Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information:
Strategic Design of a Small and Versatile Bicyclic Superorganic Base: A Density Functional Study

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B3LYP/6-311+G//B3LYP/6-31+G* SCF energies, B3LYP/6-31+G* zero point vibrational energies (ZPVE), and Cartesian coordinates for 1-7 and their monoprotonated ions**

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SCF ENERGY at B3LYP/6-311+G** = -502.66563au
ZPVE = 190.133 kcal/mol

atom	x	y	z
C1	-0.6951057180	-0.9178814080	-0.0841621238
C2	-0.7705503133	0.5005563685	-0.7407675674
C3	0.7137270750	0.5613615769	-0.2493687992
C4	0.8195527134	-0.9838380214	-0.4718131437
C5	-0.5847117829	-0.5278145422	1.4048208655
H6	-1.3960442910	-1.7158953596	-0.3403217352
N7	-1.0203601130	0.5855862578	-2.1667229275
H8	1.4380257218	1.2615904731	-0.6721139628
C9	0.4995608916	0.6068771791	1.2783819645
N10	1.1640652621	-1.4658836727	-1.7954410833
H11	-1.5338295526	-0.1605806559	1.8104733344
H12	-0.2493987862	-1.3631695268	2.0292676603
H13	1.4156015491	0.3783588389	1.8341469246
H14	0.1311984587	1.5813562080	1.6172978939
C15	-2.3777015743	0.1738058179	-2.4975526225
C16	-0.7478270425	1.9231820318	-2.6747487154
C17	2.5433986675	-1.1481285239	-2.1385551247
C18	0.9167899454	-2.8958489118	-1.9206796209
H19	-2.5215048603	0.2249805246	-3.5825889344
H20	-2.5482928363	-0.8599697807	-2.1831683962
H21	-3.1504413222	0.8127014278	-2.0185107203
H22	-0.9144330212	1.9445628447	-3.7575016107
H23	-1.3947800609	2.6993489879	-2.2123335892
H24	0.2952364530	2.1954118389	-2.4884169983
H25	2.7592053967	-1.5032882290	-3.1524095190
H26	2.6999652498	-0.0656921369	-2.1199711306
H27	3.2776685815	-1.6155119996	-1.4477790307
H28	1.1546728051	-3.2209389031	-2.9396574119
H29	1.5262246122	-3.5014413132	-1.2159048828
H30	-0.1382269212	-3.1168642392	-1.7336188930
H31	-1.4447414485	1.2011961608	-0.1998603937
H32	1.4489363716	-1.4965483527	0.2891151649

$7H^+$

SCF ENERGY at B3LYP/6-311+G** = -503.07733au
ZPVE = 198.854 kcal/mol

atom	x	y	z
C1	-0.6950180000	-0.9130460000	0.0190740000

C2	-0.7632590000	0.5006600000	-0.6381340000
C3	0.7153880000	0.5770380000	-0.1448600000
C4	0.8111170000	-0.9645380000	-0.4121400000
C5	-0.5737510000	-0.5262740000	1.5072720000
H6	-1.4026700000	-1.7061500000	-0.2299240000
N7	-0.9195780000	0.4829910000	-2.1407900000
H8	1.4319050000	1.2887670000	-0.5593960000
C9	0.5019700000	0.6092950000	1.3823540000
N10	1.0467510000	-1.3424020000	-1.8178600000
H11	-1.5223700000	-0.1721850000	1.9220190000
H12	-0.2352400000	-1.3697370000	2.1155130000
H13	1.4257530000	0.3834040000	1.9223580000
H14	0.1389710000	1.5814220000	1.7294300000
C15	-2.2784930000	0.0198760000	-2.5649000000
C16	-0.5905780000	1.8048210000	-2.7614520000
C17	2.4314890000	-1.0318200000	-2.2268820000
C18	0.7753880000	-2.7777840000	-2.0348940000
H19	-2.3144120000	-0.0178040000	-3.6553150000
H20	-2.4674570000	-0.9725320000	-2.1566140000
H21	-3.0289180000	0.7222570000	-2.1940430000
H22	-0.6742720000	1.7163610000	-3.8463120000
H23	-1.2935860000	2.5574330000	-2.3962750000
H24	0.4267640000	2.0885340000	-2.4934200000
H25	2.5661580000	-1.3007660000	-3.2781880000
H26	2.6342180000	0.0361910000	-2.1145290000
H27	3.1670870000	-1.5905830000	-1.6270310000
H28	0.9352560000	-3.0198850000	-3.0891890000
H29	1.4387040000	-3.4128970000	-1.4267900000
H30	-0.2601560000	-3.0152890000	-1.7787380000
H31	-1.4821620000	1.2248300000	-0.2400570000
H32	1.4800700000	-1.5238460000	0.2615250000
H33	-0.1867190000	-0.2415930000	-2.4259140000

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SCF ENERGY at B3LYP/6-311+G** = -581.29212 au
ZPVE = 218.478kcal/mol

atom	x	y	z
C1	-0.6949071290	-0.8969786672	0.0406165934
C2	-0.7892055432	0.5294064049	-0.6430051795
C3	0.7073075616	0.5789374149	-0.1251609277
C4	0.8331239094	-0.9819707970	-0.3684924240
C5	-0.5847834130	-0.5090805524	1.5325699622
H6	-1.3988034897	-1.6978054878	-0.2037097369
N7	-0.9230436556	0.4971976129	-2.1021242596
C8	-1.7998549670	1.5522244791	-0.0718249604
H9	1.4336084045	1.2842613452	-0.5392042776
C10	0.4938473631	0.6291248464	1.4045532863
N11	1.0644009117	-1.3631291928	-1.7646031464
C12	1.7920945273	-1.7925840705	0.5356738774
H13	-1.5347931077	-0.1580717997	1.9447961580
H14	-0.2568555151	-1.3444271805	2.1573636207
H15	1.4105783383	0.4186818735	1.9621886239
H16	0.1331007160	1.6041779429	1.7434701969
C17	-2.1569233031	-0.0560827639	-2.6224809790
C18	-0.5227740178	1.6967607950	-2.8096863954
C19	2.3349921980	-0.9673277705	-2.3374902747
C20	0.7011936235	-2.7181038070	-2.1279494946
H21	-2.0212977159	-0.3045243895	-3.6836102422
H22	-2.4152747615	-0.9796436355	-2.0960308505
H23	-3.0285841156	0.6280072841	-2.5561281464
H24	-0.3714017402	1.4562403659	-3.8705563449
H25	-1.2629263169	2.5227168002	-2.7644351658

H26	0.4254389575	2.0754643155	-2.4165678869
H27	2.2721284872	-1.0305161823	-3.4320994468
H28	2.5664475557	0.0699194310	-2.0779384753
H29	3.1941029234	-1.5959625029	-2.0229268778
H30	0.6243673507	-2.7900692339	-3.2211592277
H31	1.4283491155	-3.4899344717	-1.8000283506
H32	-0.2752289503	-2.9787419686	-1.7086744712
H33	-1.6026154177	2.5453410174	-0.4933610789
H34	-2.8184154142	1.2718493816	-0.3664543150
H35	-1.8023851419	1.6627496747	1.0125788222
H36	2.8307539765	-1.6057158465	0.2371520265
H37	1.7266743185	-1.5849964351	1.6037551587
H38	1.6061784920	-2.8657807425	0.4069908270

8H^{+}

SCF ENERGY at B3LYP/6-311+G** = -581.71529au
ZPVE = 228.604kcal/mol

atom	x	y	z
C1	-0.7064760000	-0.8906140000	0.0847820000
C2	-0.7942690000	0.5320190000	-0.6111790000
C3	0.7001770000	0.5949780000	-0.0833640000
C4	0.8216550000	-0.9643250000	-0.3121540000
C5	-0.5931920000	-0.4962180000	1.5744980000
H6	-1.4049500000	-1.6970090000	-0.1531630000
N7	-0.8662180000	0.4309150000	-2.1099180000
C8	-1.8146420000	1.5568050000	-0.1030030000
H9	1.4305880000	1.2978720000	-0.4922880000
C10	0.4825930000	0.6410960000	1.4457250000
N11	1.0068550000	-1.3080470000	-1.7949600000
C12	1.8026340000	-1.8020020000	0.5062890000
H13	-1.5466720000	-0.1489680000	1.9776480000
H14	-0.2701730000	-1.3309630000	2.2009420000
H15	1.4003980000	0.4362810000	2.0018170000
H16	0.1239470000	1.6179070000	1.7765930000
C17	-2.1532750000	-0.0812760000	-2.6238270000
C18	-0.4944710000	1.6713880000	-2.8212600000
C19	2.3397680000	-0.9377720000	-2.3588070000
C20	0.6588190000	-2.7151860000	-2.1559540000
H21	-2.0334450000	-0.3370410000	-3.6815050000
H22	-2.4506390000	-0.9811670000	-2.0803880000
H23	-2.9614710000	0.6572200000	-2.5448240000
H24	-0.3531880000	1.4403020000	-3.8819600000
H25	-1.2669350000	2.4474560000	-2.7449330000
H26	0.4414710000	2.0727070000	-2.4255660000
H27	2.2789240000	-0.9932610000	-3.4482820000
H28	2.5953320000	0.0793560000	-2.0618770000
H29	3.1096870000	-1.6274660000	-2.0088310000
H30	0.5890170000	-2.7832140000	-3.2441670000
H31	1.4292280000	-3.4033050000	-1.8039250000
H32	-0.3013470000	-2.9816710000	-1.7142150000
H33	-1.6142940000	2.5454120000	-0.5288910000
H34	-2.8301340000	1.2681340000	-0.3931600000
H35	-1.8189870000	1.6756840000	0.9788810000
H36	2.8391540000	-1.5962810000	0.2194050000
H37	1.7303050000	-1.6023680000	1.5732460000
H38	1.6179230000	-2.8733480000	0.3752070000
H39	0.2471460000	-0.6384960000	-2.2280530000

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SCF ENERGY at B3LYP/6-311+G** = -957.62808 au
ZPVE = 314.602 kcal/mol

atom	x	y	z
C1	-0.9734070000	-1.4469630000	-0.7970820000
C2	-1.1809200000	0.1090680000	-0.9185700000
C3	0.1004340000	0.1139390000	-0.0136630000
C4	0.5801890000	-1.2058250000	-0.7128840000
C5	-1.3040240000	-1.6564860000	0.6938460000
H6	-1.4057110000	-2.1402190000	-1.5261550000
N7	-1.0394260000	0.7204530000	-2.2070910000
H8	0.7496490000	0.9917440000	0.0393680000
C9	-0.4782200000	-0.4560230000	1.2956050000
N10	1.3138760000	-1.0367610000	-1.9323910000
H11	-2.3775040000	-1.5739040000	0.9010540000
H12	-0.9632140000	-2.6297060000	1.0664040000
H13	0.3019510000	-0.7903800000	1.9893580000
H14	-1.1123580000	0.2654600000	1.8239000000
C15	2.2480260000	-1.8561300000	-2.2619270000
C16	-2.0247360000	1.3332400000	-2.7604990000
N17	3.1825740000	-1.4757300000	-3.2419090000
N18	2.4897330000	-3.1251590000	-1.7037660000
N19	-3.3797550000	1.2550370000	-2.3888630000
N20	-1.7736470000	2.2238100000	-3.8199390000
C21	3.3862030000	-2.3780700000	-4.3730520000
C22	3.1751830000	-0.0711640000	-3.6336130000
C23	3.8285100000	-3.6269050000	-1.4552710000
C24	1.4175210000	-4.0782270000	-1.4919580000
C25	-4.2604220000	2.4082820000	-2.4000970000
C26	-4.0231180000	-0.0181760000	-2.1282500000
C27	-2.5187440000	2.0287160000	-5.0616980000
C28	-0.3786700000	2.5819260000	-4.0483480000
H29	2.6167140000	-2.2309880000	-5.1513740000
H30	4.3683860000	-2.1925960000	-4.8237840000
H31	3.3467840000	-3.4186770000	-4.0473260000
H32	4.0981640000	0.1391710000	-4.1871500000
H33	2.3097880000	0.1808090000	-4.2655570000
H34	3.1296270000	0.5586460000	-2.7441760000
H35	3.9123030000	-3.9782410000	-0.4154870000
H36	4.0869820000	-4.4749470000	-2.1125900000
H37	4.5565300000	-2.8303600000	-1.6157190000
H38	1.6002470000	-4.9967870000	-2.0750250000
H39	1.3257390000	-4.3667580000	-0.4337230000
H40	0.4676850000	-3.6528810000	-1.8175890000
H41	-4.7732280000	2.5002040000	-1.4304720000
H42	-3.6790820000	3.3145020000	-2.5763430000
H43	-5.0381660000	2.3342650000	-3.1796530000
H44	-4.8589200000	-0.1763220000	-2.8307510000
H45	-3.3101350000	-0.8326590000	-2.2602120000
H46	-4.4298830000	-0.0729370000	-1.1069470000
H47	-2.0544740000	1.2516170000	-5.6942490000
H48	-3.5461450000	1.7277030000	-4.8509860000
H49	-2.5415810000	2.9650840000	-5.6316880000
H50	-0.3491740000	3.4592730000	-4.7055600000
H51	0.1005500000	2.8197800000	-3.0977710000
H52	0.1911210000	1.7629820000	-4.5135670000
H53	-2.0832260000	0.4718820000	-0.3974340000
H54	1.0939910000	-1.9001880000	-0.0264170000

$9H^+$

SCF ENERGY at B3LYP/6-311+G** = -958.07671 au
ZPVE = 325.658 kcal/mol

atom	x	y	z
C1	0.0894560000	2.0605730000	-0.4538720000
C2	1.1227520000	1.3158250000	0.4793360000
C3	0.0161340000	1.6108160000	1.5547760000
C4	-1.0435960000	1.4287410000	0.4202120000
C5	0.1341780000	3.4897250000	0.1165710000
H6	0.1038890000	1.9331800000	-1.5401550000
N7	1.3289050000	-0.0937330000	0.2272240000
H8	-0.0407490000	1.0336030000	2.4812420000
C9	0.0763540000	3.1459060000	1.6501640000
N10	-1.3699520000	0.0332250000	0.1288550000
H11	1.0519420000	4.0157920000	-0.1644580000
H12	-0.7137540000	4.1009920000	-0.2116110000
H13	-0.8024440000	3.5716840000	2.1461790000
H14	0.9637470000	3.4858970000	2.1931950000
C15	-2.5809230000	-0.4792870000	-0.0990690000
C16	2.5231960000	-0.5417390000	-0.0526190000
N17	-2.8258050000	-1.7730820000	0.2298960000
N18	-3.5773650000	0.2697570000	-0.6409700000
N19	3.5870780000	0.2274250000	-0.5056090000
N20	2.8103870000	-1.8819440000	0.1455350000
C21	-3.6928900000	-2.6355220000	-0.5798190000
C22	-2.0612480000	-2.4607150000	1.2730040000
C23	-4.9797940000	0.1112510000	-0.2464160000
C24	-3.3249600000	1.2924480000	-1.6597360000
C25	4.9609840000	0.0062710000	-0.0655680000
C26	3.4210340000	1.2503250000	-1.5290940000
C27	3.5494340000	-2.6506200000	-0.8556770000
C28	1.9387400000	-2.6862690000	0.9843120000
H29	-3.1304080000	-3.5292390000	-0.8731190000
H30	-4.5776480000	-2.9512610000	-0.0153700000
H31	-4.0075120000	-2.1152590000	-1.4843070000
H32	-2.7363270000	-3.1308570000	1.8148320000
H33	-1.2460320000	-3.0588030000	0.8479270000
H34	-1.6468210000	-1.7353850000	1.9745310000
H35	-5.3885240000	1.0972180000	0.0017910000
H36	-5.5822030000	-0.3174960000	-1.0562470000
H37	-5.0538540000	-0.5258870000	0.6352070000
H38	-3.9910060000	1.1133050000	-2.5117180000
H39	-3.5209840000	2.2997220000	-1.2742880000
H40	-2.2934290000	1.2332270000	-2.0058300000
H41	5.3880310000	0.9536810000	0.2892290000
H42	4.9788720000	-0.7122100000	0.7547480000
H43	5.6000260000	-0.3672560000	-0.8789020000
H44	4.1037770000	1.0488980000	-2.3667760000
H45	2.4004590000	1.2367320000	-1.9127990000
H46	3.6447310000	2.2562830000	-1.1477030000
H47	2.8634330000	-3.2924260000	-1.4293510000
H48	4.0545710000	-1.9841100000	-1.5540100000
H49	4.2974260000	-3.2915200000	-0.3744310000
H50	2.5112680000	-3.5320990000	1.3810820000
H51	1.5640980000	-2.0850980000	1.8139500000
H52	1.0807250000	-3.0899640000	0.4223760000
H53	-0.5305790000	-0.5685530000	0.1548740000
H54	2.0655280000	1.8542130000	0.6421200000
H55	-1.9732480000	1.9937960000	0.5242900000

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SCF ENERGY at B3LYP/6-311+G** = -1036.25048 au
ZPVE = 338.051 kcal/mol

atom	x	y	z
C1	-0.8072010000	-1.1180190000	-0.1260340000
C2	-1.0075870000	0.4216400000	-0.4826160000
C3	0.3536980000	0.5073800000	0.3218480000
C4	0.7641130000	-0.9021550000	-0.2728650000
C5	-0.9780070000	-1.1026680000	1.4093290000
H6	-1.3364210000	-1.9105220000	-0.6532080000
N7	-0.8194910000	0.8636560000	-1.8549070000
C8	-2.2130920000	1.1902000000	0.1013530000
H9	1.0132160000	1.3669840000	0.1724510000
C10	-0.0855060000	0.1461990000	1.7516570000
N11	1.3364670000	-0.7517640000	-1.6005410000
C12	1.7367270000	-1.7560010000	0.5693060000
H13	-2.0233510000	-0.9793770000	1.7101560000
H14	-0.6216690000	-2.0263870000	1.8764930000
H15	0.7568140000	-0.0962610000	2.4064990000
H16	-0.6439690000	0.9503010000	2.2402170000
H17	-2.0226670000	2.2661250000	0.0009640000
H18	-3.1275550000	0.9686460000	-0.4558860000
H19	-2.4168790000	0.9895380000	1.1539260000
H20	2.7195890000	-1.2681790000	0.5670920000
H21	1.4405250000	-1.8932910000	1.6100440000
H22	1.8666850000	-2.7502480000	0.1331880000
C23	1.8501200000	-1.6644720000	-2.3396590000
C24	-1.7161410000	1.0039990000	-2.7600630000
N25	2.7862200000	-1.2808130000	-3.3243210000
N26	1.6374170000	-3.0595060000	-2.3359960000
N27	-2.9815670000	0.3907500000	-2.8841470000
N28	-1.4645680000	1.9011780000	-3.8197380000
C29	2.5849680000	-1.7370650000	-4.6967510000
C30	3.2993160000	0.0802590000	-3.2467120000
C31	2.7507750000	-3.9951500000	-2.3586770000
C32	0.3511030000	-3.6341340000	-2.0109390000
C33	-4.1759600000	1.1696830000	-3.1705220000
C34	-3.2177840000	-0.9659020000	-2.4438970000
C35	-1.6419740000	1.4366740000	-5.1923090000
C36	-0.3322010000	2.8034420000	-3.6642050000
H37	1.9027290000	-1.0683430000	-5.2509970000
H38	3.5450910000	-1.7577360000	-5.2266890000
H39	2.1607680000	-2.7420650000	-4.7046510000
H40	4.1944970000	0.1497760000	-3.8765220000
H41	2.5634360000	0.8254670000	-3.5848840000
H42	3.5614010000	0.3187790000	-2.2149200000
H43	2.8587390000	-4.5085300000	-1.3880340000
H44	2.6035560000	-4.7669230000	-3.1296390000
H45	3.6764250000	-3.4590200000	-2.5717150000
H46	0.2169610000	-4.5570860000	-2.5921480000
H47	0.2335670000	-3.8908650000	-0.9445570000
H48	-0.4431260000	-2.9405350000	-2.2897640000
H49	-4.8343230000	1.2286930000	-2.2869880000
H50	-3.8934520000	2.1826810000	-3.4598180000
H51	-4.7562190000	0.7169490000	-3.9890290000
H52	-3.9642350000	-1.4295070000	-3.1039930000
H53	-2.2951800000	-1.5426960000	-2.5183410000
H54	-3.5948430000	-1.0396170000	-1.4098150000
H55	-0.7323410000	0.9395340000	-5.5732400000
H56	-2.4689490000	0.7275490000	-5.2489700000
H57	-1.8637790000	2.2875940000	-5.8480780000
H58	-0.4284810000	3.6114320000	-4.3997110000

H59	-0.3310740000	3.2257790000	-2.6583570000
H60	0.6325750000	2.2954170000	-3.8142110000

$10H^+$

SCF ENERGY at B3LYP/6-311+G** = -1036.70252 au
ZPVE = 347.887 kcal/mol

atom	x	y	z
C1	-0.8831420000	-1.1442130000	-0.0801500000
C2	-1.0247580000	0.3925090000	-0.5105700000
C3	0.3652630000	0.4508290000	0.2503950000
C4	0.6816650000	-1.0059150000	-0.2805320000
C5	-0.9920740000	-1.0571540000	1.4570550000
H6	-1.4485140000	-1.9407360000	-0.5673160000
N7	-0.8144250000	0.7269340000	-1.9251980000
C8	-2.1556780000	1.2580520000	0.0694730000
H9	1.0594430000	1.2742700000	0.0558060000
C10	-0.0403440000	0.1683480000	1.7078800000
N11	1.1296090000	-0.9337000000	-1.6932400000
C12	1.6716660000	-1.8654430000	0.5111340000
H13	-2.0183550000	-0.8809230000	1.7893960000
H14	-0.6518140000	-1.9725990000	1.9504110000
H15	0.8113340000	-0.0689220000	2.3505300000
H16	-0.5471580000	1.0216910000	2.1639740000
H17	-1.8848100000	2.3141550000	-0.0502940000
H18	-3.0965460000	1.1012370000	-0.4606640000
H19	-2.3512170000	1.0878530000	1.1276790000
H20	2.6930040000	-1.5012130000	0.3442620000
H21	1.4882650000	-1.8270520000	1.5828890000
H22	1.6401690000	-2.9186080000	0.2243410000
C23	1.8686890000	-1.7702900000	-2.4260890000
C24	-1.7486850000	0.9875400000	-2.7997540000
N25	2.6979420000	-1.2363880000	-3.3625090000
N26	1.8153410000	-3.1235120000	-2.2976960000
N27	-3.0531800000	0.5121960000	-2.8137360000
N28	-1.4386410000	1.8265930000	-3.8570940000
C29	2.9616730000	-1.8914290000	-4.6464510000
C30	3.2316250000	0.1222020000	-3.2353560000
C31	3.0017540000	-3.9729940000	-2.4188850000
C32	0.5660520000	-3.8267520000	-2.0105180000
C33	-4.1939500000	1.3667580000	-3.1356430000
C34	-3.3861400000	-0.8239450000	-2.3511190000
C35	-1.9097670000	1.5736200000	-5.2163440000
C36	-0.2922450000	2.7176680000	-3.7708740000
H37	2.7504490000	-1.1838980000	-5.4562860000
H38	4.0087710000	-2.2059540000	-4.7269210000
H39	2.3139740000	-2.7595940000	-4.7686390000
H40	4.2679860000	0.1262560000	-3.5889290000
H41	2.6571200000	0.8378750000	-3.8363180000
H42	3.2091070000	0.4361580000	-2.1913090000
H43	3.0698280000	-4.6153720000	-1.5329770000
H44	2.9503520000	-4.6151730000	-3.3063640000
H45	3.9011440000	-3.3587960000	-2.4697250000
H46	0.4299940000	-4.6234500000	-2.7515300000
H47	0.5749940000	-4.2839150000	-1.0138150000
H48	-0.2724230000	-3.1355360000	-2.0797290000
H49	-4.8856740000	1.4058250000	-2.2823320000
H50	-3.8529920000	2.3804270000	-3.3482600000
H51	-4.7489700000	0.9879620000	-4.0045510000
H52	-4.1800790000	-1.2312110000	-2.9889280000
H53	-2.5134170000	-1.4729600000	-2.4375670000
H54	-3.7449860000	-0.8475720000	-1.3111400000
H55	-1.0630390000	1.3093080000	-5.8671900000

H56	-2.6204570000	0.7472560000	-5.2247560000
H57	-2.3953440000	2.4628130000	-5.6373750000
H58	-0.4880290000	3.6080170000	-4.3792590000
H59	-0.1295400000	3.0145280000	-2.7347010000
H60	0.6295080000	2.2456420000	-4.1465880000
H61	0.7265780000	-0.0945060000	-2.1575330000