

Dual function of living polymerization initiator through formation of chain-end-protecting cluster: density functional theory calculation

Yun Hee Jang,^{*a} Yves Lansac,^b Jae-Ki Kim,^a Hee-Soo Yoo,^a Chang-Geun Chae,^a Cheol Ho Choi,^c Shashadhar Samal,^a Jae-Suk Lee^{*a}

Electronic Supplementary Information (ESI)

Table S1. Free energy components of Na⁺, BA⁻ and (NaBA)_n in THF at 175 K (See the text for the equations).

(kcal/mol)	$\Delta E_{g,OK}$	ΔH_{trans}	$-T\Delta S_{trans}$	ΔH_{rot}	$-T\Delta S_{rot}$	$\Delta\Delta G_{0\rightarrow 175K}$	ΔG_{solv}	$\Delta G_{solv,corr}$	$\Delta G_{THF,175K}$	$\Delta\Delta G_{SA}$
NaBA	(1)	(2)	(3)	(4)	(5)	(6)=(2+3+4+5)	(7)	(8)	(9)=(1+6+7+8)	
Na ⁺	-101711.4	0.87	-4.29	0.00	0.00	-3.42	-97.83	1.08	-101811.6	
BA ⁻ (0a)	-396324.0	0.87	-5.42	0.52	-5.33	-9.35	-51.69	1.08	-396384.0	
BA ⁻ (0b)	-396335.6	0.87	-5.42	0.52	-5.35	-9.37	-47.41	1.08	-396391.3	
1a	-498178.4	0.87	-5.47	0.52	-5.45	-9.53	-31.39	1.08	-498218.2	
1b	-498179.3	0.87	-5.47	0.52	-5.41	-9.49	-27.59	1.08	-498215.4	
1c	-498166.7	0.87	-5.47	0.52	-5.47	-9.55	-40.26	1.08	-498215.4	
1d	-498167.8	0.87	-5.47	0.52	-5.42	-9.51	-34.67	1.08	-498210.9	
2a	-996400.6	0.87	-5.84	0.52	-6.29	-10.74	-27.82	1.08	-996438.1	-1.7
2b	-996390.7	0.87	-5.84	0.52	-6.22	-10.66	-33.51	1.08	-996433.8	2.6
2c	-996390.1	0.87	-5.84	0.52	-6.07	-10.51	-27.12	1.08	-996426.7	9.7
2d	-996390.2	0.87	-5.84	0.52	-6.08	-10.53	-26.97	1.08	-996426.7	9.7
3a	-1494614.3	0.87	-6.05	0.52	-6.68	-11.34	-26.31	1.08	-1494650.9	3.7
3b	-1494605.0	0.87	-6.05	0.52	-6.52	-11.18	-27.58	1.08	-1494642.7	11.9
3c	-1494603.6	0.87	-6.05	0.52	-6.45	-11.11	-27.97	1.08	-1494641.6	13.0
4a	-1992837.9	0.87	-6.20	0.52	-6.84	-11.65	-25.86	1.08	-1992874.3	-1.5
4b	-1992824.5	0.87	-6.20	0.52	-6.78	-11.59	-31.10	1.08	-1992866.1	6.6
4c	-1992822.5	0.87	-6.20	0.52	-6.49	-11.30	-30.34	1.08	-1992863.1	9.7
5a	-2491022.2	0.87	-6.32	0.52	-6.62	-11.54	-42.52	1.08	-2491075.2	15.8
5b	-2491035.8	0.87	-7.15	0.52	-6.95	-12.70	-22.36	1.08	-2491069.8	21.2
6a	-2989272.5	0.87	-6.41	0.52	-7.16	-12.18	-22.59	1.08	-2989306.2	3.0
6b	-2989222.0	0.87	-6.41	0.52	-6.75	-11.77	-55.11	1.08	-2989287.8	21.4

Table S2a. Final structures of BA⁻ optimized in THF: Cartesian coordinates (Å).

0a	x (Å)	y (Å)	z (Å)	0b	x (Å)	y (Å)	z (Å)
C1	-0.0414834969	-0.0842769104	0.1636864180	C1	-0.0031564578	-0.0035528220	-0.0281120130
C2	0.0516223697	0.3665405383	1.5052326390	O2	0.0085507133	-0.0082744991	1.2311869749
C3	1.2765586508	0.6070248390	2.1133766408	N3	1.0209607647	0.0005396400	-0.8829189749
C4	2.4715076905	0.4119181446	1.4144062796	C4	2.3448657374	0.0011128773	-0.4633594493
C5	2.4052199714	-0.0311695259	0.0911466753	C5	3.3229422009	-0.0017597218	-1.4907727280
C6	1.1826459860	-0.2732775371	-0.5258742470	H6	2.9662120541	-0.0051699642	-2.5161749062
N7	-1.2815314719	-0.1625756096	-0.4208767517	C7	4.6851017112	0.0002951636	-1.2217382773
C8	-1.6725770131	-1.0104330711	-1.3683088169	H8	5.3934879915	-0.0018719823	-2.0455489414
O9	-2.6262224218	-0.7514811666	-2.1445454909	C9	5.1471388053	0.0050896209	0.0978600503
C10	-1.0949007091	-2.4123514540	-1.5076832835	H10	6.2106976418	0.0066104308	0.3135619862
C11	-0.6072350105	-3.1433318875	-0.4198691950	C11	4.2081418764	0.0074859421	1.1296965751
C12	-0.2257650259	-4.4758754656	-0.5725667096	H12	4.5457349366	0.0112465071	2.1629633901
C13	-0.3110982928	-5.0926266694	-1.8206899006	C13	2.8382914332	0.0047960462	0.8686634157
C14	-0.7911312681	-4.3705893934	-2.9147402668	H14	2.1251039089	0.0075846749	1.6780152229
C15	-1.1890087680	-3.0471716748	-2.7524751254	C15	-1.3737394916	-0.0013398804	-0.6947858698
H16	-0.8700857500	-4.8432142038	-3.8887720504	C16	-2.5177045186	0.0001258423	0.1131201085
H17	-1.6066459176	-2.4881709707	-3.5807041340	H17	-2.3800093491	-0.0002404913	1.1872895936
H18	-0.8733988739	0.5426524554	2.0455851278	C18	-3.7942231984	0.0027152641	-0.4467532867
H19	1.3004051361	0.9595670061	3.1410574978	H19	-4.6679035611	0.0043426622	0.1979037583
H20	3.4275726752	0.6126965984	1.8849521916	C20	-3.9493749193	0.0033034497	-1.8334825406
H21	3.3205968051	-0.1722807948	-0.4770784549	H21	-4.9416087608	0.0056251248	-2.2733972544
H22	1.1537468803	-0.5814527056	-1.5652259291	C22	-2.8169063673	0.0012540783	-2.6507431083
H23	-0.5480810022	-2.6740824830	0.5543064802	H23	-2.9278226863	0.0019818142	-3.7307768925
H24	0.1318244554	-5.0342240563	0.2863807169	C24	-1.5433386372	-0.0010277505	-2.0847869923
H25	-0.0160887058	-6.1299476141	-1.9386521514	H25	-0.6563189999	-0.0023997170	-2.7049576999

Table S2b. Final structures of NaBA optimized in THF: Cartesian coordinates (Å).

1a	x (Å)	y (Å)	z (Å)	1b	x (Å)	y (Å)	z (Å)
C1	0.0678943392	-0.0220282911	0.1558876422	C1	0.1245947704	0.0538742467	-0.1878618853
C2	0.1772853799	0.3557690263	1.5094096707	O2	0.2142006627	0.6732363078	0.9277981196
C3	1.4163911785	0.4661903905	2.1331689537	N3	1.1095511516	-0.5023496819	-0.8524749360
C4	2.5925655782	0.2085969597	1.4264360339	C4	2.3813996841	-0.5289633884	-0.2768790310
C5	2.5036955025	-0.1606011669	0.0832987594	C5	3.4227664581	0.2741067357	-0.7819117183
C6	1.2669106455	-0.2722211866	-0.5445505557	H6	3.1989801645	0.9618699556	-1.5904697315
N7	-1.1861467827	-0.0103159683	-0.4559709965	C7	4.7203692846	0.1751783738	-0.2801776967
C8	-1.6301631436	-0.9336304820	-1.2976666701	H8	5.5031758782	0.8006833307	-0.6985016718
O9	-2.6514284025	-0.7050793178	-2.0193794674	C9	5.0211280278	-0.7228998029	0.7451356008
C10	-1.0463162506	-2.3256603025	-1.4188871186	H10	6.0331377153	-0.8059920729	1.1268680837
C11	-0.5801314499	-3.0454910946	-0.3131402353	C11	3.9994432680	-1.5206396668	1.2652911863
C12	-0.1361623943	-4.3588888615	-0.4595976468	H12	4.2162626550	-2.2321961391	2.0568082741
C13	-0.1372370362	-4.9657991739	-1.7151086241	C13	2.7011070953	-1.4247784557	0.7670949289
C14	-0.6039329792	-4.2574136285	-2.8228520665	H14	1.9194730595	-2.0684918427	1.1571746631
C15	-1.0666614157	-2.9529712298	-2.6707693829	C15	-1.2488654515	-0.0380816424	-0.8203978378
H16	-0.6172641736	-4.7247680915	-3.8019475719	C16	-2.3576301912	0.4767040996	-0.1393121663
H17	-1.4608685345	-2.4086231022	-3.5203266246	H17	-2.1994534917	0.9405342108	0.8259555604
H18	-0.7309926172	0.5671155042	2.0635517733	C18	-3.6378278120	0.3907860780	-0.6859321831
H19	1.4631362090	0.7603288273	3.1774095359	H19	-4.4864281643	0.7914007469	-0.1407290204
H20	3.5588153641	0.3053614263	1.9093661495	C20	-3.8289912251	-0.2103498447	-1.9292995071
H21	3.4076652174	-0.3504580857	-0.4876642940	H21	-4.8240846111	-0.2793419520	-2.3568137407
H22	1.2173370698	-0.5335972256	-1.5957445550	C22	-2.7298587654	-0.7238403930	-2.6204436475
H23	-0.5783352997	-2.5861825691	0.6675043505	H23	-2.8680829720	-1.1924013610	-3.5896207560
H24	0.2094006584	-4.9094636936	0.4088062791	C24	-1.4541077674	-0.6382471944	-2.0694525638
H25	0.2148106278	-5.9857996340	-1.8285018047	H25	-0.6007123835	-1.0366631287	-2.6001449174
Na26	-2.9882520538	1.4727209903	-1.2465084821	Na26	1.9530073629	1.2598336193	2.1679768837

1c	x (Å)	y (Å)	z (Å)	1d	x (Å)	y (Å)	z (Å)
C1	-0.0315676970	-0.1967206279	-0.0917960723	C1	-0.0090997976	0.2190584388	-0.0712287190
O2	-0.1328156893	-0.7653618914	1.0469731435	O2	0.0218892577	0.3911842817	1.1668507040
N3	1.0617895113	0.1008848773	-0.7622472499	N3	1.0186204969	0.0770122609	-0.9265150357
C4	2.3362646379	0.0003816392	-0.2089291893	C4	2.3383226786	-0.0378067334	-0.4691469860
C5	3.4055658127	-0.3602894660	-1.0576133846	C5	3.3531052986	-0.0719023668	-1.4551085659
H6	3.1743919789	-0.6178412262	-2.0866081879	H6	3.0660992517	-0.0046572698	-2.5002452695
C7	4.7226565497	-0.3752562547	-0.6087084175	C7	4.6991510746	-0.2087975589	-1.1359196850
H8	5.5177952728	-0.6606079738	-1.2922678721	H8	5.4378465317	-0.2280684491	-1.9316033183
C9	5.0274674302	-0.0140879187	0.7060263217	C9	5.1004491444	-0.3294709084	0.1958012578
H10	6.0547759046	-0.0122037181	1.0552500283	H10	6.1488829430	-0.4385688163	0.4516501420
C11	3.9847018099	0.3539867688	1.5591394455	C11	4.1205221026	-0.3089120547	1.1878367881
H12	4.2032732812	0.6481254755	2.5818996283	H12	4.4077121622	-0.4045060202	2.2311693533
C13	2.6635778628	0.3548332260	1.1189508063	C13	2.7698963901	-0.1631658392	0.8757126296
H14	1.8696632329	0.6410808795	1.7952498134	H14	2.0324013130	-0.1382010043	1.6611910706
C15	-1.3235165868	0.1686588490	-0.7982195864	C15	-1.3910833459	0.1774614547	-0.7064751815
C16	-2.4933704682	0.3550728245	-0.0518897706	C16	-2.4580738532	0.7817802822	-0.0270091820
H17	-2.4481945083	0.2409255645	1.0244172017	H17	-2.2504548916	1.2874431534	0.9077687171
C18	-3.6935357500	0.7032251629	-0.6707235149	C18	-3.7552447649	0.7174694052	-0.5273596334
H19	-4.5845731625	0.8601920368	-0.0711312763	H19	-4.5662303746	1.1969268877	0.0115024716
C20	-3.7484884605	0.8506203371	-2.0564805281	C20	-4.0171742988	0.0249989292	-1.7118636679
H21	-4.6826921317	1.1125294895	-2.5422674934	H21	-5.0305416022	-0.0390699304	-2.0943026620
C22	-2.5901634312	0.6607403030	-2.8127805025	C22	-2.9688432561	-0.5968350034	-2.3891512773
H23	-2.6234791560	0.7686443431	-3.8917810806	H23	-3.1648420026	-1.1602506991	-3.2959368136
C24	-1.3892864244	0.3337832185	-2.1875073433	C24	-1.6669978291	-0.5155967186	-1.8912051769
H25	-0.4828513984	0.2012335684	-2.7643382647	H25	-0.8648201117	-1.0432784721	-2.3930089249
Na26	-1.1437773422	-2.4184927922	2.0819188757	Na26	0.6643966564	0.9970428646	-3.0902481649

Table S2c. Final structures of (NaBA)₂ optimized in THF: Cartesian coordinates (Å).

2a	x (Å)	y (Å)	z (Å)	2b	x (Å)	y (Å)	z (Å)
C2	-0.1007780260	4.1129157461	-1.8977971175	C53	30.2526062146	-6.2497628276	-16.0132924184
C3	1.1032701328	4.7217825186	-2.2991731292	C54	29.7448125944	-6.4903453572	-17.3054634726
C4	1.1394789697	6.0513854668	-2.7097968754	C55	30.4491533232	-7.2662235981	-18.2219769527
C5	-0.0245585589	6.8219749314	-2.7217155653	C56	31.6821209250	-7.8251204746	-17.8848104727
C6	-1.2232027783	6.2385061019	-2.3085023970	C57	32.2023014919	-7.5907981721	-16.6106014455
C7	-1.2631462278	4.9087039665	-1.8984000037	C58	31.5034891598	-6.8126797604	-15.6928428198
N25	-0.0720841956	2.7954555729	-1.4173324081	N7	29.6449422927	-5.3817533105	-15.0997109950
C8	-0.9386731840	1.8657931116	-1.7693782346	C60	28.3954948843	-5.4486052588	-14.7304637761
O27	-0.9743775977	0.7467790029	-1.1461971359	O9	27.8427933431	-4.5222887536	-14.0221547693
C9	-1.8868859614	2.0098135750	-2.9379482242	C62	27.5118251806	-6.6295522040	-15.0751587289
C10	-1.4355597494	2.4369639881	-4.1915948619	C63	27.9115279413	-7.9415256728	-14.7964814961

C11	-2.3096255956	2.4996662171	-5.2750213162	C64	27.0756807665	-9.0163617236	-15.0943430009
C12	-3.6521090016	2.1561209246	-5.1147572925	C65	25.8373722785	-8.7960723997	-15.6985760417
C13	-4.1112373745	1.7322262529	-3.8672815723	C66	25.4338111727	-7.4919132137	-15.9882937024
C14	-3.2304113501	1.6461968162	-2.7909354770	C67	26.2614727962	-6.412818150	-15.6674108301
H15	-5.1542068125	1.4622487047	-3.7348402775	H68	24.4727223526	-7.3108101136	-16.4589842381
H16	-3.5836957396	1.2999746809	-1.8266701564	H69	25.9388591089	-5.4041304661	-15.8772647101
H17	2.0141202893	4.1336067963	-2.2833767426	H70	28.7968275871	-6.0498648857	-17.5899117188
H18	2.0841500646	6.4894306832	-3.0183573388	H71	30.0337191821	-7.4276186243	-19.2122961540
H19	0.0041533529	7.8598827494	-3.0361776933	H72	32.2324670744	-8.4221703293	-18.6039266984
H20	-2.1361928752	6.8262972519	-2.2962801617	H73	33.1642231529	-8.0095851199	-16.3316298877
H21	-2.1999480544	4.4784659585	-1.5631744414	H74	31.9207035486	-6.6211711015	-14.7104924279
H22	-0.3962811570	2.7130555031	-4.3234083806	H75	28.8780480040	-8.1218967025	-14.3407614663
H23	-1.9422300934	2.8197512225	-6.2444262905	H76	27.3948211632	-10.0271283677	-14.8598599855
H24	-4.3346001677	2.2139480676	-5.9565977019	H77	25.1909484149	-9.6334379024	-15.9393841600
Na1	0.8392458123	1.3559840941	0.3575964142	Na26	27.7964797296	-2.2891082097	-14.4260037347
C28	0.9386731840	-1.8657931116	1.7693782346	C79	27.3416203350	-1.2640664577	-11.0811142617
C30	1.8868859614	-2.0098135750	2.9379482242	C80	26.9985034814	0.1949426495	-10.8652122234
N31	0.0720841956	-2.7954555729	1.4173324081	N81	27.5311872863	-2.1145287259	-10.0937607622
O26	0.9743775977	-0.7467790029	1.1461971359	O30	27.5015786283	-1.6309336205	-12.3004488113
C32	1.4355597494	-2.4369639881	4.1915948619	C83	25.9243358296	0.7701709691	-11.5530540944
C33	3.2304113501	-1.6461968162	2.7909354770	C84	27.7686051625	1.0027157646	-10.0208598992
C34	0.1007780260	-4.1129157461	1.8977971175	C85	27.2240983578	-1.8113627094	-8.7547361712
C35	2.3096255956	-2.4996662171	5.2750213162	C86	25.6086042879	2.1166519067	-11.3799803489
H36	0.3962811570	-2.7130555031	4.3234083806	H87	25.3294125094	0.1576582411	-12.2198438898
C37	4.1112373745	-2.1732262529	3.8672815723	C88	27.4689336318	2.3552106688	-9.8664396287
H38	3.5836957396	-1.2999746809	1.8266701564	H89	28.6077676658	0.5743661797	-9.4855187847
C39	-1.1032701328	-4.7217825186	2.2991731292	C90	25.9635370870	-1.3352083533	-8.3451546738
C40	1.2631462278	-4.9087039665	1.8984000037	C91	28.1759040546	-2.0752194140	-7.7525226367
C41	3.6521090016	-2.1561209246	5.1147572925	C92	26.3820314603	2.9144584691	-10.5370009472
H42	1.9422300934	-2.8197512225	6.2444262905	H93	24.7615968738	2.5441789475	-11.9059030751
H43	5.1542068125	-1.4622487047	3.7348402775	H94	28.0820202412	2.9713978149	-9.2176736196
C44	-1.1394789697	-6.0513854668	2.7097968754	C95	25.6832558102	-1.1049098163	-7.0007983293
H45	-2.0141202893	-4.1336067963	2.2833767426	H96	25.1993199710	-1.1527357973	-9.0921899005
C46	1.2232027783	-6.2385061019	2.3085023970	C97	27.8933311833	-1.8418699276	-6.4089524712
H47	2.1999480544	-4.4784659585	1.5631744414	H98	29.1465879089	-2.4629453102	-8.0415022415
H48	4.3346001677	-2.2139480676	5.9565977019	H99	26.1416473389	3.9645387458	-10.4070374346
C49	0.0245585589	-6.8219749314	2.7217155653	C100	26.6456051899	-1.3511869048	-6.0210787627
H50	-2.0841500646	-6.4894306832	3.0183573388	H101	24.7021723244	-0.7359576292	-6.7172370250
H51	2.1361928752	-6.8262972519	2.2962801617	H102	28.6530314758	-2.0465944520	-5.6609009264
H52	-0.0041533529	-7.8598827494	3.0361776933	H103	26.4250116154	-1.1727071737	-4.9744131734
Na29	-0.8392458123	-1.3559840941	-0.3575964142	Na52	28.0189351787	-3.9290251782	-11.7937411596

2c	x (Å)	y (Å)	z (Å)	2d	x (Å)	y (Å)	z (Å)
C1	0.4004660840	-0.1498733375	-0.4626520733	C1	-4.3410017464	-0.3322918600	-0.0312462532
O2	0.1061785079	-0.6122456908	0.6781474816	O2	-4.0723136632	0.1877705522	1.0916631329
N3	1.6182910021	0.0797043150	-0.9543367130	N3	-5.1931927853	-1.3172511348	-0.3020494951
C4	2.7311812975	0.1395732561	-0.1066194779	C4	-6.1071486396	-1.8021373720	0.6394992038
C5	4.0046956374	-0.1318870096	-0.6444505239	C5	-6.5487503390	-1.1401579379	1.8017157884
H6	4.0768488578	-0.4682148253	-1.6726330044	H6	-6.1271232870	-0.1820923407	2.0443048422
C7	5.1673175193	0.0226829031	0.1022093561	C7	-7.5388284648	-1.6940951469	2.6137725633
H8	6.1256161002	-0.2022842869	-0.3537632582	H8	-7.8657342727	-1.1503577837	3.4897418122
C9	5.1092666031	0.4610614304	1.4246682015	C9	-8.1139482286	-2.9217473243	2.3201628422
H10	6.0158258177	0.5884975117	2.0068552352	H10	-8.8783185332	-3.3446433491	2.9628086895
C11	3.8597824223	0.7406611947	1.9796394490	C11	-7.6960901642	-3.5882736400	1.1735867791
H12	3.7895827601	1.0988570007	3.0029945483	H12	-8.1381472959	-4.5393357958	0.9130491642
C13	2.6917039043	0.5792003613	1.2380766124	C13	-6.7221313761	-3.0347510573	0.3517050985
H14	1.7384410611	0.8228330591	1.6862133820	H14	-6.4331009047	-3.5443580579	-0.5555923075
C15	-0.7511668266	0.1688394029	-1.3957993026	C15	-3.5940133826	0.1950373722	-1.2425500088
C16	-2.0402455530	-0.2741766426	-1.0754827220	C16	-2.4063456942	0.9145213743	-1.0671499623
H17	-2.1721545258	-0.8719877237	-0.1844426129	H17	-2.0209457326	1.0413665974	-0.0658872294
C18	-3.1276929203	0.0466408441	-1.8840816540	C18	-1.7237232264	1.4419544702	-2.1600926465
H19	-4.1194244907	-0.3067505157	-1.6215653129	H19	-0.8005276554	1.9874425982	-2.0052766201
C20	-2.9470140792	-2.879922391	-3.0255270816	C20	-2.2233953498	1.2712779553	-3.4509417854
H21	-3.7954912478	1.0840011685	-3.6516818170	H21	-1.6957632250	1.6900855271	-4.3010067826
C22	-1.6697677621	1.2856009666	-3.3503910988	C22	-3.4099273953	0.5634036437	-3.6405803187
H23	-1.5211611149	1.9062490301	-4.2280203471	H23	-3.8139394307	0.4362281071	-4.6393475437
C24	-0.5825315056	0.9571806945	-2.5416260103	C24	-4.0856813191	0.0261951957	-2.5450804996
H25	0.4050736496	1.3345189406	-2.7720204586	Na25	-3.7067141004	-3.0046053670	-1.1884766466
Na26	1.0450532266	-2.3246480044	1.7991007292	C27	-2.5396032901	-3.1826160014	1.8678128054
C27	0.5559721636	-3.7448111514	-0.8072501558	O27	-2.7539455669	-3.6746424013	0.7206527023
O28	0.5510099302	-3.2914040940	-1.9889440161	N29	-1.7209972211	-2.1846838858	2.1982718349
N29	1.6093087152	-3.9000973675	-0.0051413929	C30	-0.7765743029	-1.6534681876	1.3135446461
C30	2.9104383832	-3.8697174146	-0.5213908339	C31	-0.3223418744	-2.2333917406	0.1091605654
C31	3.9665964987	-3.5001922549	0.3344543705	H32	-0.7638650730	-3.1571452847	-0.2214338261
H32	3.7308200498	-3.1711954053	1.3407777787	C33	0.6944426443	-1.6395026560	-0.6374045214

C33	5.2958915560	-3.5583381321	-0.0685509189	H34	1.0259564017	-2.1210193453	-1.5501446290
H34	6.0760368322	-3.2586234316	0.6236442270	C35	1.2874576515	-0.4479664518	-0.2358201445
C35	5.6296720365	-3.9975240204	-1.3490867787	H36	2.0743670133	0.0063216754	-0.8265224561
H36	6.6667707023	-4.0526791544	-1.6623775035	C37	0.8566624643	0.1393140080	0.9525201346
C37	4.6013071901	-4.3751223491	-2.2140024992	H38	1.3133419710	1.0577803724	1.2988038616
H38	4.8374685185	-4.7375491952	-3.2101189498	C39	-0.1444495962	-0.4565499843	1.7090012545
C39	3.2677434455	-4.3079010408	-1.8179336000	H40	-0.4381874657	-0.0106583439	2.6506426746
H40	2.4910982074	-4.6274162598	-2.4993354756	C41	-3.3131202446	-3.7765120065	3.0310192856
C41	-0.7801335048	-4.1450067264	-0.2135549297	C42	-2.9345534238	-3.5555507070	4.3642302022
C42	-1.9619259554	-3.8026580896	-0.8816193402	H43	-2.0713182687	-2.9336271139	4.5625614792
H43	-1.8893411898	-3.2217339680	-1.7907896100	C44	-3.6303028168	-4.1535571760	5.4135836433
C44	-3.2021861143	-4.1999915508	-0.3884779830	H45	-3.3127222376	-3.9809014749	6.4382727981
H45	-4.1078300668	-3.9244081047	-0.9186776686	C46	-4.7223685993	-4.9826610157	5.1464965655
C46	-3.2827845057	-4.9573574055	0.7807874170	H47	-5.2628111112	-5.4520153940	5.9613686142
H47	-4.2484745579	-5.2728726191	1.1616524313	C48	-5.1102520721	-5.2083032427	3.8239388065
C48	-2.1122510396	-5.3151198863	1.4504756001	H49	-5.9607158717	-5.8475948452	3.6073712404
H49	-2.1630897478	-5.9168785816	2.3523527200	C49	-4.4084254177	-4.6143404417	2.7786397606
C50	-0.8730507088	-4.9112934580	0.9562747987	Na50	-3.2067926131	-0.4646291428	3.0422651741
H51	0.0393115806	-5.2106719047	1.4559562440	H51	-4.7073470382	-4.7816745205	1.7519583134
Na52	1.6387546673	-1.5071203575	-2.8243902311	H52	-5.0171991603	-0.5056120322	-2.6834054625

Table S2d. Final structures of (NaBA)₃ optimized in THF: Cartesian coordinates (Å).

3a	x (Å)	y (Å)	z (Å)	3b	x (Å)	y (Å)	z (Å)
C1	-1.1489050762	1.6824995521	2.2326913673	C1	12.3455943295	-5.3686700465	3.7697786261
C2	-0.3250678574	1.6303437664	3.3568603513	C2	11.2924054293	-5.9301594301	3.0460777212
C3	0.9067951650	0.9813500826	3.3077933059	C3	9.9697684449	-5.6573346259	3.3879544256
C4	1.3531699529	0.3473179946	2.1312737840	C4	9.6618228872	-4.8024562021	4.4648278721
C5	0.5199603338	0.4342485666	1.0032175951	C5	10.7367261269	-4.2678111903	5.2029390643
C6	-0.7115440496	1.0833326396	1.0524603650	C6	12.0571451852	-4.5374899197	4.8537572102
N7	2.6167932803	-0.2801654372	2.0388767120	N7	8.3513661235	-4.5590083478	4.9128839042
C8	2.9827954701	-1.2123753242	2.8973711267	C8	7.3795151962	-4.1166351765	4.1233890883
C9	1.9981533202	-1.8482149384	3.8535225594	C9	7.5942643985	-3.6468938859	2.6977911293
C10	0.7745776091	-2.3598042068	3.4041299181	C10	6.6424875789	-3.9836018707	1.7271075107
C11	-0.1190746650	-2.9490895173	4.2953183473	C11	6.7412840153	-3.4866514879	0.4296686635
C12	0.1848786526	-3.0118637882	5.6549887561	C12	7.7782317407	-2.6159742878	0.0908545307
C13	1.3941840912	-2.4912731192	6.1145752727	C13	8.7208901648	-2.2600725456	1.0546967170
C14	2.2983255479	-1.9245393306	5.2170313439	C14	8.6361519347	-2.7816578148	2.3446587868
Na15	4.8790444592	0.0591732504	1.2332396751	Na15	6.4718598005	-6.6146425554	8.7657696126
O16	4.1970728363	-1.6228109793	2.9488118601	O16	6.1983343998	-3.9888437587	4.5653270794
C17	8.4972756508	-8.6472089228	5.7849575678	C17	7.2950679631	-11.3245977236	4.0901976803
C18	7.5395392298	-8.6807900092	4.7711324574	C18	7.0606970201	-11.4335582490	5.4618035143
C19	7.2308671303	-7.5289731188	4.0513612252	C19	6.7630799418	-10.3036689136	6.2196293039
C20	7.8752144917	-6.3091555444	4.3175616521	C20	6.6805479028	-9.0367610008	5.6214617802
C21	8.8285845946	-6.2883004626	5.3526148896	C21	6.9245004080	-8.9388417480	4.2411953542
C22	9.1369220493	-7.4406771649	6.0692767276	C22	7.2280236341	-10.0690454334	3.4865487046
N23	7.4789387579	-5.1413229134	3.6357861508	N23	6.4476944752	-7.8939320528	6.4205176978
C24	8.3458141637	-4.3421781773	3.0546966886	C24	5.3970512552	-7.1136546349	6.2231199085
C25	9.7909934117	-4.7108461158	2.8105125807	C25	4.2757847696	-7.4136631731	5.2555686108
C26	10.1504647883	-5.9438427423	2.2552679385	C26	3.5777805744	-8.6254531921	5.2660712929
C27	11.4886849385	-6.2489367144	2.0191807104	C27	2.4772822786	-8.8130077995	4.4301018700
C28	12.4863381543	-5.3340758671	2.3528574375	C28	2.0792213862	-7.8026670527	3.5563937192
C29	12.1393651187	-4.1023418104	2.9072974376	C29	2.7822797870	-6.5975451965	3.5296437236
C30	10.7986498569	-3.7903715502	3.1246332447	C30	3.8655678999	-6.3984289761	4.3818914123
Na31	5.7142011169	-3.3646781167	3.3498796083	Na31	8.5182190923	-6.3663885735	6.3663885735
O32	7.9858619510	-3.1810907041	2.6346937657	O32	5.2618537736	-6.0466991332	6.9103502268
C33	12.1725136451	0.5326061143	-3.3838432587	C33	5.9884217714	-0.8541499974	11.6626267599
C34	11.5633157381	1.5555482700	-2.6557961200	C34	5.2551965237	-2.0414686401	11.6603527076
C35	10.4573163402	1.2951698652	-1.8515540972	C35	5.6707722160	-3.1263771960	10.8906498912
C36	9.9203686674	-0.0032972630	-1.7553721069	C36	6.8373927753	-3.0608927718	10.1081967092
C37	10.5566952378	-1.0264975349	-2.4818723232	C37	7.5567157618	-1.8523692242	10.1088942962
C38	11.6596510962	-0.7615427406	-3.2882786263	C38	7.1391282806	-0.7691538019	10.8783195598
N39	8.8716042032	-0.3438285456	-0.8890633201	N39	7.1809944480	-4.1722221296	9.3070266779
C40	7.7521815232	0.3356743188	-0.7461029361	C40	8.3819314652	-4.7215871475	9.2867192535
C41	7.3358227591	1.4060509901	-1.7275677216	C41	9.5151068231	-4.3414927603	10.2135379488
C42	7.4186426348	1.1933758823	-3.1104586910	C42	9.3184338905	-4.1341150548	11.5848311767
C43	7.0115786437	2.1792879617	-4.0054291726	C43	10.3971696925	-3.8549858813	12.4214825134
C44	6.5399393506	3.4037646621	-3.5320263439	C44	11.6857164922	-3.7550471039	11.8967905251
C45	6.4636310434	3.6291514095	-2.1572713313	C45	11.8914134053	-3.9538756221	10.5314654355
C46	6.8469482801	2.6312768649	-1.2624309306	C46	10.8153483087	-4.2584044798	9.7004863081
Na47	8.4414857886	-1.7066485687	1.0034557176	Na47	6.2637821438	-4.0215834651	6.8581773272
O48	6.9624928825	0.0688862995	0.2411569822	O48	8.6223159559	-5.6907792067	8.4783422694
H49	-2.1072095262	2.1900314746	2.2727412797	H49	13.3740646899	-5.5811427825	3.4989205324
H50	-0.6395961717	2.1041168706	4.2817377208	H50	11.5010809914	-6.5869690911	2.2073364944

H51	1.5389636559	0.9650615782	4.1884194897	H51	9.1612815579	-6.1009909867	2.8183111152
H52	0.8354128779	-0.0273609456	0.0802896353	H52	10.5111227045	-3.6221194652	6.0446342938
H53	-1.3298294440	1.1209871062	0.1607892936	H53	12.8646673781	-4.0944732992	5.4285556611
H54	0.5219370985	-2.3062418710	2.3520378827	H54	5.8147387978	-4.6250360245	2.0040574241
H55	-1.0549746698	-3.3563137060	3.9282278027	H55	6.0004072265	-3.7645312486	-0.3130997272
H56	-0.5167614027	-3.4604385207	6.3505305978	H56	7.8458311795	-2.2117350565	-0.9139330774
H57	1.6363915547	-2.5294436400	7.1715903726	H57	9.5209645672	-1.5706939275	0.8052172925
H58	3.2401559673	-1.5259881952	5.5760558301	H58	9.3702387083	-2.4903659322	3.0863493820
H59	8.7326512937	-9.5424812973	6.3502138079	H59	7.5288060536	-12.2041547034	3.5006594086
H60	7.0257262298	-9.6086003199	4.5397690933	H60	7.1062350321	-12.4046743437	5.9440187384
H61	6.4808850892	-7.5639010223	3.2685572326	H61	6.5803633516	-10.3913760452	7.2850941798
H62	9.3203448135	-5.3541539060	5.5992828424	H62	6.8687703668	-7.9667553184	3.7645496805
H63	9.8760547716	-7.3918135178	6.8627959737	H63	7.4087370232	-9.9678943372	2.4212863958
H64	9.3828908057	-6.6646814680	2.0017818838	H64	3.8783327636	-9.4184423448	5.9397086200
H65	11.7526285358	-7.2055148047	1.5808884865	H65	1.9295668265	-9.7489730880	4.4635685838
H66	13.5291876421	-5.5783939970	2.1802750930	H66	1.2242918712	-7.9509240399	2.9048156094
H67	12.9105360956	-3.3868493309	3.1728956184	H67	2.4777149208	-5.8062540621	2.8526887526
H68	10.5274846316	-2.8326056259	3.5554422634	H68	4.4069820065	-5.4589036906	4.3787978812
H69	13.0392257530	0.7374345744	-4.0025599323	H69	5.6649187421	-0.0074048086	12.2592356618
H70	11.9586370840	2.5654393174	-2.7037824290	H70	4.3534441200	-2.1244254270	12.2600102807
H71	10.0132509806	2.0982056365	-1.2752746263	H71	5.0921966926	-4.0442107443	10.8876250427
H72	10.1744925604	-2.0379125048	-2.4015907592	H72	8.4506910224	-1.7637643773	9.5022686819
H73	12.1257877764	-1.5727991072	-3.8391143664	H73	7.7170897852	0.1499585294	10.8627370289
H74	7.7978538491	0.2514164397	-3.4882283261	H74	8.3230576858	-4.1989972307	12.0061106079
H75	7.0682446722	1.9926374435	-5.0728701244	H75	10.2302912396	-3.7134139985	13.4840903622
H76	6.2346034792	4.1764367256	-4.2294452170	H76	12.5239095932	-3.5297581812	12.5479400920
H77	6.1028073204	4.5811796415	-1.7813396290	H77	12.8916930797	-3.8813607789	10.1168525445
H78	6.7934944885	2.8093243407	-0.1945156830	H78	10.9775211375	-4.4361388819	8.6441218287

3c	x (Å)	y (Å)	z (Å)	3c	x (Å)	y (Å)	z (Å)
C1	-4.1422174349	0.6129083963	-3.5426186442	C40	0.6860190527	1.0203047192	2.5286820791
C2	-2.9569198994	0.6043931242	-4.2800946928	C41	1.9104328918	0.2768931342	3.0150742104
C3	-1.7724343928	1.1009285564	-3.7393765948	C42	3.1042918406	0.3773823216	2.2898830552
C4	-1.7339474204	1.6334726127	-2.4279710027	C43	4.2554747163	-0.2762616262	2.7214807693
C5	-2.9428728896	1.6376025542	-1.7052128455	C44	4.2390307834	-1.0247720073	3.8998961049
C6	-4.1225974669	1.1408831338	-2.2515817743	C45	3.0620609885	-1.1125626024	4.6421082529
N7	-0.6021852288	2.2352188429	-1.8650676343	C46	1.9052580984	-0.4700197841	4.1993074371
C8	0.6024579795	1.7285053751	-2.1286581230	Na47	-0.3186617851	-1.9116800943	2.7389725382
C9	1.7785222011	2.5831337595	-1.7069801410	O48	0.8882564132	2.0527118335	1.8288923659
C10	3.0116568476	1.9716425010	-1.4521800322	H49	-5.0615333706	0.2259152353	-3.9686356036
C11	4.1220197783	2.7328448777	-1.0997777140	H50	-2.9545031420	0.2199921138	-5.2959080560
C12	4.0220597910	4.1227927474	-1.0129371313	H51	-0.8748663255	1.1134072871	-4.3427876284
C13	2.8038897710	4.7443240409	-1.2825809309	H52	-2.9487985808	2.0367046078	-0.6971277304
C14	1.6883803882	3.9783632961	-1.6235724686	H53	-5.0333374467	1.1663891399	-1.6617727758
Na15	-0.3531545850	3.1849079505	0.3481033951	H54	3.0789435273	0.8946334309	-1.5420205414
O16	0.8610665630	0.6157721700	-2.6670122014	H55	5.0711094132	2.2463352172	-0.9000221348
C17	-4.4453011698	-3.1939002502	0.9504941460	H56	4.8900308641	4.7167461924	-0.7462874097
C18	-4.2484032532	-2.2044643666	-0.0123127200	H57	2.7224770532	5.8257030112	-1.2380345115
C19	-3.0019645071	-2.0323920931	-0.6098422012	H58	0.7511185566	4.4629868716	-1.8701585996
C20	-1.9067314512	-2.8456758009	-0.2689648754	H59	-5.4175174716	-3.3318499216	1.4113599992
C21	-2.1209996926	-3.8417930005	0.7089048036	H60	-5.0707534629	-1.5601503613	-0.3052990929
C22	-3.3698077010	-4.0126471909	1.3011210555	H61	-2.8686586739	-1.2502898633	-1.3479380203
N23	-0.7014573821	-2.7128010224	-0.9769497864	H62	-1.3065027994	-4.5039740841	0.9740219881
C24	0.4509801323	-2.7728729727	-0.3147737138	H63	-3.5049151038	-4.8014069638	2.0355864199
C25	1.6887281647	-2.8437740888	-1.1799435051	H64	0.7587335123	-3.9495866576	-2.7704538069
C26	1.6768475005	-3.4895228939	-2.4231727713	H65	2.8176551943	-4.1072172650	-4.1399819939
C27	2.8401124256	-3.5869556000	-3.1877911913	H66	4.9344313061	-3.0992597865	-3.3164783287
C28	4.0292104172	-3.0279804667	-2.7225393612	H67	4.9766299370	-1.9545957073	-1.1152732951
C29	4.0511231261	-2.3846223878	-1.4834579865	H68	2.9058096398	-1.8259253013	0.2574538687
C30	2.8936662740	-2.3041210742	-0.7138177945	H69	-5.0691693802	3.0734762088	2.0444037255
Na31	-0.2609177331	-1.3031775039	-2.8803094189	H70	-3.0845524112	4.3009005976	2.9207254355
O32	0.6266391859	-2.7522296359	0.9364522898	H71	-0.9551786091	3.1231729987	3.2879329562
C33	-4.1261674465	2.5588387793	2.1939361879	H72	-2.7277162496	-0.5206098731	1.8778879771
C34	-3.0102436700	3.2445187383	2.6785978723	H73	-4.8600932971	0.6403232649	1.5458808482
C35	-1.7984521275	2.5851907714	2.8756993289	H74	3.1100655492	0.9782520542	1.3891340124
C36	-1.6598285518	1.2066815398	2.5976280982	H75	5.1715549090	-0.1966702337	2.1452578320
C37	-2.7978750144	0.5346245809	2.1152871824	H76	5.1386503823	-1.5268049868	4.2404933388
C38	-4.0068181879	1.1967679291	1.9187471324	H77	3.0447612731	-1.6740847556	5.5707379930
N39	-0.4882907073	0.4826526179	2.8623974333	H78	1.0000254687	-0.5142519062	4.7925505649

Table S2e. Final structures of (NaBA)₄ optimized in THF: Cartesian coordinates (Å).

4a	x (Å)	y (Å)	z (Å)	4b	x (Å)	y (Å)	z (Å)
----	-------	-------	-------	----	-------	-------	-------

C1	-1.9091631784	3.2033000458	1.8136577082	N1	-0.1431541409	-1.0269043320	3.7550629983
C2	-1.3535546658	4.4273397255	2.2197148333	N2	3.2258313215	-3.4803557506	-0.6204031521
C3	-1.9185963139	5.1589667621	3.2593542137	N3	1.2362782539	-5.4807380631	1.8463741611
C4	-3.0427511038	4.6810259145	3.9311548294	N4	3.3430968575	-0.1481916635	2.9641839246
C5	-3.5895501771	3.4564550903	3.5515850778	C5	-0.8998636623	-1.6491069972	2.8683846190
C6	-3.0305316732	2.7225086997	2.5106034809	C6	2.9766068016	-2.2072891571	-0.8726082866
N7	-1.2692486192	2.4575168634	0.8113090687	C7	1.2965798857	-5.2030480371	3.1375000578
C8	-1.8703805109	1.9174052272	-0.2164893731	C8	4.3155106903	-0.7247651392	2.7662436104
O9	-1.2278529737	1.0691315004	-0.9599648448	Na9	0.7759814187	-3.4819176608	0.4394192827
C10	-3.2677553640	2.2592583442	-0.6717143767	Na10	2.1240825850	-1.9575552824	4.1144964893
C11	-3.7754372468	3.5618624947	-0.5938509129	Na11	3.4645144475	-3.9596368427	1.8019340930
C12	-5.0384984191	3.8599154264	-1.0985744591	Na12	1.3274442048	-0.3972053720	1.6023418945
C13	-5.8209885890	2.8590712793	-1.6710403406	O13	-0.3925727505	-2.0808079597	1.7794912345
C14	-5.3258542783	1.5591041911	-1.7517654876	O14	2.1425034471	-1.5635596415	-0.1504037778
C15	-4.0539074030	1.2681389057	-1.2693313619	O15	1.8505818759	-4.1227599665	3.5320409053
H16	-5.9255697723	0.7752280790	-2.2005141704	O16	4.0471585490	-1.9716753901	2.6930668996
H17	-3.6566008661	0.2663078504	-1.3567820045	C17	-0.5964766247	-0.6295409934	5.0271093344
H18	-0.4750922429	4.7977941533	1.7022141603	C18	4.2181076444	-4.2252970526	-1.2870438542
H19	-1.4751705526	6.1056880096	3.5490071071	C19	0.5438473691	-6.5866041307	1.3170515803
H20	-3.4789430116	5.2484656785	4.7451038310	C20	3.5290155113	1.5437244403	2.9394611973
H21	-4.4556342905	3.0641500418	4.0740939663	C21	-0.3207248807	0.6781162646	5.4652471522
H22	-3.4545976304	1.7644752763	2.2336032803	C22	5.5614602310	-3.8154117616	-1.3723985039
H23	-3.1821470883	4.3452857931	-0.1410157673	C23	-0.8120074403	-6.8483419501	1.5913467840
H24	-5.4124548005	4.8760041132	-1.0409147144	C24	4.1249256830	2.2237679903	1.8614555007
H25	-6.8076185073	3.0916356551	-2.0558727022	C25	-0.6830719652	1.1025895331	6.7409434156
Na26	0.8682305042	1.6401533384	0.2358934145	C26	6.5201542030	-4.6191772988	-1.9853389211
C27	1.2185012371	-1.3957166958	1.3088818365	C27	-1.4724169519	-7.9178802096	0.9899107572
C28	2.0525981391	-1.3180941640	2.5615368443	C28	4.2234477679	3.6127152855	1.8565538476
N29	0.2082408820	-2.2078945686	1.1352777821	C29	-1.3199672846	0.2281846417	7.6229945497
O30	1.5160924669	-0.5435127154	0.3755744659	C30	6.1712735650	-5.8585162175	-2.5224164187
C31	1.4869507781	-1.4496484897	3.8351437561	C31	-0.8061637548	-8.7474343289	0.0867059801
C32	3.4183196382	-1.0279042201	2.4571201203	C32	3.7202043528	4.3650787046	2.9183865902
C33	-0.0956345102	-3.3072438694	1.9542775567	C33	-1.5826322639	-1.0782854555	7.2094717722
C34	2.2712271198	-1.2976230437	4.9750648164	C34	4.8466791632	-6.2680573651	-2.4627362323
H35	0.4314792959	-1.6652781024	3.9364740319	C35	0.5330931620	-8.4876819726	-0.2100517954
C36	4.2077337299	-0.9027708218	3.5961075107	C36	3.1083057189	3.7058017890	3.9849236265
H37	3.8557225272	-0.8999991411	1.4747514969	C37	-1.2223702548	-1.5052679599	5.9337305224
C38	-1.4164321641	-3.4832401859	2.3983673055	C38	3.8868408851	-5.4878246054	-1.8109801325
C39	0.8437783813	-4.3059846997	2.2610683248	C39	1.1959438883	-7.4199537231	0.3909586237
C40	3.6344233151	-1.0338453881	4.8598104362	C40	3.0078304857	2.3170764272	3.9916001931
H41	1.8158803315	-1.3883592702	5.9546844506	H41	0.1758470640	1.3557768647	4.7802473936
H42	5.2673466540	-0.6942612110	3.4984912244	H42	5.8472963600	-2.8527233240	-0.9666182700
C43	-1.7757247781	-4.5969167105	3.1506169386	H43	-1.3424616570	-6.2118226300	2.2900713091
H44	-2.1536479478	-2.7261128710	2.1528114750	H44	4.5211578293	1.6542346865	1.0291343296
C45	0.4782696847	-5.4195884616	3.0107989921	H45	-0.4674577936	2.1214004589	7.0479265994
H46	1.8613253525	-4.2033488809	1.9026955325	H46	7.5472410861	-4.2728957166	-2.0445781831
H47	4.2451829589	-0.9256523326	5.7491099589	H47	-2.5168302624	-8.1005376026	1.2252342126
C48	-0.8305705864	-5.5722049555	3.4652881675	H48	4.6937488015	4.1107051766	1.0143763015
H49	-2.8004466683	-4.7046309071	3.4901390045	H49	-1.5996790886	0.5568553249	8.6178840665
H50	1.2220578039	-6.1764446015	3.2365847293	H50	6.9196621845	-6.4810463585	-3.0012060443
H51	-1.1119170301	-6.4423893311	4.0470342342	H51	-1.3235775864	-9.574469523	-0.3830163803
Na52	-0.5680649023	-1.1141361525	-0.8020171277	H52	3.7971902307	5.4466647829	2.9113466508
C53	-0.6584585580	-0.2912798846	-6.0581255405	H53	-2.0691947250	-1.7733609689	7.8868522472
C54	-0.2618251136	0.7178760857	-6.9505265541	H54	4.5580997037	-7.2516199708	-2.8353966396
C55	-0.7421362772	0.7477867876	-8.2558763203	H55	1.0653696373	-9.1205743808	-0.9136713599
C56	-1.6433325271	-0.2188193873	-8.6999892266	H56	2.7072772130	4.2761508757	4.8172425481
C57	-2.0608450564	-1.2129428835	-7.8167116227	H57	-1.4343606697	-2.5226869532	5.6271048157
C58	-1.5807534208	-1.2492572242	-6.5114327413	H58	2.8599148910	-5.8253611338	-1.7353313492
N59	-0.2092363945	-0.2409587845	-4.7284422003	H59	2.2358520445	-7.2194763487	0.1588566107
C60	0.3067682878	-1.2468559428	-4.0709815588	H60	2.5296207868	1.8068180191	4.8193993823
O61	0.5007077341	-1.1383832618	-2.7915174934	C61	-2.3923126564	-1.8416151873	3.0266837821
C62	0.7775142609	-2.5398345354	-4.6891643300	C62	3.5703944561	-1.4452631176	-2.0386865601
C63	1.4076533845	-2.5765549024	-5.9390376472	C63	0.8049145324	-6.1338486243	4.2239765594
C64	1.9042221318	-3.7745150724	-6.4457202035	C64	5.7801731585	-0.3574471313	2.6689035274
C65	1.7616659493	-4.9568254017	-5.7222378738	C65	-2.9532570434	-3.0885425205	2.7277127630
C66	1.1344644167	-4.9319945358	-4.4779390186	C66	4.0037272654	-0.1287419582	-1.8409073378
C67	0.6613746802	-3.7301266155	-3.9604845033	C67	1.0771335227	-7.5070403236	4.2069566760
H68	1.0219906101	-5.8466668206	-3.9064894843	C68	6.3920998060	-0.5170075064	3.5737582846
H69	0.1983444980	-3.7067827292	-2.9819751965	C69	-4.3281845801	-3.2920425650	2.8216268391
H70	0.4367549715	1.4725610562	-6.6055646480	C70	4.5047082517	0.6243436598	-2.9003587484
H71	-0.4132348302	1.5326212296	-8.9287492115	C71	0.6739543071	-8.3231671353	5.2618026492
H72	-2.0215819007	-0.1920843990	-9.7154549693	C72	7.7590755278	-0.7279246102	3.4929678472
H73	-2.7710650236	-1.9651044081	-8.1438349080	C73	-5.1665968415	-2.2391259794	3.1907298564
H74	-1.9211834028	-2.0199750334	-5.8306768227	C74	4.5491177790	0.0804372772	-4.1845306593
H75	1.5160584874	-1.6675662142	-6.5156055791	C75	-0.0287784779	-7.7829417474	6.3381573267
H76	2.4011314649	-3.7835648088	-7.4092957488	C76	8.5292538265	0.1871729214	2.4922798216

H77	2.1410627730	-5.8901300647	-6.1233703099	C77	-4.6193611000	-0.9877112587	3.4715492590
Na78	-0.0844995052	1.2490668940	-2.9003976310	C78	4.0971823110	-1.2214935014	-4.3969182725
C79	3.0889005214	2.1344929029	-2.0631678639	C79	-0.3080545800	-6.4159687586	6.3630004380
C80	3.4718862683	3.5930387356	-2.021920546	C80	7.9278250861	-0.6844750519	1.5846575928
N81	3.9239012647	1.1473079202	-2.2602833291	C81	-3.2409268556	-0.7928738936	3.4014886374
O82	1.8411312587	1.8788788802	-1.8204370839	C82	3.6222847781	-1.9830590224	-3.3304503251
C83	4.6630941178	4.0277199511	-1.4295648087	C83	0.1200559581	-5.5974721920	5.3202513554
C84	2.5779866210	4.5504695427	-2.5157011255	C84	6.5671518226	-0.9658166624	1.6848889673
C85	5.2415985307	1.2784134410	-2.7247794322	H85	-2.3018016131	-3.8965948164	2.4155483129
C86	4.9509054065	5.3867200252	-1.3355996731	H86	3.9375295142	0.3023538754	-0.8498585894
H87	5.3659267243	3.3035669480	-1.0389071048	H87	1.6125245371	-7.9414895954	3.3723835456
C88	2.8766979264	5.9073869411	-2.4459079991	H88	5.8025066630	0.9922076206	4.3473907065
H89	1.6447240293	4.2226479579	-2.9557899047	H89	-4.7476462872	-4.2679969781	2.5998328863
C90	6.2703015939	0.5967076830	-2.0541233063	H90	4.8502894169	1.6385158486	-2.7283743455
C91	5.5660972913	1.9731479991	-3.9020630301	H91	0.9074740564	-9.3825049669	5.2413025186
C92	4.0639801515	6.3300337599	-1.8506081043	H92	8.2223458480	1.4457313098	4.2113065441
H93	5.8724774156	5.7079874989	-0.8632726426	H93	-6.2389943692	-2.3919226679	3.2540781249
H94	2.1802611672	6.6349335942	-2.8476765798	H94	4.9266786395	0.6692970061	-5.0138973105
C95	7.5794854047	0.6375434386	-2.5224340829	H95	-0.3502329658	-8.4207746742	7.1545990001
H96	6.0254028140	0.0397677204	-1.1557863434	H96	9.5910380325	0.3999625578	2.4233124347
C97	6.8764733189	2.0073889523	-4.3682579277	H97	-5.2663622003	-0.1614988257	3.7483399291
H98	4.7806413698	2.4787143084	-4.4514120050	H98	4.1151058627	-1.6465630325	-5.3949167557
H99	4.2946913759	7.3875286543	-1.7856761205	H99	-0.8505971383	-5.9885034480	7.1998312356
C100	7.8931133169	1.3458637210	-3.6814393272	H100	8.5217302501	-1.1497831239	0.8052662283
H101	8.3576579527	0.1096044123	-1.9815259333	H101	-2.8264329186	0.1847647477	3.637823278
H102	7.1026541526	2.5505751032	-5.2796337356	H102	3.2837036690	-2.9960961907	-3.5079010575
H103	8.9120067306	1.3724463954	-4.0499271735	H103	-0.0677433678	-4.5309418669	5.3500336809
Na104	2.4080311520	-0.5536202928	-1.7112971790	H104	6.1025957975	-1.6639150624	1.0006327518

4c	x (Å)	y (Å)	z (Å)	4c	x (Å)	y (Å)	z (Å)
N1	0.0693120939	4.6773848152	0.1282330830	H53	-1.4029989539	8.5874682292	1.9565686000
N2	-4.6773848152	0.0693120939	0.1282330830	H54	-8.5874682292	-1.4029989539	1.9565686000
N3	-0.0693120939	-4.6773848152	0.1282330830	H55	1.4029989539	-8.5874682292	1.9565686000
N4	4.6773848152	-0.0693120939	0.1282330830	H56	8.5874682292	1.4029989539	1.9565686000
C5	1.1685631958	3.9901350161	-0.0576940630	H57	-1.1281049011	6.1265437545	1.9428317707
C6	-3.9901350161	1.1685631958	-0.0576940630	H58	-6.1265437545	-1.1281049011	1.9428317707
C7	-1.1685631958	-3.9901350161	-0.0576940630	H59	1.1281049011	-6.1265437545	1.9428317707
C8	3.9901350161	-1.1685631958	-0.0576940630	H60	6.1265437545	1.1281049011	1.9428317707
Na9	-1.2089807479	2.7211363496	-0.0418337814	C61	2.5552465871	4.5861237303	-0.0767415755
Na10	-2.7211363496	-1.2089807479	-0.0418337814	C62	-4.5861237303	2.5552465871	-0.0767415755
Na11	1.2089807479	-2.7211363496	-0.0418337814	C63	-2.5552465871	-4.5861237303	-0.0767415755
Na12	2.7211363496	1.2089807479	-0.0418337814	C64	4.5861237303	-2.5552465871	-0.0767415755
O13	1.1126400121	2.7067077119	-0.1904886041	C65	3.4604341572	4.1984102378	-1.0727740835
O14	-2.7067077119	1.1126400121	-0.1904886041	C66	-4.1984102378	3.4604341572	-1.0727740835
O15	-1.1126400121	-2.7067077119	-0.1904886041	C67	-3.4604341572	-4.1984102378	-1.0727740835
O16	2.7067077119	-1.1126400121	-0.1904886041	C68	4.1984102378	-3.4604341572	-1.0727740835
C17	-0.0058531426	6.0795300567	0.1150159214	C69	4.7671303337	4.6801710196	-1.0725796567
C18	-6.0795300567	-0.0058531426	0.1150159214	C70	-4.6801710196	4.7671303337	-1.0725796567
C19	0.0058531426	-6.0795300567	0.1150159214	C71	-4.7671303337	-4.6801710196	-1.0725796567
C20	6.0795300567	0.0058531426	0.1150159214	C72	4.6801710196	-4.7671303337	-1.0725796567
C21	0.5038159776	6.8648340238	-0.9330390274	C73	5.1913060483	5.5415119684	-0.0626438769
C22	-6.8648340238	0.5038159776	-0.9330390274	C74	-5.5415119684	5.1913060483	-0.0626438769
C23	-0.5038159776	-6.8648340238	-0.9330390274	C75	-5.1913060483	-5.5415119684	-0.0626438769
C24	6.8648340238	-0.5038159776	-0.9330390274	C76	5.5415119684	-5.1913060483	-0.0626438769
C25	0.3421960321	8.2474042899	-0.9298048669	C77	4.3001750184	5.9263846217	0.9371107196
C26	-8.2474042899	0.3421960321	-0.9298048669	C78	-5.9263846217	4.3001750184	0.9371107196
C27	-0.3421960321	-8.2474042899	-0.9298048669	C79	-4.3001750184	-5.9263846217	0.9371107196
C28	8.2474042899	-0.3421960321	-0.9298048669	C80	5.9263846217	-4.3001750184	0.9371107196
C29	-0.3364789625	8.8812428578	0.1094464141	C81	2.9880679245	5.4601711292	0.9261646023
C30	-8.8812428578	-0.3364789625	0.1094464141	C82	-5.4601711292	2.9880679245	0.9261646023
C31	0.3364789625	-8.8812428578	0.1094464141	C83	-2.9880679245	-5.4601711292	0.9261646023
C32	8.8812428578	0.3364789625	0.1094464141	C84	5.4601711292	-2.9880679245	0.9261646023
C33	-0.8638467361	8.1102220741	1.1448375217	H85	3.1278960747	3.5358494322	-1.8650738205
C34	-8.1102220741	-0.8638467361	1.1448375217	H86	-3.5358494322	3.1278960747	-1.8650738205
C35	0.8638467361	-8.1102220741	1.1448375217	H87	-3.1278960747	-3.5358494322	-1.8650738205
C36	8.1102220741	0.8638467361	1.1448375217	H88	3.5358494322	-3.1278960747	-1.8650738205
C37	-0.7087270868	6.7280340299	1.1440486521	H89	5.4537705798	4.3789869929	-1.8554386992
C38	-6.7280340299	-0.7087270868	1.1440486521	H90	-4.3789869929	5.4537705798	-1.8554386992
C39	0.7087270868	-6.7280340299	1.1440486521	H91	-5.4537705798	-4.3789869929	-1.8554386992
C40	6.7280340299	0.7087270868	1.1440486521	H92	4.3789869929	-5.4537705798	-1.8554386992
H41	1.0222151025	6.3825600275	-1.7535594126	H93	6.2110979639	5.9090479614	-0.0543630341
H42	-6.3825600275	1.0222151025	-1.7535594126	H94	-5.9090479614	6.2110979639	-0.0543630341
H43	-1.0222151025	-6.3825600275	-1.7535594126	H95	-6.2110979639	-5.9090479614	-0.0543630341
H44	6.3825600275	-1.0222151025	-1.7535594126	H96	5.9090479614	-6.2110979639	-0.0543630341
H45	0.7467296762	8.8324606660	-1.7491010149	H97	4.6261243825	6.5943704913	1.7265435568

H46	-8.8324606660	0.7467296762	-1.7491010149	H98	-6.5943704913	4.6261243825	1.7265435568
H47	-0.7467296762	-8.8324606660	-1.7491010149	H99	-4.6261243825	-6.5943704913	1.7265435568
H48	8.8324606660	-0.7467296762	-1.7491010149	H100	6.5943704913	-4.6261243825	1.7265435568
H49	-0.4609129231	9.9581480598	0.1080280258	H101	2.2971077830	5.7729392071	1.6991271749
H50	-9.9581480598	-0.4609129231	0.1080280258	H102	-5.7729392071	2.2971077830	1.6991271749
H51	0.4609129231	-9.9581480598	0.1080280258	H103	-2.2971077830	-5.7729392071	1.6991271749
H52	9.9581480598	0.4609129231	0.1080280258	H104	5.7729392071	-2.2971077830	1.6991271749

Table S2f. Final structures of (NaBA)₅ optimized in THF: Cartesian coordinates (Å).

5a	x (Å)	y (Å)	z (Å)	5b	x (Å)	y (Å)	z (Å)
N1	2.3858413652	5.1041053448	0.0356653723	N1	2.7429238143	0.5929475804	1.2645855006
N2	-4.1170271203	3.8463252698	0.0356653723	N2	-2.2426013912	2.4168081500	1.2284166171
N3	-4.9303040581	-2.7269455962	0.0356653723	N3	-3.0951995516	-0.6208467383	-0.5860362323
N4	1.0699316375	-5.5316703338	0.0356653723	N4	0.5614466119	-3.3025587058	0.0453505285
N5	5.5915581757	-0.6918146846	0.0356653723	N5	1.0495314642	-1.1690945777	3.9631249368
C6	3.2840459800	4.1702559902	0.2810581570	C6	2.1416743296	1.4200955018	0.4239045922
C7	-2.9513231159	4.4119933010	0.2810581570	C7	-1.7567114010	2.7903452070	2.3952123810
C8	-5.1080639774	-1.4434941720	0.2810581570	C8	-4.0079366981	-1.2388334218	0.1406339160
C9	-0.2056340388	-5.3041217618	0.2810581570	C9	0.5644040824	-2.4026374121	-0.9312459812
C10	4.9809751522	-3.3824633573	0.2810581570	C10	-0.1411348922	-1.6596783262	3.7103947402
Na11	0.4054843266	3.8858837068	0.5571909552	Na11	-2.6016942449	0.1833943884	2.3681828228
Na12	-3.5703934731	1.5864426147	0.5571909552	Na12	-1.0124220484	0.7718011911	-0.3459839381
Na13	-2.6121088462	-2.9054082498	0.5571909552	Na13	-1.5947836546	-2.3209128888	0.8316261248
Na14	1.9560214238	-3.3820836642	0.5571909552	Na14	1.3922844572	-1.4041140132	1.4498471285
Na15	3.8209965688	0.8151655925	0.5571909552	Na15	0.7313145680	1.0625811163	2.8605526547
O16	2.9318872446	2.9505312777	0.4598530245	O16	0.8831967707	1.6012537807	0.5150110706
O17	-1.9001190140	3.7001547763	0.4598530245	O17	-1.3251730180	1.9122859726	3.2285030083
O18	-4.1062253780	-0.6637098624	0.4598530245	O18	-3.7491101960	-1.5165551342	1.3670892239
O19	-0.6376678350	-4.1103500299	0.4598530245	O19	0.1739572374	-1.2137487578	-0.6598199056
O20	3.7121249824	-1.8766261618	0.4598530245	O20	-0.7687613919	-1.2449258143	2.6564235134
C21	2.6998596765	6.3904737050	-0.4307496670	C21	4.0851596673	0.1816746725	1.1504184453
C22	-5.2433991369	4.5424841154	-0.4307496670	C22	-2.9088582712	3.3113339813	0.3581084476
C23	-5.9404585597	-3.5830641284	-0.4307496670	C23	-3.3365987142	-0.0735499016	-1.8605705141
C24	1.5719938383	-6.7569395306	-0.4307496670	C24	1.2146943477	-4.5502194079	-0.0152514766
C25	6.9120041818	-0.5929541615	-0.4307496670	C25	1.7665218532	-1.4472115884	5.1471066858
C26	3.6048729191	6.6324346202	-1.4838885306	C26	4.6194162761	-0.3712528941	-0.0289336210
C27	-5.1938531699	5.4779728918	-1.4838885306	C27	-2.3212126947	3.7059899721	-0.8539396484
C28	-6.8148507106	-3.2468611836	-1.4838885306	C28	-4.4201480648	0.7806062146	-2.1364290625
C29	0.9820438024	-7.4846434600	-1.4838885306	C29	2.5654744577	-4.6763179819	-0.3875291679
C30	7.4217871590	-1.3789028684	-1.4838885306	C30	3.1153924684	-1.8237016758	5.0531516065
C31	3.8165951402	7.9198724176	-1.9691557366	C31	5.9257406538	-0.5837692106	-0.0647781414
C32	-6.3528535120	6.0771728485	-1.9691557366	C32	-3.0097236935	4.5114160958	-1.7571660992
C33	-7.7428745362	-4.1639730417	-1.9691557366	C33	-4.5703613769	1.3520290436	-3.3942794608
C34	1.5674938780	-8.6506497165	-1.9691557366	C34	3.2046920013	-5.9127575436	-0.3546993222
C35	8.7116390299	-1.1824225079	-1.9691557366	C35	3.8759588942	-2.0485918997	6.1976661651
C36	3.1294510725	9.0077775886	-1.4296558026	C36	6.7314218925	-0.8084614226	1.0728194083
C37	-7.5998520085	5.7598411913	-1.4296558026	C37	-4.3051304847	4.9409117055	-1.4748373174
C38	-7.8264179232	-5.4479999626	-1.4296558026	C38	-3.6405152545	1.1062429611	-4.4061941988
C39	2.7628597218	-9.1268903389	-1.4296558026	C39	2.5210780946	-7.0547791910	0.0627882388
C40	9.5339591374	-0.1927284785	-1.4296558026	C40	3.3142079243	-1.8855352388	7.4636834795
C41	2.2133276861	8.7817914499	-0.4018767560	C41	6.2079388443	-0.2795103030	2.2533929576
C42	-7.6680241141	4.8187225177	-0.4018767560	C42	-4.9017941962	4.5546331900	-0.2754328782
C43	-6.9524272152	-5.8036571517	-0.4018767560	C43	-2.5440943638	0.2901861270	-4.1349623697
C44	3.3711877908	-8.4055798965	-0.4018767560	C44	1.1892167786	-6.9387104592	0.4602756560
C45	9.0359358523	0.6087230805	-0.4018767560	C45	1.9819251524	-1.4878898009	7.5685097860
C46	1.9971398121	7.4951580529	0.0838191998	C46	4.9019952241	0.2016787803	2.2946291400
C47	-6.5111687648	4.2155240461	0.0838191998	C47	-4.2154646056	3.7469311574	0.6276059767
C48	-6.0212634152	-4.8898209120	0.0838191998	C48	-2.3884593080	-0.2882454221	-2.8758977417
C49	2.7898233189	-7.2375995686	0.0838191998	C49	0.5481006163	-5.7028322309	0.4291994071
C50	7.7454690490	0.4167383816	0.0838191998	C50	1.2163678693	-1.2684602578	6.4262607459
H51	4.1307290686	5.7993364819	-1.9350995501	H51	4.0044488535	-0.4182791853	-0.9200866421
H52	-4.2390312699	5.7206503267	-1.9350995501	H52	-1.3003498044	3.4069939180	-1.0708738159
H53	-6.7505944728	-2.2637801422	-1.9350995501	H53	-5.1349386859	1.0011565950	-1.3533865235
H54	0.0669344415	-7.1197433977	-1.9350995501	H54	3.1158961880	-3.7954392331	-0.6987395166
H55	6.7919622326	-2.1364632688	-1.9350995501	H55	3.5626364706	-1.9359405945	4.0719711349
H56	4.5177658707	8.0712433718	-2.7845058781	H56	6.3140740046	-1.2712081917	-0.9882753674
H57	-6.2801421727	-6.7908020380	-2.7845058781	H57	-2.5295436447	4.8054566558	-2.6843327487
H58	-8.3991071876	-3.8742969014	-2.7845058781	H58	-5.4150354388	2.0066415040	-3.5810666086
H59	1.0892084556	-9.1852492056	-2.7845058781	H59	4.2468458611	-5.9819824533	-0.6495856238
H60	9.0722750340	-1.8024993028	-2.7845058781	H60	4.9139428013	-2.3487830311	6.0986698918
H61	3.2932531871	10.0093583215	-1.8127131184	H61	7.7473015741	-1.1866464094	1.0425273105
H62	-8.5017942540	6.2251317275	-1.8127131184	H62	-4.8419988501	5.5668195209	-2.1789540815
H63	-8.5476510014	-6.1620153294	-1.8127131184	H63	-3.7628780131	1.5561049873	-5.3854290307

H64	3.2190554111	-10.0334666403	-1.8127131184	H64	3.0222008786	-8.0161848492	0.0900896044
H65	10.5371366572	-0.0390080793	-1.8127131184	H65	3.9087252616	-2.0559873903	8.3543900664
H66	1.6589775117	9.6128516360	0.0236415964	H66	6.8188242797	-0.2435314324	3.1497280210
H67	-8.6297129442	4.5843158928	0.0236415964	H67	-5.9099534204	4.8814897009	-0.0403159913
H68	-6.9924334243	-6.8018378227	0.0236415964	H68	-1.8059751302	0.0936019951	-4.9056671420
H69	4.3081514239	-8.7520828532	0.0236415964	H69	0.6457946035	-7.8145309836	0.8003316631
H70	9.6550174330	1.3927531471	0.0236415964	H70	1.5337182582	-1.3423574110	8.5460538601
H71	1.2642270351	7.3293103623	0.8641914987	H71	4.4949848327	0.6021565183	3.2159297507
H72	-6.5799207414	3.4672328188	0.8641914987	H72	-4.6884539135	3.4429003023	1.5547701836
H73	-5.3308416966	-5.1864426333	0.8641914987	H73	-1.5367703544	-0.9232189353	-2.6645470417
H74	3.2852793842	-6.6726306469	0.8641914987	H74	-0.4815316011	-5.6182179860	0.7577898844
H75	7.3612560186	1.0625300991	0.8641914987	H75	0.1841805673	-0.9565054876	6.5203615015
C76	4.7500117245	4.5013824252	0.4515383932	C76	2.8695810792	2.2320416919	-0.6200782732
C77	-2.8132347414	5.9085332706	0.4515383932	C77	-1.6700790347	4.2411511820	2.8072793066
C78	-6.4886864130	-0.8497080403	0.4515383932	C78	-5.3455765334	-1.7110343889	-0.3854275104
C79	-1.1969940042	-6.4336817200	0.4515383932	C79	0.9657929037	-2.677070412	-2.358178477
C80	5.7489034341	-3.1265259355	0.4515383932	C80	-0.7866827675	-2.7628401130	4.5099691536
C81	5.7351476628	3.7882794255	-0.2376280172	C81	4.0634526288	2.9015640642	-0.3307580058
C82	-1.8306097401	6.6250922786	-0.2376280172	C82	-2.1449732114	4.6291624904	4.0649763930
C83	-6.8665267024	0.3062527812	-0.2376280172	C83	-6.4294500027	-1.7758193689	0.4992423344
C84	-2.4131371466	-6.4358176506	-0.2376280172	C84	0.7093333912	-3.8996833298	-2.9893814236
C85	5.3751259263	-4.2838068347	-0.2376280172	C85	-0.0764662417	-3.9315049133	4.8121612889
C86	7.0830570950	4.1043438582	-0.0769069553	C86	4.6782663394	3.7007946420	-1.2920115472
C87	-1.7146779569	8.0046996085	-0.0769069553	C87	-2.0493085437	5.9523947221	4.4869276362
C88	-8.1427863522	8.6808232696	-0.0769069553	C88	-7.6681665730	-2.2545785076	0.0799624233
C89	-3.3178407718	-7.4838004336	-0.0769069553	C89	1.0346935564	-4.0844344340	-4.3307978136
C90	6.0922479859	-5.4680756026	-0.0769069553	C90	-0.6950819500	-4.9835349419	5.4824828038
C91	7.4657045808	5.1146581196	0.8042703236	C91	4.1212653163	3.8224669941	-2.5641698249
C92	-2.5572993428	8.6808232697	0.8042703236	C92	-1.4419559324	6.9040445126	3.6679131310
C93	-9.0462024941	0.2503857114	0.8042703236	C93	-7.8352549888	-2.7087841675	-1.2281057869
C94	-3.0335612677	-8.5260763897	0.8042703236	C94	1.6425926398	-3.0588080170	-5.0538415427
C95	7.1713585237	-5.5197907109	0.8042703236	C95	-2.0258950623	-4.8740997007	5.8820194221
C96	6.4915016751	5.8120119033	1.5183641305	C96	2.9338996007	3.1549148364	-2.8638347508
C97	-3.5215674568	7.9697954182	1.5183641305	C97	-0.9395164586	6.5225653363	2.4256188937
C98	-8.6679500571	-0.8864074515	1.5183641305	C98	-6.7570321930	-2.6732340529	-2.1114662646
C99	-1.8355202912	-8.5176253511	1.5183641305	C99	1.9069220081	-1.8384599579	-4.4326016803
C100	7.5335361300	-4.3777745190	1.5183641305	C100	-2.7404654712	-3.7129087195	5.5895716699
C101	5.1435407236	5.5153882631	1.3336201964	C101	2.3061220053	2.3797279895	-1.8923462361
C102	-3.6560044527	6.5961466259	1.3336201964	C102	-1.0631506565	5.2032109547	1.9926670398
C103	-7.4030757384	-1.4387454535	1.3336201964	C103	-5.5264791710	-2.1684001469	-1.6969042944
C104	-0.9193479749	-7.4853402174	1.3336201964	C104	1.5566261295	-1.6456744959	-3.0989940887
C105	6.8348874424	3.1874492182	1.3336201964	C105	-2.1286157247	-2.6731575719	4.8929157596
H106	5.4488148832	3.0016605144	-0.9259766251	H106	4.5116442326	2.8031863914	0.6500401219
H107	-1.1709723938	6.1096950110	-0.9259766251	H107	-2.5912170563	3.8863858605	4.7121706960
H108	-6.1725156224	0.7743386633	-0.9259766251	H108	-6.2870879965	-1.4560149637	1.5228998055
H109	-2.6438520570	-5.6311273983	-0.9259766251	H109	0.2570690737	-4.7112231927	-2.4358691585
H110	4.5385251900	-4.2545667905	-0.9259766251	H110	0.9611047803	-4.0233156114	4.5165786752
H111	7.8315103596	3.5587773689	-0.6398147580	H111	5.5960023294	4.2249432967	-1.0475675306
H112	-0.9645286140	8.5479316462	-0.6398147580	H112	-2.4407660085	6.2389543103	5.4575380965
H113	-8.4276218262	1.7241349219	-0.6398147580	H113	-8.4997318362	-2.2834228180	0.7764182873
H114	-4.2440281189	-7.4823576632	-0.6398147580	H114	0.8179576252	-5.0331343150	-4.8101024912
H115	5.8046681995	-6.3484862738	-0.6398147580	H115	-0.1350059039	-5.8873055520	5.6962116601
H116	8.5150561922	5.3579616120	0.9327822714	H116	4.6062692910	4.4366534253	-3.3153499436
H117	-2.4644272337	9.7540008715	0.9327822714	H117	-1.3575051673	7.9334773746	3.9991892641
H118	-10.0381559854	0.6703424529	0.9327822714	H118	-8.7965880702	-3.0920176347	-1.5543961865
H119	-3.7394943496	-9.3397064515	0.9327822714	H119	1.9056311864	-3.2094257552	-6.0955324154
H120	7.7270213766	-6.4425984849	0.9327822714	H120	-2.5046188654	-5.6897155065	6.4131759261
H121	6.7799174098	6.5950462473	2.2120082700	H121	2.4930722118	3.2467799595	-3.8505593762
H122	-4.1771520087	8.4860660017	2.2120082700	H122	-0.4529289286	7.2532716203	1.7887898578
H123	-9.3615393274	-1.3503690275	2.2120082700	H123	-6.8741888348	-3.0358042685	-3.1272197979
H124	-1.6085974826	-9.3206399580	2.2120082700	H124	2.3797936283	-1.0362434815	-4.9886385955
H125	8.3673714089	-4.4101032635	2.2120082700	H125	-3.7773319955	-3.6201328455	5.8940821742
H126	4.3901261808	6.0751433406	1.8749886502	H126	1.3724070707	1.8797573555	-2.1199197066
H127	-4.4211810642	6.0525806471	1.8749886502	H127	-0.6768329954	4.9194429248	1.0230253953
H128	-7.1225663489	-2.3344427810	1.8749886502	H128	-4.7062237773	-2.1336839386	-2.4014763096
H129	0.0191929734	-7.4953456306	1.8749886502	H129	1.7365223684	-0.6925615985	-2.6183131695
H130	7.1344282588	-2.2979355761	1.8749886502	H130	-2.6967501140	-1.7826569848	4.6567057311

Table S2g. Final structures of (NaBA)₆ optimized in THF: Cartesian coordinates (Å).

6a	x (Å)	y (Å)	z (Å)	6b	x (Å)	y (Å)	z (Å)
C1	-0.3486482452	0.6354069863	0.1719904426	N1	5.6154169829	2.9748317607	0.1913430609
C2	-0.2161945078	0.8568926406	1.5425791554	N2	0.2314286147	6.3505096404	0.1913430609
C3	0.9926305525	0.6086029034	2.1861182131	N3	-5.3839883682	3.3756778797	0.1913430609

C4	2.0996485636	0.1224689657	1.4706686995	N4	-5.6154169829	-2.9748317607	0.1913430609
C5	1.9634523696	-0.0725778229	0.0865171986	N5	-0.2314286147	-6.3505096404	0.1913430609
C6	0.7506936933	0.1724533611	-0.5516409566	N6	5.3839883682	-3.3756778797	0.1913430609
N7	3.3540643760	-0.0659117158	2.0764394260	C7	5.7357550446	0.6222304573	-0.0726601294
C8	3.5461085094	-0.7841607941	3.1499675726	C8	1.4023629572	5.8134248072	-0.0726601294
C9	2.5433556337	-1.7557737294	3.7219218310	C9	-4.3333920874	4.1211943499	-0.0726601294
C10	1.8097568300	-2.6169306128	2.8974207452	C10	-5.7357550446	-1.6922304573	-0.0726601294
C11	0.9485886882	-3.5624185282	3.448455139	C11	-1.4023629572	-5.8134248072	-0.0726601294
C12	0.7914541363	-3.6486005538	4.8306186581	C12	4.3333920874	-4.1211943499	-0.0726601294
C13	1.5120135467	-2.7914554340	5.6611131363	Na13	3.2343885296	3.0219653762	-0.0624765787
C14	2.3905881438	-1.8623850952	5.1095365632	Na14	-0.9999045203	4.3120453205	-0.0624765787
Na15	5.5345920592	0.8005300991	2.0317426399	Na15	-4.2342930500	1.2900799443	-0.0624765787
O16	4.6846461347	-0.7248174728	3.7719688929	Na16	-3.2343885296	-3.0219653762	-0.0624765787
C17	6.5938858722	-8.4164551935	4.4335191393	Na17	0.9999045203	-4.3120453205	-0.0624765787
C18	5.6410392469	-7.5915086538	3.8353054699	Na18	4.2342930500	-1.2900799443	-0.0624765787
C19	5.8570575137	-6.2199820544	3.7370994485	O19	4.6865913277	0.9632883977	-0.2407242880
C20	7.0425688990	-5.6409127551	4.2192864813	O20	1.5090634402	4.5403513458	-0.2407242880
C21	7.9857866379	-6.4778815332	4.8388351774	O21	-3.1775278874	3.5770629480	-0.2407242880
C22	7.7627302151	-7.8484505226	4.9388801104	O22	-4.6865913277	-0.9632883977	-0.2407242880
N23	7.1896782490	-4.2434085273	4.1564743127	O23	-1.5090634402	-4.5403513458	-0.2407242880
C24	8.2534188782	-3.6392327634	3.7004335181	O24	3.1775278874	-3.5770629480	-0.2407242880
C25	9.3737056880	-4.3129152353	2.9459194916	C25	6.6812124035	3.8888829115	0.1780584693
C26	9.1200767338	-5.2351141644	1.9242876749	C26	-0.0272651919	7.7305411253	0.1780584693
C27	10.1672845309	-5.7713493185	1.1787075920	C27	-6.7084775954	3.8416582138	0.1780584693
C28	11.4845295451	-1.045391666	1.4563276182	C28	-6.6812124035	-3.8888829115	0.1780584693
C29	11.7497615628	-4.5004257423	2.4786535470	C29	0.0272651919	-7.7305411253	0.1780584693
C30	10.6999946934	-3.9470365846	3.2078938965	C30	6.7084775954	-3.8416582138	0.1780584693
Na31	6.0852183647	-2.2241683937	4.6855490562	C31	7.5633408090	4.0217831450	-0.9098400069
O32	8.3730169698	-2.3520398271	3.8272881505	C32	0.2987040324	8.5609368506	-0.9098400069
C33	12.0114200920	-0.4035135850	-3.1769445873	C33	-7.2646367766	4.5391537056	-0.9098400069
C34	11.6349629080	0.8430486664	-2.6777323317	C34	-7.5633408090	-4.0217831450	-0.9098400069
C35	10.7358197722	0.9408474695	-1.6197762558	C35	-0.2987040324	-8.5609368506	-0.9098400069
C36	10.1819843374	-0.2131584089	-1.0400486580	C36	7.2646367766	-4.5391537056	-0.9098400069
C37	10.5883769857	-1.4641697061	-1.5323655405	C37	8.5612331889	4.9928526566	-0.9078215949
C38	11.4846707991	-1.5562612780	-2.5935908705	C38	-0.0433206435	9.9106717576	-0.9078215949
N39	9.3281592037	-0.1627036103	0.0746595128	C39	-8.6045538324	4.9178191010	-0.9078215949
C40	8.2571728188	0.5799695467	0.1540074665	C40	-8.5612331889	-4.9928526566	-0.9078215949
C41	7.5977505050	1.2685993561	-1.0145493301	C41	0.0433206435	-9.9106717576	-0.9078215949
C42	7.4414968696	0.6279372270	-2.2492975844	C42	8.6045538324	-4.9178191010	-0.9078215949
C43	6.7637899172	1.2541342125	-3.2922511471	C43	8.7060258901	5.8634155792	0.1724587653
C44	6.2491908167	2.5386329586	-3.1247678428	C44	-0.7248538995	10.4713473764	0.1724587653
C45	6.4034329735	3.1880162141	-1.9009485716	C45	-9.4308797896	4.6079317972	0.1724587653
C46	7.0593322851	2.5501777319	-0.8508292667	C46	-8.7060258901	-5.8634155792	0.1724587653
Na47	9.1986016801	-0.8985286739	2.3002285510	C47	0.7248538995	-10.4713473764	0.1724587653
O48	7.6533718647	0.7202029136	1.2970746119	C48	9.4308797896	-4.6079317972	0.1724587653
H49	-1.2908694238	0.8324613376	-0.3272154527	C49	7.8261335387	5.7546932970	1.2494364965
H50	-1.0580253868	1.2321211905	2.1155493087	C50	-1.0706438169	9.6549771064	1.2494364965
H51	1.0969323306	0.8051647654	3.2469700463	C51	-8.8967773555	3.9002838094	1.2494364965
H52	2.8200585599	-0.4221083735	-0.4798470215	C52	-7.8261335387	-5.7546932970	1.2494364965
H53	0.6656072915	0.0060761263	-1.6207079603	C53	1.0706438169	-9.6549771064	1.2494364965
H54	1.9156207828	-2.5513333945	1.8222434451	C54	8.8967773555	-3.9002838094	1.2494364965
H55	0.3961370054	-4.2297352137	2.7961413504	C55	6.8255739492	4.7884841771	1.2484938290
H56	0.1133357906	-4.3792206472	5.2578568404	C56	-0.7341619684	8.3053625239	1.2484938290
H57	1.3906769689	-2.8494935207	6.7373709198	C57	-7.5597359176	3.5168783469	1.2484938290
H58	2.9552609386	-1.2043024657	5.7593657245	C58	-6.8255739492	-4.7884841771	1.2484938290
H59	6.4226178951	-9.4840661348	4.5148781796	C59	0.7341619684	-8.3053625239	1.2484938290
H60	4.7212286341	-8.0169025558	3.4474312862	C60	7.5597359176	-3.5168783469	1.2484938290
H61	5.1104780723	-5.5778078794	3.2820991602	H61	7.4583124461	3.3573656168	-1.7599308995
H62	8.8907556002	-6.0461015784	5.2496781825	H62	0.8215923091	8.1377708561	-1.7599308995
H63	8.5061416711	-8.4751245002	5.4208683940	H63	-6.6367201370	4.7804052393	-1.7599308995
H64	8.1016326530	-5.5318034487	1.7077029510	H64	-7.4583124461	-3.3573656168	-1.7599308995
H65	9.9533432914	-6.4758127390	0.3824481543	H65	-0.8215923091	-8.1377708561	-1.7599308995
H66	12.2989099912	-5.8350001144	0.8796346923	H66	6.6367201370	-4.7804052393	-1.7599308995
H67	12.7729420307	-4.2199600188	2.7037944342	H67	9.2303011263	5.7035111423	-1.7596190041
H68	10.9067374745	-3.2371953787	4.0005607932	H68	0.2240976678	10.5288508311	-1.7596190041
H69	12.7140612401	-0.4761389305	-3.9996831288	H69	-9.0062034584	5.4584996888	-1.7596190041
H70	12.0487415027	1.7483336407	-3.1101392736	H70	-9.2303011263	-5.0703511423	-1.7596190041
H71	10.4652221141	1.9130870654	-1.2251521529	H71	-0.2240976678	-10.5288508311	-1.7596190041
H72	10.1877928901	-2.3607051422	-1.0717552415	H72	9.0062034584	-5.4584996888	-1.7596190041
H73	11.7770424416	-2.5338493245	-2.9634568899	H73	9.4851808714	6.6181331241	0.1716317057
H74	7.8465900119	-0.3653323754	-2.3946181528	H74	-0.9888809754	11.5234741561	0.1716317057
H75	6.6418241083	0.7390648989	-4.2388786052	H75	-10.4740618468	4.9053410320	0.1716317057
H76	5.7305441810	3.0293071174	-3.9412164468	H76	-9.4851808714	-6.6181331241	0.1716317057
H77	6.0095790142	4.1893839728	-1.7651754014	H77	0.9888809754	-11.5234741561	0.1716317057
H78	7.1651432049	3.0551145965	0.1015769403	H78	10.4740618468	-4.9053410320	0.1716317057
C79	1.7063772434	5.6360317416	6.8400675274	H79	7.9157194139	6.4297450897	2.0952638530

C80	1.7091721588	5.3986740365	5.4657867666	H80	-1.6104628806	10.0700866465	2.0952638530
C81	2.6750741259	4.5780302321	4.8900882293	H81	-9.5261822945	3.6403415568	2.0952638530
C82	3.6702489697	3.9792247339	5.6805584346	H82	-7.9157194139	-6.4297450897	2.0952638530
C83	3.6417487532	4.2028763658	7.0660963398	H83	1.6104628806	-10.0700866465	2.0952638530
C84	2.6776893443	5.0291773392	7.6367903642	H84	9.5261822945	-3.6403415568	2.0952638530
N85	4.6208513765	3.0872050575	5.1519812780	H85	6.1367573239	4.7199003248	2.0819005673
C86	5.3883107556	3.3577330169	4.1309227651	H86	-1.0191749227	7.6745379018	2.0819005673
C87	5.5677919475	4.7358116184	3.5446772586	H87	-7.1559322466	2.9546375769	2.0819005673
C88	5.8217441256	5.8417635841	4.3634394646	H88	-6.1367573239	-4.7199003248	2.0819005673
C89	6.0557147476	7.0965140025	3.8058530599	H89	1.0191749227	-7.6745379018	2.0819005673
C90	6.0161722043	7.2681184651	2.4231536821	H90	7.1559322466	-2.9546375769	2.0819005673
C91	5.7544731931	6.1739242053	1.5994841196	C91	7.0683678091	0.9844739465	-0.1233846668
C92	5.5471953653	4.9146987047	2.1570997671	C92	2.6816044575	6.6136230592	-0.1233846668
Na93	5.3088519770	0.8512980662	5.3345851679	C93	-4.3867633515	5.6291491127	-0.1233846668
O94	6.1025473830	2.4164394468	3.5901241805	C94	-7.0683678091	-0.9844739465	-0.1233846668
C95	13.4317773406	5.4396029438	2.4205736160	C95	-2.6816044575	-6.6136230592	-0.1233846668
C96	12.3256265406	5.7940543303	3.1932570632	C96	4.3867633515	-5.6291491127	-0.1233846668
C97	11.3706934357	4.8417006165	3.5396368983	C97	7.3412089028	0.0753586678	-1.1499536947
C98	11.5112829882	3.5032268738	3.1368575690	C98	3.6053419307	6.3953527382	-1.1499536947
C99	12.6163602892	3.1623310382	2.3387682553	C99	-3.7358669721	6.3199940704	-1.1499536947
C100	13.5651442959	4.1195229341	1.9908252611	C100	-7.3412089028	-0.0753586678	-1.1499536947
N101	10.5030300838	2.5740043663	3.4479449115	C101	-3.6053419307	-6.3953527382	-1.1499536947
C102	10.7348017531	1.4072328046	3.9866753464	C102	3.7358669721	-6.3199940704	-1.1499536947
C103	12.0375219504	1.0094568850	4.6355929607	C103	8.5572057347	-0.6018724203	-1.1944107660
C104	12.7525346930	1.8986226237	5.4469541556	C104	4.7998396732	7.1098213415	-1.1944107660
C105	13.9167689100	1.4892850182	6.0917714611	C105	-3.7573660615	7.7116937618	-1.1944107660
C106	14.3959444628	0.1917507518	5.9204145786	C106	-8.5572057347	0.6018724203	-1.1944107660
C107	13.6939816068	-0.7017846505	5.1125542717	C107	-4.7998396732	-7.1098213415	-1.1944107660
C108	12.5168632160	-0.2975533492	4.4876140472	C108	3.7573660615	-7.7116937618	-1.1944107660
Na109	8.2500310637	2.1757244445	2.9883136110	C109	9.5088183893	-0.3952462555	-0.1975095215
O110	9.7926192163	0.5162691414	4.0275971877	C110	5.0967024926	8.0372551573	-0.1975095215
C111	10.0623074914	-2.0283833375	11.4999983812	C111	-4.4121158966	8.4325014128	-0.1975095215
C112	8.9080755012	-2.6866189945	11.0770720098	C112	-9.5088183893	0.3952462555	-0.1975095215
C113	8.3073357801	-2.3574710163	9.8650385423	C113	-5.0967024926	-8.0372551573	-0.1975095215
C114	8.8463456270	-1.3505966167	9.0460465776	C114	4.4121158966	-8.4325014128	-0.1975095215
C115	10.0229107325	-0.7110014600	9.4714135148	C115	9.2389328404	0.4940047416	0.8412339613
C116	10.6167484508	-1.0399964531	10.6865384217	C116	4.1916457644	8.2481529144	0.8412339613
N117	8.3203536330	-1.0429198570	7.7788631997	C117	-5.0472870760	7.7541481728	0.8412339613
C118	7.0632742883	-0.7727290944	7.5448563828	C118	-9.2389328404	-0.4940047416	0.8412339613
C119	6.0363976038	-0.4721624562	8.6087357695	C119	-4.1916457644	-8.2481529144	0.8412339613
C120	6.3296702226	0.3612458151	9.6943597984	C120	5.0472870760	-7.7541481728	0.8412339613
C121	5.3444616510	0.6893402193	10.6223098011	C121	8.0309074275	1.857258676	0.8735298248
C122	4.0564455470	0.1733856364	10.4916619779	C122	2.9885849905	7.5478327815	0.8735298248
C123	3.7543929977	-0.6622120487	9.4175145018	C123	-5.0423224370	6.3621069138	0.8735298248
C124	4.7340896623	-0.9692904047	8.4765571544	C124	-8.0309074275	-1.1857258676	0.8735298248
Na125	8.9551265065	-0.9206196215	5.5226215616	C125	-2.9885849905	-7.5478327815	0.8735298248
O126	6.6368112894	-0.6897482150	6.3209243029	C126	5.0423224370	-6.3621069138	0.8735298248
H127	0.9515919172	6.2747388479	7.2852978465	H127	6.5996744544	-0.0897240219	-1.9221605325
H128	0.9505898358	5.8513306090	4.8353251642	H128	3.3775405094	5.6706237233	-1.9221605325
H129	2.6574804359	4.3841002957	3.8240678053	H129	-3.2221339449	5.7603477451	-1.9221605325
H130	4.3889065453	3.7212644447	7.6882125138	H130	-6.5996744544	0.0897240219	-1.9221605325
H131	2.6820303915	5.1955036851	8.7092783743	H131	-3.3775405094	-5.6706237233	-1.9221605325
H132	5.8366877268	5.7215073348	5.4389068156	H132	3.2221339449	-5.7603477451	-1.9221605325
H133	6.2623127823	7.9419336185	4.4530640983	H133	8.7552366714	-1.3018572917	-1.9977840673
H134	6.1877508313	8.2476738265	1.9902002504	H134	5.5050598224	6.9313287277	-1.9977840673
H135	5.7138528024	6.3028325160	0.5233094768	H135	-3.2501768490	8.2331860194	-1.9977840673
H136	5.3463943003	4.0673331175	1.5127899328	H136	-8.7552366714	1.3018572917	-1.9977840673
H137	14.1711904771	6.1840686168	2.1466961639	H137	-5.5050598224	-6.9313287277	-1.9977840673
H138	12.2020842876	6.8198723874	3.5252478018	H138	3.2501768490	-8.2331860194	-1.9977840673
H139	10.5058067663	5.1228063110	4.1308378245	H139	10.4505397767	-0.9316397173	-0.2244273880
H140	12.7146359389	2.1431439294	1.9828947432	H140	6.0320935507	8.5846130712	-0.2244273880
H141	14.4111423446	3.8320362288	1.3748873659	H141	-4.4184462260	9.5162527885	-0.2244273880
H142	12.3966215059	2.9122531858	5.5780418785	H142	-10.4505397767	0.9316397173	-0.2244273880
H143	14.4530141203	2.1873643244	6.7251893944	H143	-6.0320935507	-8.5846130712	-0.2244273880
H144	15.3083658554	-0.1223507926	6.4153509297	H144	4.4184462260	-9.5162527885	-0.2244273880
H145	14.0622373095	-1.7123682195	4.9730019342	H145	9.9707809372	0.6518335097	1.6268531531
H146	11.9675575381	-0.9968554189	3.8687635102	H146	4.4208860901	8.9608663420	1.6268531531
H147	10.5289457181	-2.2894773463	12.4432841329	H147	-5.5498948470	8.3090328323	1.6268531531
H148	8.4736382267	-3.4685002952	11.6916174792	H148	-9.9707809372	-0.6518335097	1.6268531531
H149	7.4198710164	-2.8869717801	9.5384816046	H149	-4.4208860901	-8.9608663420	1.6268531531
H150	10.4658459489	0.0478833360	8.8359780536	H150	5.5498948470	-8.3090328323	1.6268531531
H151	11.5207957875	-0.5257931603	10.9960634658	H151	7.8329491486	1.8845623684	1.6770664751
H152	7.3299494792	0.7577993444	9.8133292266	H152	2.2843956883	7.7258141334	1.6770664751
H153	5.5857580575	1.3451213885	11.4514562952	H153	-5.5485534603	5.8412517650	1.6770664751
H154	3.2929447097	0.4217575775	11.2206760500	H154	-7.8329491486	-1.8845623684	1.6770664751
H155	2.7550653045	-1.0702321534	9.3114776346	H155	-2.2843956883	-7.7258141334	1.6770664751

H156

4.4940015511

-1.6111143427

7.6371866827

H156

5.5485534603

-5.8412517650

1.6770664751
