Table S10. Cartesian coordinates (Angstroms) of the optimized $(BGA\text{-}12)_6$/PHEAA SP-DN eutectogels.

Atom	X	Y	Z	Atom	X	Y	Z
C(1)	14.7648	0.5923	-3.9103	**H(350)**	11.4212	-2.9316	2.4013
O(2)	14.0835	-0.4208	-3.9618	**H(351)**	11.5649	-1.747	1.0598
N(3)	14.2708	1.8013	-4.3074	**C(352)**	10.2643	-1.1106	2.7191
H(4)	14.7681	2.6831	-4.1506	**H(353)**	10.2737	-1.1594	3.8263
C(5)	12.9102	1.8704	-4.8463	**H(354)**	10.3035	-0.0331	2.4725
H(6)	12.7698	1.0482	-5.5893	**C(355)**	9.0094	-1.7764	2.1621
H(7)	12.794	2.8327	-5.3897	**H(356)**	8.9539	-1.6299	1.0665
C(8)	11.8568	1.7442	-3.7295	**H(357)**	9.0674	-2.8732	2.3237
H(9)	12.0264	0.8103	-3.1558	**C(358)**	7.7466	-1.2359	2.8373
H(10)	11.9779	2.5649	-2.9959	**H(359)**	7.6689	-0.1414	2.7018
C(11)	10.4605	1.7401	-4.3547	**H(360)**	7.7981	-1.3986	3.9299
H(12)	10.3507	2.587	-5.0581	**C(361)**	6.5223	-1.9425	2.2506
H(13)	10.3267	0.8266	-4.9672	**H(362)**	6.4566	-1.739	1.1637
C(14)	9.3701	1.8083	-3.2819	**H(363)**	6.637	-3.0401	2.3508
H(15)	9.5556	2.6612	-2.5999	**C(364)**	5.2346	-1.4989	2.9477
H(16)	9.3985	0.8978	-2.6512	**H(365)**	5.1508	-0.3959	2.9428
C(17)	7.99	1.9494	-3.9355	**H(366)**	5.2547	-1.7917	4.0132
H(18)	7.9682	2.8376	-4.5936	**C(367)**	4.0306	-2.1291	2.2428
H(19)	7.7902	1.0834	-4.5938	**H(368)**	4.0022	-1.8016	1.1846
C(20)	6.8993	2.0592	-2.8668	**H(369)**	4.1403	-3.231	2.2183
H(21)	7.1571	2.8555	-2.14	**C(370)**	2.723	-1.7575	2.9454
H(22)	6.846	1.1184	-2.2831	**H(371)**	2.6736	-0.6663	3.1201
C(23)	5.5359	2.3593	-3.4993	**H(372)**	2.6846	-2.2209	3.9482
H(24)	5.5734	3.3141	-4.0546	**C(373)**	1.5319	-2.2147	2.0992
H(25)	5.28	1.5856	-4.2465	**H(374)**	1.5449	-1.702	1.1174
C(26)	4.4616	2.4179	-2.4099	**H(375)**	1.6159	-3.2968	1.8764
H(27)	4.7764	3.1123	-1.6052	**C(376)**	0.2128	-1.9412	2.8268
H(28)	4.3611	1.4222	-1.9316	**H(377)**	0.1822	-0.9044	3.21
C(29)	3.108	2.864	-2.9725	**H(378)**	0.1394	-2.5912	3.7195
H(30)	3.1811	3.8852	-3.3876	**C(379)**	-0.9662	-2.1937	1.886
H(31)	2.8066	2.2153	-3.8157	**H(380)**	-1.0338	-1.4071	1.1139
C(32)	2.0571	2.8078	-1.8596	**H(381)**	-0.8239	-3.1461	1.3331
H(33)	2.4188	3.3634	-0.9706	**C(382)**	-2.2685	-2.2601	2.7013
H(34)	1.9244	1.7541	-1.5353	**H(383)**	-2.3864	-1.3456	3.3245
C(35)	0.7164	3.3814	-2.3156	**H(384)**	-2.2286	-3.1327	3.3949
H(36)	0.8129	4.4426	-2.6024	**N(385)**	-3.4418	-2.3841	1.8291
H(37)	0.3463	2.8542	-3.2182	**C(386)**	-3.6721	-3.5755	1.2039
C(38)	-0.3034	3.2162	-1.1744	**H(387)**	-4.1437	-1.6425	1.9003
H(39)	0.0704	3.6886	-0.2383	**O(388)**	-2.8288	-4.4524	1.1291
H(40)	-0.4493	2.1247	-0.9708	**C(389)**	-5.0458	-3.7881	0.5544
N(41)	-1.5838	3.8278	-1.529	**C(390)**	-5.5672	-5.149	1.051
C(42)	-2.4478	3.1609	-2.3371	**H(391)**	-4.9763	-3.7435	-0.561
H(43)	-1.8631	4.6777	-1.0271	**C(392)**	-7.0172	-5.4815	0.6186
O(44)	-2.2162	2.0361	-2.7636	**H(393)**	-4.874	-5.9569	0.7042
C(45)	-3.7451	3.8728	-2.7272	**C(394)**	-7.9826	-5.5706	1.824
C(46)	-4.9176	3.0935	-2.1003	**H(395)**	-7.041	-6.4363	0.0323
H(47)	-3.8245	3.9304	-3.8386	**H(396)**	-7.8332	-4.737	2.5462

C(48)	-6.2504	3.4134	-2.8059	**C(397)**	-9.4567	-5.6642	1.4145
H(49)	-4.7169	1.9946	-2.1121	**H(398)**	-9.798	-6.7156	1.3341
C(50)	-7.4393	2.8594	-1.9904	**H(399)**	-9.6965	-5.1648	0.4606
H(51)	-6.244	3	-3.8414	**O(400)**	-10.2187	-5.0974	2.4679
H(52)	-7.5247	3.3874	-1.0105	**H(401)**	-10.5589	-4.203	2.2126
C(53)	-8.7625	2.9399	-2.7544	**O(402)**	-7.587	-6.769	2.4796
H(54)	-8.8068	2.241	-3.6084	**H(403)**	-8.2205	-6.9865	3.1913
H(55)	-8.967	3.9708	-3.1071	**O(404)**	-7.5125	-4.5535	-0.3024
O(56)	-9.8301	2.6683	-1.8739	**H(405)**	-7.4469	-3.62	0.0117
H(57)	-9.7336	1.7944	-1.4385	**O(406)**	-5.4613	-5.0446	2.4558
O(58)	-7.1182	1.5028	-1.7858	**H(407)**	-5.7018	-5.9001	2.8816
H(59)	-7.5842	1.1227	-0.9937	**O(408)**	-5.9037	-2.7215	0.8825
O(60)	-6.5069	4.79	-2.9336	**H(409)**	-6.3482	-2.8602	1.7573
H(61)	-5.7259	5.3151	-2.6311	**C(410)**	14.3192	-0.9929	4.6025
O(62)	-4.9338	3.5115	-0.754	**C(411)**	15.6378	-1.2489	3.8392
H(63)	-5.5982	2.9639	-0.2436	**H(412)**	14.4129	-1.3049	5.6736
O(64)	-3.7571	5.2113	-2.3142	**C(413)**	16.8417	-0.9398	4.752
H(65)	-3.6423	5.2595	-1.3201	**H(414)**	15.6901	-2.3007	3.465
C(66)	16.1949	0.5982	-3.3583	**C(415)**	18.1633	-0.8374	3.9618
C(67)	16.8721	-0.7778	-3.469	**H(416)**	16.9139	-1.7051	5.5597
H(68)	16.1692	0.9607	-2.3007	**H(417)**	18.0508	-0.1481	3.09
C(69)	18.1515	-0.9066	-2.5976	**C(418)**	19.3261	-0.3937	4.8653
H(70)	16.1468	-1.5894	-3.1917	**H(419)**	20.3089	-0.6394	4.4179
C(71)	19.4016	-1.3193	-3.407	**H(420)**	19.2638	-0.817	5.8819
H(72)	17.9609	-1.6216	-1.7619	**O(421)**	19.3278	1.0185	4.9437
H(73)	19.5771	-0.6097	-4.2484	**H(422)**	18.4589	1.3191	5.3154
C(74)	20.6538	-1.4365	-2.5166	**O(423)**	14.0428	0.3775	4.6943
H(75)	20.765	-0.5823	-1.8309	**H(424)**	13.6781	0.7496	3.8448
H(76)	21.5653	-1.5374	-3.1378	**O(425)**	15.6152	-0.3629	2.7441
O(77)	20.5814	-2.6621	-1.8215	**H(426)**	16.1526	-0.7288	1.999
H(78)	20.4129	-2.5449	-0.8607	**O(427)**	16.7227	0.3001	5.414
O(79)	16.9114	1.5779	-4.0858	**H(428)**	15.8529	0.7291	5.2001
H(80)	17.2656	1.1858	-4.9241	**O(429)**	18.4633	-2.0734	3.3657
O(81)	17.1639	-0.8903	-4.8459	**H(430)**	18.6851	-2.7935	4.0138
H(82)	17.5772	-1.7637	-5.0409	**C(431)**	12.4106	-5.9601	2.1108
O(83)	18.504	0.3517	-2.0512	**O(432)**	12.2319	-7.1258	2.4186
H(84)	18.2699	0.3761	-1.0921	**N(433)**	11.6962	-5.3087	1.1536
O(85)	19.143	-2.5498	-4.0432	**H(434)**	11.9468	-4.356	0.8571
H(86)	19.3403	-3.3005	-3.4378	**C(435)**	10.6165	-5.947	0.3956
C(87)	13.4857	-2.4297	-0.821	**H(436)**	10.5108	-7.0163	0.686
O(88)	12.8392	-3.3738	-0.3653	**H(437)**	10.8746	-5.9229	-0.6874
N(89)	13.0437	-1.665	-1.8381	**C(438)**	9.3052	-5.1792	0.661
H(90)	13.6809	-0.992	-2.2962	**H(439)**	8.975	-5.3718	1.6999
C(91)	11.8117	-2.0278	-2.5493	**H(440)**	9.4909	-4.089	0.595
H(92)	11.8303	-3.1096	-2.8163	**C(441)**	8.2115	-5.5765	-0.3355
H(93)	11.7794	-1.4553	-3.5044	**H(442)**	8.4498	-5.1781	-1.3392
C(94)	10.58	-1.7243	-1.6773	**H(443)**	8.1688	-6.6758	-0.4461
H(95)	10.5761	-2.4025	-0.7991	**C(444)**	6.8496	-5.0477	0.137
H(96)	10.6477	-0.698	-1.2744	**H(445)**	6.9313	-3.9763	0.4025
C(97)	9.2934	-1.901	-2.4858	**H(446)**	6.5513	-5.5701	1.0659
H(98)	9.2804	-1.204	-3.3452	**C(447)**	5.769	-5.2285	-0.937
H(99)	9.2517	-2.9166	-2.9223	**H(448)**	5.9614	-4.5458	-1.7855
C(100)	8.0691	-1.667	-1.5927	**H(449)**	5.8115	-6.2506	-1.3558
H(101)	8.1682	-0.7074	-1.0508	**C(450)**	4.3758	-4.9652	-0.349

H(102)	8.0155	-2.4572	-0.8174	**H(451)**	4.3634	-3.9943	0.1808
C(103)	6.7806	-1.6641	-2.4217	**H(452)**	4.1445	-5.731	0.4155
H(104)	6.8248	-0.8712	-3.1923	**C(453)**	3.2977	-4.9722	-1.4408
H(105)	6.6826	-2.6148	-2.9779	**H(454)**	3.4282	-4.1006	-2.1089
C(106)	5.5592	-1.4571	-1.5186	**H(455)**	3.4132	-5.8645	-2.0831
H(107)	5.6932	-0.5559	-0.8916	**C(456)**	1.8951	-4.9582	-0.8184
H(108)	5.4641	-2.3093	-0.8166	**H(457)**	1.7903	-4.103	-0.1252
C(109)	4.2833	-1.327	-2.3565	**H(458)**	1.7552	-5.8655	-0.2002
H(110)	4.3508	-0.4417	-3.0171	**C(459)**	0.8048	-4.8866	-1.8979
H(111)	4.1847	-2.1959	-3.0342	**H(460)**	0.7484	-3.8643	-2.3154
C(112)	3.0475	-1.2243	-1.4554	**H(461)**	1.0617	-5.5467	-2.7464
H(113)	3.161	-0.3884	-0.7409	**C(462)**	-0.5524	-5.2972	-1.3151
H(114)	2.9523	-2.1426	-0.842	**H(463)**	-0.8064	-4.6646	-0.4387
C(115)	1.785	-1.029	-2.3016	**H(464)**	-0.4944	-6.3311	-0.9251
H(116)	1.8499	-0.0807	-2.8682	**C(465)**	-1.6718	-5.191	-2.3583
H(117)	1.7124	-1.8279	-3.064	**H(466)**	-1.8884	-4.1259	-2.5706
C(118)	0.5291	-1.0347	-1.4226	**H(467)**	-1.3677	-5.6368	-3.3195
H(119)	0.6046	-0.254	-0.6435	**C(468)**	-2.9294	-5.8998	-1.8196
H(120)	0.4443	-2.0016	-0.8854	**H(469)**	-3.0336	-5.6957	-0.7231
C(121)	-0.7142	-0.8074	-2.283	**H(470)**	-2.8264	-7.0014	-1.9349
H(122)	-0.6183	0.1319	-2.8649	**N(471)**	-4.1576	-5.4319	-2.4685
H(123)	-0.8211	-1.6168	-3.0298	**C(472)**	-4.9231	-6.2663	-3.2344
C(124)	-1.9756	-0.7471	-1.4061	**H(473)**	-4.3235	-4.4113	-2.4672
H(125)	-1.888	0.0674	-0.6514	**O(474)**	-4.6045	-7.398	-3.5452
H(126)	-2.1133	-1.7048	-0.8475	**C(475)**	-6.2648	-5.6652	-3.6918
N(127)	-3.1589	-0.464	-2.225	**C(476)**	-7.4014	-6.6969	-3.6005
C(128)	-3.9413	-1.4821	-2.6673	**H(477)**	-6.174	-5.2663	-4.7297
H(129)	-3.1858	0.4665	-2.6802	**C(478)**	-8.7993	-6.0585	-3.8694
O(130)	-3.771	-2.6508	-2.3383	**H(479)**	-7.2106	-7.532	-4.3123
C(131)	-5.1578	-1.1119	-3.5308	**C(480)**	-9.6747	-6.0294	-2.5936
C(132)	-6.3846	-1.6484	-2.776	**H(481)**	-9.3201	-6.6041	-4.6875
H(133)	-5.0658	-1.5393	-4.5521	**H(482)**	-9.0823	-5.712	-1.697
C(134)	-7.7307	-1.389	-3.4659	**C(483)**	-10.9135	-5.127	-2.7081
H(135)	-6.2605	-2.7472	-2.6015	**H(484)**	-11.8408	-5.7211	-2.8058
C(136)	-8.8846	-1.6373	-2.4606	**H(485)**	-10.8695	-4.3879	-3.5251
H(137)	-7.8296	-2.03	-4.3721	**O(486)**	-10.9213	-4.4364	-1.4707
H(138)	-8.8362	-0.9312	-1.6009	**H(487)**	-11.7025	-3.8413	-1.3566
C(139)	-10.2391	-1.5398	-3.1683	**O(488)**	-10.0855	-7.3739	-2.4255
H(140)	-10.3956	-2.3821	-3.8696	**H(489)**	-10.6013	-7.4796	-1.5888
H(141)	-10.3494	-0.5832	-3.708	**O(490)**	-8.6673	-4.7632	-4.387
O(142)	-11.2776	-1.7004	-2.2287	**H(491)**	-8.3568	-4.1329	-3.6751
H(143)	-11.4088	-0.8944	-1.6783	**O(492)**	-7.3154	-7.2202	-2.2937
O(144)	-8.6402	-2.9279	-1.9607	**H(493)**	-8.0542	-7.8526	-2.1324
H(145)	-9.4838	-3.4005	-1.7202	**O(494)**	-6.5424	-4.5344	-2.9204
O(146)	-7.8721	-0.0861	-3.9568	**H(495)**	-6.8609	-4.7597	-2.0034
H(147)	-7.6241	0.5607	-3.2464	**C(496)**	13.4268	-5.105	2.8841
O(148)	-6.3896	-0.9904	-1.5238	**C(497)**	14.7755	-5.8347	3.0397
H(149)	-6.1368	-1.6245	-0.8114	**H(498)**	12.9603	-4.8674	3.8813
O(150)	-5.1741	0.2754	-3.7202	**C(499)**	15.5576	-5.3884	4.305
H(151)	-5.7539	0.6973	-3.0368	**H(500)**	14.6197	-6.9396	3.0781
C(152)	14.8298	-2.0986	-0.17	**C(501)**	17.0579	-5.1575	4.0009
C(153)	15.7424	-3.3252	-0.375	**H(502)**	15.4227	-6.1555	5.1032
H(154)	14.6732	-1.8897	0.9199	**H(503)**	17.1848	-4.3542	3.2316
C(155)	16.9325	-3.3164	0.5986	**C(504)**	17.8377	-4.8293	5.2783

H(156)	15.1687	-4.278	-0.2217	**H(505)**	18.0083	-5.7149	5.9118
C(157)	18.1672	-3.9991	-0.0188	**H(506)**	17.3596	-4.0346	5.8868
H(158)	16.6347	-3.7873	1.5678	**O(507)**	19.0901	-4.2601	4.9372
H(159)	18.4965	-3.4524	-0.9331	**H(508)**	19.6076	-4.8789	4.3763
C(160)	19.3299	-4.153	0.9764	**O(509)**	13.6386	-3.8504	2.3075
H(161)	20.0979	-4.8509	0.5903	**H(510)**	13.7364	-3.9143	1.3223
H(162)	18.9947	-4.504	1.967	**O(511)**	15.4802	-5.5219	1.8608
O(163)	20.0123	-2.9203	1.0776	**H(512)**	16.2448	-6.128	1.7255
H(164)	19.6405	-2.3911	1.8184	**O(513)**	15.1798	-4.1758	4.8963
O(165)	15.3143	-0.9386	-0.7945	**H(514)**	14.2741	-3.845	4.651
H(166)	16.1833	-0.6861	-0.3975	**O(515)**	17.6322	-6.285	3.379
O(167)	16.1744	-3.2717	-1.7151	**H(516)**	17.5309	-7.0938	3.9173
H(168)	16.4433	-4.1714	-2.0091	**C(517)**	-10.6875	6.671	-0.7727
O(169)	17.267	-1.9654	0.8471	**C(518)**	-12.0446	5.9639	-0.6252
H(170)	17.7763	-1.9196	1.6869	**H(519)**	-9.8508	5.9454	-0.6474
O(171)	17.7008	-5.2848	-0.389	**H(520)**	-10.6046	7.0558	-1.8111
H(172)	18.4167	-5.8082	-0.8021	**C(521)**	-11.999	4.5934	-1.321
C(173)	13.338	5.2366	-2.3297	**H(522)**	-12.8095	6.6226	-1.1096
O(174)	12.9996	4.4019	-1.4981	**C(523)**	-13.3819	4.0624	-1.7356
N(175)	12.5215	5.7375	-3.2852	**H(524)**	-11.3464	4.6516	-2.2212
H(176)	12.9089	6.4332	-3.9291	**H(525)**	-11.5144	3.8503	-0.6487
C(177)	11.1287	5.317	-3.4495	**C(526)**	-13.2455	2.7471	-2.5239
H(178)	11.1016	4.2397	-3.7429	**C(527)**	-13.9279	1.5836	-1.7936
H(179)	10.6876	5.8975	-4.2901	**H(528)**	-12.1721	2.5069	-2.7024
C(180)	10.3075	5.5218	-2.1647	**H(529)**	-13.6757	2.8573	-3.541
H(181)	10.5588	4.734	-1.4257	**C(530)**	-13.9839	0.3101	-2.6462
H(182)	10.5815	6.4754	-1.677	**H(531)**	-14.9779	1.8831	-1.5378
C(183)	8.815	5.497	-2.4995	**C(532)**	-14.7207	-0.7949	-1.8652
H(184)	8.546	6.39	-3.0949	**H(533)**	-14.5003	0.5099	-3.6078
H(185)	8.575	4.6237	-3.1385	**H(534)**	-12.9603	-0.0235	-2.9129
C(186)	7.9687	5.4441	-1.2225	**C(535)**	-14.5977	-2.1554	-2.5532
H(187)	8.3035	6.2176	-0.5067	**C(536)**	-14.9644	-3.3341	-1.6262
H(188)	8.1144	4.4733	-0.7098	**H(537)**	-13.5468	-2.2817	-2.9037
C(189)	6.4893	5.6506	-1.5658	**H(538)**	-15.2351	-2.182	-3.4605
H(190)	6.3457	6.6484	-2.0212	**C(539)**	-14.4897	-4.6467	-2.2734
H(191)	6.169	4.9205	-2.3349	**H(540)**	-16.0726	-3.3691	-1.4867
C(192)	5.6105	5.5118	-0.3185	**C(541)**	-14.4405	-5.8154	-1.2825
H(193)	5.9941	6.1569	0.4932	**H(542)**	-15.1636	-4.8987	-3.1201
H(194)	5.6604	4.4748	0.0674	**H(543)**	-13.4784	-4.4995	-2.7084
C(195)	4.1615	5.8864	-0.6487	**C(544)**	-13.9364	-7.1021	-1.9527
H(196)	4.1198	6.923	-1.0325	**H(545)**	-12.9372	-6.9266	-2.4148
H(197)	3.7793	5.2462	-1.4682	**H(546)**	-14.6189	-7.3925	-2.7785
C(198)	3.2649	5.7472	0.5861	**C(547)**	-12.3966	5.7274	0.8356
H(199)	3.6998	6.3026	1.4373	**O(548)**	-11.5821	5.3268	1.6498
H(200)	3.2222	4.687	0.904	**N(549)**	-13.7204	5.9068	1.1701
C(201)	1.856	6.2681	0.2812	**H(550)**	-14.3315	6.4766	0.5673
H(202)	1.906	7.3226	-0.0488	**C(551)**	-14.1802	5.7334	2.5526
H(203)	1.4209	5.7063	-0.5691	**H(552)**	-13.3214	5.6044	3.2598
C(204)	0.9509	6.1444	1.5122	**H(553)**	-14.749	4.7751	2.611
H(205)	1.4203	6.6378	2.383	**C(554)**	-15.0461	6.9253	2.9956
H(206)	0.8452	5.0767	1.7881	**H(555)**	-14.9566	7.7943	2.3118
C(207)	-0.4212	6.7628	1.2277	**H(556)**	-16.1107	6.6575	3.0999
H(208)	-0.3432	7.859	1.1208	**O(557)**	-14.5841	7.445	4.2319
H(209)	-0.8066	6.3979	0.2542	**H(558)**	-14.7088	6.7885	4.9483

C(210)	-1.408	6.3994	2.352	**C(559)**	-13.1155	1.3045	-0.5372
H(211)	-1.1254	6.9069	3.299	**O(560)**	-12.0407	0.7437	-0.5445
H(212)	-1.3688	5.2983	2.5414	**N(561)**	-13.7268	1.6793	0.668
N(213)	-2.785	6.7671	2.009	**H(562)**	-14.5961	2.2506	0.6021
C(214)	-3.4595	6.0928	1.0478	**C(563)**	-14.2592	-3.1134	-0.2994
H(215)	-3.2479	7.5243	2.5045	**O(564)**	-13.0424	-3.2032	-0.1881
O(216)	-2.934	5.2048	0.3774	**N(565)**	-15.0171	-2.7324	0.7725
C(217)	-4.9404	6.4313	0.858	**H(566)**	-16.0395	-2.8697	0.8171
C(218)	-5.7558	5.3549	1.611	**C(567)**	-12.8459	2.0599	1.7872
H(219)	-5.2032	6.46	-0.2285	**H(568)**	-12.4441	3.0869	1.6095
C(220)	-7.1309	5.1611	0.9465	**H(569)**	-11.9648	1.3779	1.8277
H(221)	-5.2091	4.3793	1.6333	**C(570)**	-13.6369	2.0354	3.1083
C(222)	-8.1642	4.5135	1.8902	**H(571)**	-14.7277	2.1705	2.9577
H(223)	-7.0065	4.5754	-0.0044	**H(572)**	-13.4648	1.109	3.6828
H(224)	-8.6534	5.2712	2.5456	**C(573)**	-14.3763	-2.2707	2.0086
C(225)	-9.1863	3.7113	1.0818	**H(574)**	-13.3955	-1.7849	1.7751
H(226)	-8.729	2.8919	0.4982	**H(575)**	-14.1546	-3.1274	2.6842
H(227)	-9.7564	4.3551	0.3828	**C(576)**	-15.2869	-1.2525	2.7067
O(228)	-10.0406	3.0608	1.9991	**H(577)**	-16.3386	-1.5898	2.7924
H(229)	-10.7448	3.705	2.2637	**H(578)**	-14.9015	-0.9834	3.7071
O(230)	-7.4461	3.6248	2.7413	**O(579)**	-13.2949	3.1455	3.91
H(231)	-8.0685	2.9564	3.1316	**H(580)**	-12.3292	3.1799	4.068
O(232)	-7.6624	6.361	0.4786	**O(581)**	-15.3715	-0.0739	1.938
H(233)	-7.7451	7.0363	1.2085	**H(582)**	-14.4831	0.1878	1.5425
O(234)	-5.8526	5.8413	2.9286	**H(583)**	-13.9918	3.8954	-0.815
H(235)	-6.357	5.2036	3.4855	**H(584)**	-14.2508	-0.8542	-0.8499
O(236)	-5.1052	7.7314	1.3641	**H(585)**	-13.7308	-5.5567	-0.4529
H(237)	-5.9683	7.8245	1.8511	**C(586)**	-15.8486	-6.06	-0.7635
C(238)	14.7582	5.8244	-2.3229	**O(587)**	-16.8028	-6.2674	-1.4788
C(239)	15.7763	4.6762	-2.3844	**N(588)**	-15.9595	-6.1042	0.622
H(240)	14.9038	6.4491	-1.4093	**H(589)**	-15.2343	-5.6595	1.2081
C(241)	17.1802	5.1487	-1.9484	**C(590)**	-16.1784	-0.3654	-1.7682
H(242)	15.4352	3.8388	-1.72	**O(591)**	-16.8535	-0.0971	-2.7395
C(243)	18.2658	4.1414	-2.3864	**N(592)**	-16.6966	-0.2676	-0.4873
H(244)	17.194	5.3057	-0.8445	**H(593)**	-16.1105	-0.4443	0.3398
H(245)	18.4677	4.2127	-3.4772	**C(594)**	-14.0293	5.1317	-2.6028
C(246)	19.5549	4.2599	-1.5569	**O(595)**	-13.6617	5.4086	-3.7226
H(247)	19.3418	4.2907	-0.4713	**N(596)**	-15.0895	5.8095	-2.0114
H(248)	20.1653	5.1322	-1.8459	**H(597)**	-15.3402	5.6291	-1.0484
O(249)	20.393	3.1569	-1.8217	**C(598)**	-15.44	7.1446	-2.5102
H(250)	19.8828	2.3135	-1.7972	**H(599)**	-14.5756	7.5985	-3.0527
O(251)	14.8113	6.7052	-3.419	**H(600)**	-16.2614	7.0552	-3.2559
H(252)	15.6369	6.5499	-3.9448	**C(601)**	-15.8639	8.0349	-1.3293
O(253)	15.7539	4.2128	-3.7161	**H(602)**	-15.9933	9.0865	-1.6381
H(254)	16.3411	3.4156	-3.8112	**H(603)**	-16.7884	7.6745	-0.8399
O(255)	17.4133	6.3696	-2.6149	**O(604)**	-14.9055	7.9585	-0.2992
H(256)	18.1386	6.8699	-2.1929	**H(605)**	-14.0537	8.4196	-0.5408
O(257)	17.7198	2.8834	-2.0737	**C(606)**	-17.8553	0.5938	-0.2596
H(258)	18.0049	2.1643	-2.7136	**H(607)**	-18.6119	0.4392	-1.0657
C(259)	13.0728	2.1276	1.4133	**H(608)**	-18.3348	0.2965	0.6992
O(260)	12.6927	1.3674	2.3039	**C(609)**	-17.4318	2.0757	-0.2192
N(261)	12.3742	2.2942	0.268	**H(610)**	-16.9957	2.4066	-1.1813
H(262)	12.6849	2.9281	-0.4777	**H(611)**	-18.274	2.7348	0.055
C(263)	11.0869	1.6152	0.083	**O(612)**	-16.4167	2.319	0.7395

H(264)	11.1581	0.5709	0.476	**H(613)**	-16.314	1.5568	1.3543
H(265)	10.8873	1.5475	-1.0106	**C(614)**	-17.287	-6.1673	1.2335
C(266)	9.9465	2.3649	0.7989	**H(615)**	-17.1837	-6.6616	2.2271
H(267)	10.1442	2.3741	1.89	**H(616)**	-17.9654	-6.806	0.6183
H(268)	9.9301	3.4248	0.4884	**C(617)**	-17.8871	-4.7598	1.3845
C(269)	8.606	1.6887	0.4971	**H(618)**	-18.0953	-4.2909	0.403
H(270)	8.3909	1.746	-0.5873	**H(619)**	-18.8031	-4.7628	2.0006
H(271)	8.6667	0.6084	0.7421	**O(620)**	-16.9831	-3.8708	2.0162
C(272)	7.4558	2.3259	1.2903	**H(621)**	-16.2399	-4.3467	2.4488
H(273)	7.414	3.4138	1.0992	**C(622)**	-13.8378	-8.2488	-0.9359
H(274)	7.6399	2.2196	2.3756	**H(623)**	-14.8637	-8.4287	-0.5236
C(275)	6.1206	1.6694	0.9125	**C(624)**	-10.4865	7.8159	0.2297
H(276)	5.9208	1.8262	-0.1648	**H(625)**	-10.2226	7.3537	1.2209
H(277)	6.1895	0.5716	1.0509	**C(626)**	-9.3416	8.7315	-0.2281
C(278)	4.9526	2.2182	1.7445	**H(627)**	-8.4648	8.108	-0.5173
H(279)	4.9024	3.3188	1.6539	**H(628)**	-9.638	9.2591	-1.1597
H(280)	5.1214	2.0137	2.8174	**C(629)**	-13.3298	-9.5338	-1.6037
C(281)	3.6292	1.5891	1.2868	**H(630)**	-13.957	-9.7648	-2.4899
H(282)	3.4874	1.7724	0.2042	**H(631)**	-12.2972	-9.3805	-1.9868
H(283)	3.6778	0.4879	1.4026	**C(632)**	-8.9234	9.7712	0.8257
C(284)	2.4285	2.1392	2.0691	**H(633)**	-9.6921	10.582	0.8547
H(285)	2.3785	3.2388	1.9613	**C(634)**	-13.3463	-10.7342	-0.6378
H(286)	2.5591	1.9483	3.1494	**H(635)**	-12.6075	-10.5582	0.1819
C(287)	1.1226	1.4997	1.5743	**C(636)**	-12.9854	-12.0234	-1.3692
H(288)	1.0627	1.582	0.4726	**H(637)**	-12.962	-12.8793	-0.6839
H(289)	1.1291	0.4133	1.7924	**H(638)**	-13.7248	-12.2612	-2.1486
C(290)	-0.1074	2.1526	2.219	**H(639)**	-12.0018	-11.952	-1.8483
H(291)	-0.0868	3.2452	2.0422	**C(640)**	-7.563	10.3674	0.4652
H(292)	-0.0697	2.0221	3.3165	**H(641)**	-7.2547	11.1382	1.1799
C(293)	-1.4098	1.5592	1.6682	**H(642)**	-6.7743	9.5945	0.4692
H(294)	-1.4068	1.5672	0.5609	**H(643)**	-7.5727	10.819	-0.5327
H(295)	-1.5131	0.4949	1.964	**C(644)**	-12.8623	-7.8442	0.1596
C(296)	-2.6224	2.3535	2.1862	**O(645)**	-11.6749	-7.6854	-0.038
H(297)	-2.4407	3.4497	2.0876	**N(646)**	-13.3915	-7.7371	1.4388
H(298)	-2.7828	2.1356	3.2666	**H(647)**	-14.4184	-7.7214	1.5793
N(299)	-3.8491	2.0442	1.4394	**C(648)**	-14.7617	-10.8555	-0.0913
C(300)	-4.5809	0.9409	1.7501	**O(649)**	-15.6996	-11.289	-0.7207
H(301)	-4.0458	2.6331	0.6122	**N(650)**	-14.9476	-10.4027	1.2178
O(302)	-4.2167	0.114	2.5761	**H(651)**	-14.2035	-9.8879	1.6759
C(303)	-5.93	0.7672	1.04	**C(652)**	-11.7426	8.6583	0.3413
C(304)	-6.9153	-0.0617	1.8917	**O(653)**	-12.3364	9.1336	-0.6201
H(305)	-5.765	0.3233	0.0229	**N(654)**	-12.2093	8.8612	1.6129
C(306)	-8.0941	-0.5572	1.0381	**H(655)**	-11.76	8.4158	2.435
H(307)	-6.404	-0.9187	2.3921	**C(656)**	-8.7875	9.1206	2.1962
C(308)	-9.1194	-1.3671	1.8645	**O(657)**	-7.9374	8.2727	2.4443
H(309)	-7.7242	-1.1713	0.1744	**N(658)**	-9.6456	9.5507	3.1708
H(310)	-9.5763	-0.7679	2.6799	**H(659)**	-10.3977	10.2243	2.9692
C(311)	-10.1619	-1.948	0.9055	**C(660)**	-13.2327	9.8641	1.887
H(312)	-9.7306	-2.7073	0.2224	**H(661)**	-14.0836	9.7657	1.1714
H(313)	-10.6566	-1.1558	0.3096	**H(662)**	-13.6387	9.6895	2.9129
O(314)	-11.1363	-2.5924	1.7143	**C(663)**	-12.6471	11.2836	1.7776
H(315)	-11.886	-2.8678	1.1143	**H(664)**	-13.4338	12.0522	1.8538
O(316)	-8.3625	-2.4012	2.4638	**H(665)**	-12.0684	11.4169	0.8443
H(317)	-8.9428	-3.1655	2.687	**C(666)**	-16.3127	-10.0097	1.5958

O(318)	-8.7743	0.495	0.4065	**H(667)**	-16.9784	-10.9035	1.5297
H(319)	-9.0934	1.1679	1.0586	**H(668)**	-16.7184	-9.2663	0.8686
O(320)	-7.4617	0.79	2.8824	**C(669)**	-16.3204	-9.4282	3.0165
H(321)	-6.8841	0.7801	3.6758	**H(670)**	-17.2592	-8.8843	3.229
O(322)	-6.4892	2.0199	0.775	**H(671)**	-16.1549	-10.1989	3.7878
H(323)	-6.7854	2.4925	1.6131	**C(672)**	-9.7244	8.8548	4.4608
C(324)	14.3889	2.8808	1.6085	**H(673)**	-9.1248	9.4109	5.2151
C(325)	15.5447	2.0687	0.9712	**H(674)**	-9.2782	7.8304	4.3843
H(326)	14.5612	3.0473	2.7011	**C(675)**	-11.1909	8.7404	4.9145
C(327)	16.9016	2.4951	1.5619	**H(676)**	-11.2613	8.408	5.9649
H(328)	15.3821	0.9689	1.0962	**H(677)**	-11.7533	9.6829	4.7815
C(329)	18.0874	1.9013	0.7756	**C(678)**	-12.6255	-7.0701	2.4955
H(330)	16.9537	2.2264	2.6408	**H(679)**	-12.7717	-7.6277	3.4469
H(331)	18.0582	2.2635	-0.284	**H(680)**	-11.5256	-7.1095	2.2848
C(332)	19.4577	2.2374	1.3923	**C(681)**	-13.0692	-5.6105	2.6544
H(333)	19.4294	3.1598	1.9963	**H(682)**	-12.5943	-5.127	3.5284
H(334)	20.2374	2.3392	0.6088	**H(683)**	-12.8764	-5.0036	1.7466
O(335)	19.8986	1.1369	2.1481	**O(684)**	-14.4801	-5.5308	2.8423
H(336)	19.7108	1.2522	3.1129	**H(685)**	-14.8404	-6.3635	3.2145
O(337)	14.3373	4.1817	1.0921	**O(686)**	-15.3114	-8.4297	3.11
H(338)	14.0089	4.1987	0.1521	**H(687)**	-14.4917	-8.8091	3.4938
O(339)	15.417	2.2991	-0.4064	**O(688)**	-11.7611	11.4096	2.8853
H(340)	16.2826	2.4725	-0.8482	**H(689)**	-11.4509	12.3304	2.9777
O(341)	17.1125	3.8908	1.4583	**O(690)**	-11.7461	7.7332	4.0869
H(342)	16.2488	4.3604	1.3626	**H(691)**	-12.7269	7.6657	4.1952
O(343)	17.8746	0.5079	0.677				
H(344)	18.596	0.0114	1.1459				
C(345)	13.1604	-1.7585	3.9509				
O(346)	12.7127	-2.7524	4.5088				
N(347)	12.7239	-1.2961	2.7512				
H(348)	13.0445	-0.3929	2.3811				
C(349)	11.4987	-1.8419	2.1667				