339443
S	-15.3441236413	5.6076838835	0.5116477168	H	-1.2753196627	-1.1799656371	14.4770770997
H	-15.8578040525	9.0512757536	1.4873240749	H	3.0999746614	-0.3084672408	13.3090603522
H	-13.3387749631	8.3843451977	1.667736227	H	3.1978459248	1.4377402625	13.2099155867
C	-29.8549793263	3.8764207703	-2.5172914691	C	3.8503658601	0.6278967175	15.0825163065
C	-28.9841330432	2.7537564574	-2.5454226411	C	-3.15749096	1.2702214641	15.8893619455
C	-27.1466281636	4.0901586626	-1.8054276067	H	-2.8484423409	3.3823597792	15.5995673232
C	-28.0187269349	5.2115460257	-1.769112174	H	-3.2131113837	-0.8810913478	15.983957575
C	-29.36162776	5.1250900703	-2.1063364933	H	3.7283692034	1.5479483897	15.6696012655
C	-31.1714619026	3.5365223347	-2.9477490028	H	3.617953038	-0.1928325832	15.7747919787
H	-31.9737657025	4.2623490788	-3.0250381229	C	5.3041664065	0.5097207142	14.6960547637
C	-25.8167814269	4.4398403927	-1.4294285799	H	-4.0116352147	1.4025692331	16.547720631
S	-27.1778000683	6.65579965	-1.2795065245	O	5.7241391851	0.382798708	13.570321397
H	-25.0011059605	3.7251666332	-1.4112398483	O	6.0944400789	0.5615717508	15.7812757958
S	-29.8084037317	1.3214397716	-3.0925574355	C	7.4899440043	0.4523034788	15.512681322
C	-27.6466217319	2.8354079841	-2.1872624055	H	7.7165329906	-0.5019214888	15.0291584595
C	-31.3113598376	2.2167405618	-3.2836685814	H	7.8221764884	1.2640221773	14.8597562028
O	-26.8340207072	1.7384969361	-2.2432349901	H	7.9836725443	0.5156265544	16.4826799146

Table S28. The coordinate of **11/PC₇₁BM** (338 atoms).

Atom	Coordinates (Angstroms)			Atom	Coordinates (Angstroms)		
	X	Y	Z		X	Y	Z
C	17.6090924627	6.2543797091	2.7448084304	H	-31.9802979198	8.0513667353	-3.6137726377
C	20.1068251645	5.9512919463	2.6078123629	H	-31.8908174965	7.1310593327	-2.083139408
C	18.780323925	5.6671453863	2.2357840595	H	-30.4596618948	8.024361518	-2.6766038533
C	16.2885222654	5.8281933803	2.191419243	C	-26.3495975731	6.0640001805	-3.5987299652
C	15.1388891308	6.0601258288	2.9558235897	C	-22.671479418	7.1487714954	-4.5000187899
C	13.8888922171	5.6701059246	2.502292366	C	-23.5420264118	8.0362997013	-5.0824384383
C	13.7355045141	5.0496248584	1.2533516827	C	-24.9008076181	7.7444785937	-4.833107081
C	14.8844659269	4.8525954409	0.4711629164	C	-25.1070264371	6.6355196992	-4.0508765564
C	16.1356561256	5.227092842	0.9348973307	S	-23.5721541661	5.9473216861	-3.6159866126
H	18.6475862839	4.9109329059	1.4752343339	S	-38.7747794958	0.7304516901	2.7357925655

H	15.2474131056	6.5506042598	3.917664134	C	-40.2675538265	1.6400485797	-0.6195703438
H	13.0188598836	5.8327366349	3.1335397711	C	-38.0884898921	1.9816123589	-1.7217939652
H	14.7891339526	4.4264949312	-0.5233158164	C	-39.5081995467	1.9571750724	-1.7212418885
H	16.9957205044	5.0850664584	0.2877100253	C	-39.5093898664	1.3157942904	0.554737515
C	21.2169263266	5.1738503391	1.9753238935	C	-38.0633422073	1.3562665253	0.5584328753
C	21.032568165	3.907588329	1.4069446582	C	-37.3177791163	1.6854734511	-0.6222733711
C	22.5018299142	5.7307993737	1.9737296967	N	-37.5324733807	1.0597906904	1.741455998
C	22.1014801483	3.2259666553	0.835244022	N	-40.0275316806	0.9578235838	1.7263596812
H	20.0568618732	3.4319828475	1.4366385561	C	-35.8656043002	1.7055044102	-0.6439267427
C	23.567439677	5.0543477728	1.3927487093	C	-34.9959108891	0.8270643714	-0.0474086543
H	22.6459387326	6.6995911517	2.441249793	C	-33.6363462469	1.1607336789	-0.2339378918
C	23.3703002733	3.8001508672	0.8185315206	C	-33.4288930417	2.292473335	-0.9823786227
H	21.9436553472	2.2396672478	0.4071863131	S	-34.9632389907	2.9517138276	-1.4609264608
H	24.5563613625	5.5049332983	1.3915475237	C	-49.7265509848	-0.0341400747	-3.685605683
H	24.2037577828	3.2681170529	0.3675920256	C	-48.8524014679	-0.4280236016	-4.7343207119
O	17.5353689633	7.106719854	3.6867106348	C	-46.9391064585	0.1861815931	-3.4408009389
O	20.4878357604	6.8519716563	3.4208496767	C	-47.8123693535	0.5758795612	-2.39086831
Ir	19.205794175	8.0749482547	4.6517244162	C	-49.1927282268	0.4647696003	-2.4894002063
C	20.7834233526	8.8193986652	5.5952463676	C	-51.1033591687	-0.2138421759	-4.0482767597
C	21.4617893937	10.0057500885	5.3026656628	H	-51.9309584058	0.0475219981	-3.3992423407
C	21.2678393498	8.0011970342	6.6554528862	C	-45.5721787754	0.4101497115	-3.1006210342
C	22.5891469702	10.3528486154	6.0291650316	S	-46.9367241201	1.2053085739	-1.0244086281
H	21.1280394634	10.6706277694	4.5131794391	H	-44.7536616692	0.2009877175	-3.7811924607
C	22.4120607933	8.4038600701	7.3511576554	S	-49.7422648665	-1.001025132	-6.1190895354
C	23.0928055646	9.5700096742	7.0604161316	C	-47.4702134386	-0.336836119	-4.6285498846
H	23.9759650882	9.8582201932	7.6170981549	O	-46.6552606128	-0.7077687958	-5.660355784
C	20.4927190901	6.7990815249	6.9252276101	O	-50.0025002408	0.8668940809	-1.4642797272
C	20.7291906025	5.8395747033	7.9184127333	C	-46.2445309936	-2.0683108686	-5.6052046956
C	19.8691165101	4.7622151763	8.0571815572	H	-45.6116400209	-2.2341880684	-6.4792472564
H	21.5830995224	5.9529848159	8.5709268481	H	-45.6700733704	-2.2712532472	-4.6924331292
C	18.5846345889	5.6149242457	6.2406945204	H	-47.1069417068	-2.7450786846	-5.6454975922
C	18.7717983792	4.6427277631	7.2073544246	C	-50.3432452342	-0.1778062326	-0.5619988739
H	20.0535918655	4.0197369272	8.8284710658	H	-50.9750658126	0.2726601489	0.2061043453
H	17.7516008779	5.5924093339	5.5468027099	H	-50.8978671272	-0.97591809	-1.0715664715
H	18.0731920413	3.8169667279	7.2861119185	H	-49.4478178989	-0.6045084736	-0.0932594917
C	18.1270622841	10.5573070316	3.5916579808	C	-45.4050488493	0.9397964718	-1.8500478861
C	19.6521349373	9.575153834	2.1008744275	C	-41.7196072012	1.6246558675	-0.6363184261
C	17.8992153264	11.5910658101	2.6741824273	C	-42.5852226783	2.0599183749	0.3357531693
C	19.4650327325	10.5745731243	1.1623487512	C	-43.9459757247	1.8594516341	0.014875011
H	20.3366346168	8.7487533186	1.9440089084	C	-44.1588597637	1.2765650675	-1.209260071
C	18.5672119145	11.5973107856	1.4602650263	S	-42.6283824871	0.9728260883	-1.9726466807
H	17.2027726771	12.378129077	2.9257798006	C	-51.2488640864	-0.719455072	-5.2979127265
H	20.0103766317	10.545719446	0.2254145849	H	-52.175912368	-0.9391390463	-5.8125548563
H	18.3892472864	12.399903523	0.7501359714	F	-40.086440081	2.2643851091	-2.8808412984

C	17.5393882792	10.4044696732	4.9147591411	F	-20.9220350541	6.4583388256	-2.3561338844
C	16.6209624576	11.2794982801	5.5031769285	F	-1.549888461	4.1784481735	-2.3204587514
C	17.969166793	9.2628093787	5.6493840292	F	0.9981362009	4.004916647	-2.6039308942
C	16.1154853859	11.0896582887	6.7747030064	F	-18.3603254981	6.4577104595	-2.4795578366
C	17.4698374977	9.0704803179	6.9403767861	F	-37.5220038787	2.3182459959	-2.8789698967
C	16.563070669	9.9738174073	7.4705266801	C	0.5033361137	4.9872307782	8.3138928233
H	15.4057566069	11.7849062563	7.2058362041	C	1.5630893789	4.2241883303	9.028511197
H	17.7747544141	8.2240925429	7.546612067	C	2.7697333885	4.4058738465	8.1724858735
N	19.0035751383	9.5638192218	3.2733183493	C	2.5049951556	5.4410022169	7.2112180953
N	19.4172721027	6.6554771413	6.1009537886	C	-0.6293333929	0.5396453966	1.6756642597
F	16.0897994062	9.7726844866	8.7072704437	C	-1.2469164836	-0.311968748	2.6675574842
F	16.1885558811	12.3636619771	4.8319288339	C	-0.2313397229	-1.2016579807	3.1871280397
F	22.8999694194	7.6477759992	8.3531371593	C	1.0138721355	-0.8960702831	2.5172806799
F	23.2307081227	11.4905141781	5.7332134161	C	0.7663444659	0.1790121243	1.5832513929
C	10.7572107798	3.4616934638	-0.391106348	C	1.113280548	5.7993730308	7.3010882338
C	9.9675814088	4.338718062	0.400812355	C	-0.7726011407	4.4962291177	8.1021858481
C	7.9555052685	3.4580195461	-0.5374826409	C	1.1882153025	2.6931524145	9.3580483008
C	8.7427358496	2.5722641423	-1.3208430802	C	3.6020238454	3.362536291	7.8048456421
C	10.1291957321	2.5524856239	-1.2553719258	C	3.1432222367	5.4567837628	5.9679142259
C	12.1531717948	3.6502381286	-0.154930467	C	-1.0037658237	1.8801756612	1.5876817364
H	12.9181759821	3.0660298775	-0.6531673434	C	-2.2115681279	0.2115492073	3.5245849998
C	6.562850568	3.285132445	-0.785228311	C	-0.2256610526	-1.5309987878	4.5392714304
S	7.7543106159	1.5582878345	-2.334465406	C	2.2100938138	-0.9326052159	3.2294182837
H	5.7976003389	3.8737637617	-0.2904258872	C	1.7278576647	1.1733376456	1.405502809
S	10.961581094	5.3661114008	1.3923922785	C	0.4112713203	6.1628811708	6.1492142716
C	8.5810029342	4.3476446547	0.3495565126	C	-1.1080177253	3.1096211063	8.4083207599
C	12.42568331	4.6171266303	0.7712805254	C	2.095397115	1.6699078718	8.7776174838
O	7.8538343811	5.2169030084	1.1110981313	C	4.2392942307	3.3552150396	6.5147617592
O	10.8585914699	1.6969573115	-2.0329552245	C	2.4076362983	5.8096239561	4.7782110022
C	7.4038107345	4.6660824543	2.3440015628	C	-1.9971882558	2.4174704567	2.4834993185
H	6.834217772	5.4523460386	2.8431385932	C	-2.1953526251	-0.1263198303	4.9269807044
H	6.7547550361	3.7971946331	2.1788302529	C	1.0163877776	-1.5618637753	5.274257915
H	8.2502356623	4.3695670723	2.9756775364	C	3.1965207533	0.1040243473	3.0461415327
C	11.1480928297	0.4566874265	-1.3998710442	C	1.3338943877	2.5570289029	1.3186705401
H	11.718903083	-0.1312962533	-2.121401905	C	-0.0037222371	2.9029724465	1.4093664179
H	11.7467206702	0.6061584946	-0.4923662173	C	-2.5882484201	1.6013193929	3.432716928
H	10.2275796796	-0.0801277214	-1.1393447947	C	-1.2256594848	-0.9827494703	5.4237502452
S	-0.5937456536	-1.6874397767	-1.7838009751	C	2.2084494015	-1.2663242771	4.6325296263
C	-1.8618650602	1.8684543558	-2.0088981008	C	2.9595185637	1.134609574	2.1522447987
C	0.3617018551	2.8516230322	-2.412661159	C	1.0702414733	6.1554475856	4.8666453094
C	-1.0458968658	2.9486297719	-2.2469363132	C	-1.4870356196	4.8376598384	6.8994775889
C	-1.1879775238	0.6030494678	-1.9727648703	C	-0.1582438182	2.2529512976	8.9164245679
C	0.2454623144	0.5051156766	-2.1349178047	C	3.2598779903	1.978161193	8.1108029825
C	1.055625909	1.6663654404	-2.363600978	C	4.0274649175	4.3889113183	5.615047302

N	0.7020237754	-0.7402288075	-2.0363793233	C	-0.9149717152	5.6673614966	5.9461540424
N	-1.7777064775	-0.573902323	-1.7828549337	C	-2.0277322651	2.6392049597	7.4005362651
C	6.2927302904	2.3092491359	-1.7059416973	C	1.3087263618	0.5643341106	8.3057335761
C	2.5020653465	1.5889172087	-2.473948618	C	4.3144798031	1.9978379009	6.0375463302
C	3.2590534258	0.6643434865	-3.1473534146	C	2.8606699009	4.9735161731	3.6924376437
C	4.6503894291	0.8308495512	-2.9654804636	C	-1.6194546124	3.7678222774	2.8337904287
C	4.9904338281	1.8813128575	-2.1497871903	C	-2.5811884861	1.0397754996	5.685641641
S	3.5475276539	2.6899632281	-1.6228049799	C	0.775989103	-1.0529295058	6.6020000559
C	-11.4553595328	4.7021973984	-3.2429332473	C	3.8104410656	0.3875295088	4.3220882363
C	-10.647634777	5.5314184873	-4.0669161591	C	2.3300111808	3.3661467016	1.9847202928
C	-8.6649897921	4.4287442206	-3.3172358044	C	-0.3928991621	4.0703149072	2.1675334092
C	-9.4724592629	3.5992773303	-2.493043446	C	-2.8227709413	2.1050230952	4.7658157509
C	-10.8550459667	3.7119223257	-2.449957671	C	-0.6051560365	-0.6968902722	6.6939742884
C	-12.8366422789	5.0357908213	-3.3521518255	C	3.2015936522	-0.458142873	5.2987095349
H	-13.6110632821	4.5353981644	-2.7806294255	C	3.3307241474	2.4867857072	2.5009048893
C	-7.2795074941	4.12648722	-3.1740308823	C	0.1377160447	5.678645964	3.8735789899
S	-8.5109572806	2.4829375706	-1.5659490337	C	-2.2678000554	3.7018734134	6.478861796
H	-6.4997999922	4.670731038	-3.6961245264	C	-0.0694900509	0.9215614028	8.3932286347
S	-11.6012168153	6.6945848892	-4.9423685148	C	3.7072435996	1.1541097293	7.0150149858
C	-9.2671026959	5.4052011789	-4.1256053718	C	3.8601741769	4.0934224526	4.2097521755
C	-13.0780691052	6.0667088905	-4.2201900091	C	-1.0874096945	5.3726864338	4.5417247638
O	-8.5162498285	6.2303307947	-4.9132025387	C	-2.0509984962	1.2886268982	6.9751608322
O	-11.6060965479	2.9130448544	-1.6355845417	C	1.7685138413	-0.3307792568	7.3056859291
C	-8.2746482547	5.7162374857	-6.2177756661	C	4.2565043729	1.6893106122	4.6557047666
H	-7.6762930374	6.466881414	-6.7376047778	C	1.9840592026	4.5624344145	2.6570033755
H	-7.719801755	4.7705654544	-6.1736249959	C	0.56890821	4.9286558054	2.7511561003
H	-9.2140139741	5.5577091421	-6.761600709	C	-2.537914457	3.4485806992	5.1107665861
C	-12.0299843737	1.7026043713	-2.2515856802	C	-1.0270289124	0.3926799611	7.4904927812
H	-12.6065223837	1.1607488728	-1.4994106871	C	3.0233167398	-0.0256472362	6.6354972745
H	-12.6633145939	1.9049171044	-3.1245810539	C	4.0143984446	2.7785877662	3.7067781869
H	-11.1721304604	1.0935830626	-2.5619981453	C	-1.9194283532	4.3146045164	4.1049456962
C	-7.0349388218	3.111607517	-2.2885391124	C	1.4516282981	3.714798987	10.4428474527
C	-3.2937254314	1.987894487	-1.7943013004	C	0.237001662	4.1816442952	11.212902136
C	-4.0674025572	1.3350801867	-0.867937919	C	2.6206468221	3.6404610913	11.435927006
C	-5.4413888618	1.6514143382	-0.9532636729	C	-0.0133299577	5.5461726807	11.3714094911
C	-5.7521050735	2.5591085868	-1.9348092177	C	-0.5782028807	3.26241359	11.8761884486
S	-4.3007338184	3.0181847962	-2.7714638973	H	2.6800887047	4.6430840023	11.8829873851
S	-19.9145568641	7.8808140422	-8.0597781635	H	2.2689811662	2.9872527761	12.2471125643
C	-21.2229969466	7.1292720752	-4.5910082627	C	4.0256071994	3.203036906	11.037902475
C	-18.9876231991	6.7905953573	-3.6067601002	C	-1.0671619837	5.9843811315	12.1679736579
C	-20.40560856	6.7912463576	-3.5382049101	H	0.6186208616	6.2700647202	10.8623680962
C	-20.5289236319	7.4284826068	-5.8110618834	C	-1.6326579465	3.6984783647	12.6731246756
C	-19.0844070301	7.4267074425	-5.8815243525	H	-0.3888551563	2.1975996328	11.7629250635
C	-18.2753263824	7.1275369896	-4.7339791544	H	4.0268203728	2.1881459901	10.631998622

N	-18.6182911477	7.6667446806	-7.1039517834	H	4.4399199605	3.8494682784	10.2598575954
N	-21.1118129301	7.6706720735	-6.981853187	C	4.9448311479	3.2463283933	12.2515151457
C	-16.8249757693	7.1456745489	-4.7829972529	C	-1.8808833489	5.0609128993	12.8191599114
C	-16.0127257428	8.0238042252	-5.4573607332	H	-1.2535812844	7.0492379276	12.2771881738
C	-14.6368349562	7.7309521094	-5.3373004535	H	-2.2625076789	2.9715479803	13.1786071432
C	-14.3576771675	6.6336484552	-4.5612912267	H	4.99257966	4.2546157198	12.6841839842
S	-15.8443944218	5.9528573807	-3.9748906201	H	4.5743423378	2.5997863884	13.0586967972
C	-30.6601724802	4.3711582601	-2.3620269262	C	6.3522489787	2.8140106725	11.920629602
C	-29.7789682487	3.469704949	-1.7064111408	H	-2.7063612112	5.4018191441	13.4379150614
C	-27.874977058	4.6474244702	-2.541761146	O	6.7379681339	2.4473855209	10.8358196894
C	-28.756356268	5.5515429947	-3.1934968767	O	7.1429468664	2.8861240461	13.0039796954
C	-30.1367100704	5.4389765512	-3.1073937068	C	8.4958659525	2.4933749814	12.7866209039
C	-32.0253520845	4.0191602261	-2.1544084513	H	8.5467652653	1.4545345615	12.4492415111
H	-32.8495022	4.569684671	-2.5954228194	H	8.9663501982	3.1307193206	12.0329616136
C	-26.5095417788	4.9666244332	-2.7958675537	H	8.9951524341	2.6075468244	13.7490584436
S	-27.8876724592	6.7611602821	-4.0942518874	F	-44.9159651232	2.2323386917	0.8455848636
H	-25.6846631459	4.380283147	-2.4052896988	F	-42.2332624845	2.6602329948	1.4613288069
S	-30.647898801	2.2218322377	-0.8594015965	F	-35.3439291847	-0.2681875127	0.6085739185
C	-28.3986767392	3.5959271697	-1.7735355684	F	-32.662108147	0.4091389202	0.2717355451
C	-32.1855923144	2.9059883138	-1.3738212859	F	-25.8749092551	8.5105177588	-5.3166374465
O	-27.5763016241	2.7027619302	-1.1480688028	F	-23.1918054575	9.1042106415	-5.7806537104
O	-30.9588632663	6.3120741806	-3.760633789	F	-16.4255913598	9.0854490631	-6.1302173368
C	-27.2149208519	3.0841407754	0.1743210192	F	-13.7132982212	8.4864030187	-5.9251308111
H	-26.5701947714	2.2908181536	0.5573415661	F	-6.3313732517	1.1112607195	-0.1252322303
H	-26.6674050295	4.0350848952	0.1755579182	F	-3.6135979711	0.5161071634	0.0690347632
H	-28.0996931968	3.1768087724	0.8160230405	F	2.7792929007	-0.2907341328	-3.9284153623
C	-31.3369128544	7.4392913436	-2.9788411314	F	5.5302920267	0.0196681854	-3.5475204034