Supporting Information

A Theoretical and Experimental Study on meridional−facial Isomerization of Tris(quinolin-8-olate)aluminium (Alq3).

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Experimental detail

1. General Information. Commercially available boehmite (Wako chemicals), and Hq (Sigma-Aldrich) were used as received. All manipulations were carried out under ambient atmosphere and temperatures. X-ray powder diffraction (XRPD) was recorded on Rigaku RINT-Ultima III X-ray diffractometer. ^{13}C CP/MAS NMR spectra were obtained on a JEOL EX-270WB Fourier-transform spectrometer at room temperatures. A HORIBA model F-21 pH meter was used for pH measurements, and pH of weak acid was obtained by drawing a calibration curve using HCl aqueous solutions (0.010~10.0 mM).

2. Configuration specific synthesis of meridional and facial Alq_3. Each Alq_3 isomer was prepared by the previously described method developed in our laboratory.[1] Briefly, boehmite (0.20 g, 3.3 mmol) and Hq (1.45 g, 10.0 mmol) were suspended in deionized water (30 mL) and charged in a round-bottom flask equipped with a water-cooled condenser. The suspension was stirred vigorously and heated under reflux. Formation of *mer*-Alq_3 is judged by the development of bright yellow color, which typically occurred within 1 h. Then, the suspension gradually changed its color to yellowish crème that indicates formation of *fac*-Alq_3. The resulting solid products were isolated by filtration and rinsed with cold acetone to remove residual Hq, then characterized by ^{13}C CP/MAS NMR and XRPD.

1. Katakura, R.; Koide, Y., *Inorg. Chem.* **2006**, *45*, 5730.

3. Computational Methods. Gas-phase calculations were carried out at DFT-B3LYP levels. All calculations were performed using Gaussian 09 program[5], except for intrinsic reaction coordinate (IRC) calculations which were carried out using GAUSSIAN 03 program[6], and 6-31+G* split-valence double-zeta plus polarization basis sets were employed for geometry optimizations. The starting geometries of *mer*-Alq_3[2] and *fac*-Alq_3[3] were obtained from literatures mentioned in the manuscript. Although each Alq_3 isomer exists as enantiomers (Δ and Λ), chirality change was excluded from consideration, and all calculations employed Δ-*mer*-Alq_3 or Δ-*fac*-Alq_3.[4] The frequency calculations were performed for all of the stationary structures obtained at the same level. It was confirmed that all of the frequencies were real for the ground state (GS) and there is only one imaginary frequency for the transition state (TS1 and TS3). Vectors of the imaginary frequencies directed the reaction mode, and IRC calculations were further performed to confirm that the rate-determining-TS was on the saddle point of the energy surface between the reactant and product.

4. Computational Results

Total calculation energies (in Hartree) for the energy minima are shown in the following.

***mer*-Alq$_3$**

¥RB3LYP¥6-31+G(d)¥C27H18Al1N3O3¥0,1

¥Al,0.1565821508,0.0137474613,0.0808557436¥N,0.0194404458,-0.0491768907,2.1545294957¥C,0.934545768,-0.039494197,3.1144278082¥H,1.9731516229,0.0026370633,2.8018217585¥C,0.5875507948,-0.0819192382,4.4816602083¥H,1.3735076392,-0.0703444147,5.2304685195¥C,-0.7448079715,-0.1367366179,4.8424134407¥H,-1.0313480555,-0.1693868633,5.8913888694¥C,-1.752400438,-0.1520608245,3.8442880341¥C,-3.1482634409,-0.2105283234,4.0903344229¥H,-3.5154269466,-0.2455253125,5.1123350965¥C,-4.0211800732,-0.2229963361,3.0137168396¥H,-5.0916771278,-0.2682161863,3.2014088925¥C,-3.5768660694,-0.1795349287,1.6734999185¥H,-4.288555377,-0.1918317033,0.8533160928¥C,-2.2134899045,-0.1201726224,1.3810241964¥C,-1.301834338,-0.1060302865,2.4933000768¥O,-1.6987787185,-0.0772941812,0.1745541608¥N,2.2527419836,0.3204013066,0.151785409¥C,3.2524271667,-0.5506870971,0.2172524139¥H,2.9716007087,-1.5988319329,0.2468901842¥C,4.6009797307,-0.1309874452,0.2498238559¥H,5.3882946518,-0.876772448,0.3013500306¥C,4.8977700348,1.2191788166,0.2158132591¥H,5.9317208538,1.5566471592,0.2416541342¥C,3.8526071407,2.1769027275,0.1446613802¥C,4.018533404,3.585741887,0.1034162842¥H,5.0165268675,4.0144892947,0.1285586233¥C,2.8937992942,4.3932096628,0.0319110456¥H,3.020641013,5.4730683936,0.0021413443¥C,1.579274092,3.872475004,-0.006263114¥H,0.7225086346,4.5376437412,-0.0627399626¥C,1.36708012,2.4935770444,0.0295096926¥C,2.5292388745,1.6534681306,0.1112550745¥O,0.1983837649,1.8948206183,-0.014306436¥N,0.1020801583,-0.1842976918,-1.9706543309¥C,-0.1257767271,0.7171659814,-2.9156889316¥H,-0.2515518646,1.7425568126,-2.5821255499¥C,-0.2078589315,0.3546547056,-4.2781437474¥H,-0.3949842182,1.1225245086,-5.0223150211¥C,-0.0534745387,-0.9699413957,-4.6419440507¥H,-0.1155660461,-1.2645466757,-5.6873895932¥C,0.1821293704,-1.9596180685,-3.6522064838¥C,0.3486429452,-3.3489191398,-3.8930252616¥H,0.3021543189,-3.7312311066,-4.908999877¥C,0.5622100903,-4.1969390837,-2.8183524273¥H,0.6852759445,-5.2619706592,-3.0018591989¥C,0.6219505363,-3.7358110695,-1.4820124674¥H,0.7796307857,-4.4330415792,-0.6640803244¥C,0.4656259016,-2.3795199268,-1.196743336¥C,0.2484486001,-1.4959468063,-2.3093401081¥O,0.5109343991,-1.8376118842,0.0027452552

¥HF=-1672.381819 Hartrees

PCM : HF=-1672.40183448 Hartrees

TS1

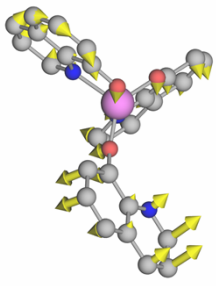
¥RB3LYP¥6-31+G(d)¥C27H18Al1N3O3¥0,1

¥H,-0.1714452585,-0.1238988931,0.0901795558¥C,0.0820791474,-0.2024701904,1.1417398311¥N,1.3585734607,-0.0194990948,1.4679291282¥C,-0.545477701,-0.5648064592,3.4431400374¥C,1.7272876926,-

0.093334651,2.7836451508¥C,-0.9032038194,-0.480675354,2.1101566978¥C,0.8034183292,-
0.3689092919,3.8323718284¥C,3.1236450475,0.1363850545,3.0290833845¥H,-1.9316402387,-
0.6227823412,1.7938436902¥H,0.6091434873,-0.6325587808,5.9807331384¥H,-1.2953059836,-
0.7780881525,4.2016979852¥C,3.5579614531,0.0739568187,4.3536730079¥H,4.6079319546,0.2448946363,4.5705
454063¥C,2.6416648465,-0.203868543,5.3928932831¥H,3.0163589883,-
0.2440877379,6.4129961542¥C,1.2922003935,-
0.4229867315,5.1625566969¥O,3.8800398644,0.3836515792,1.9863963451¥H,8.1675134005,-2.1181398736,-
4.4029250447¥C,7.5110711639,-2.0851396458,-3.5374237923¥H,8.5925411094,-3.5459594286,-
2.3878770058¥C,7.7421462433,-2.8679972348,-2.4289145355¥N,5.5407628051,-1.118071258,-
2.5239254565¥C,6.8621247762,-2.7946172371,-1.3169068331¥C,6.3868837097,-1.2209324537,-
3.5307986445¥C,5.7562889099,-1.8852070665,-1.4175157879¥C,7.0419047734,-3.5719524015,-
0.1420506428¥H,6.185158321,-0.5905126937,-4.3972352134¥C,6.1458492453,-
3.4457137299,0.8989078968¥H,7.88522679,-4.2557258709,-0.0782558581¥H,6.2773105839,-
4.0358403006,1.8030598859¥C,5.0505635046,-2.5561724129,0.8177249741¥H,4.361523734,-
2.4666485148,1.6517567669¥C,4.8359707433,-1.7743197628,-0.3112603375¥O,3.7868761157,-0.9610536194,-
0.4337020177¥H,3.0491580053,4.8321899424,-0.517464679¥C,2.5130766201,4.145425669,-
1.1653448756¥C,2.5274039219,2.7863036093,-0.8768380192¥C,1.1489956533,3.7765325471,-
3.1769643603¥C,1.814896346,1.9113700801,-1.7576428781¥C,1.8191655128,4.6194560187,-
2.3061811417¥C,1.1440740375,2.3795330501,-2.9207783509¥N,1.8747611186,0.5975452376,-
1.4061836725¥H,1.8278531738,5.6881585926,-2.5066889592¥H,0.0183361644,1.6775502686,-
4.6399490519¥H,0.640898514,4.1669582244,-4.0543530553¥C,1.3355392695,-0.3128228671,-
2.206774783¥H,1.4602487719,-1.3511871883,-1.9146461966¥C,0.6505807323,0.0491457244,-
3.3870380771¥H,0.22139142,-0.7281677653,-4.0114083081¥C,0.5447574827,1.3842959584,-
3.7343066703¥O,3.1593967922,2.2216333394,0.1420131552¥Al,3.01734

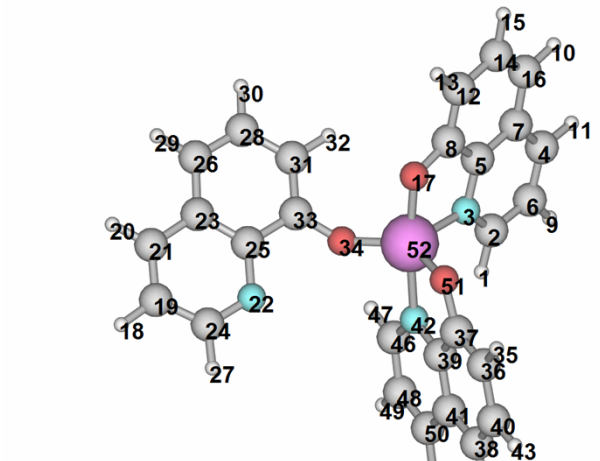
¥HF=-1672.3496197 Hartrees PCM : HF=-1672.37349940 Hartrees

i=-15.5026 cm^{-1}



IRC Calculation

Note that IRC calculations were carried out by applying perturbations to the TS geometries found in previous calculations, but not by performing full IRC calculations.



¥RB3LYP¥6-31+G(d) IRC=forward ¥C27H18Al1N3O3¥0,1
Pt1 HF = -1672.34962002 Hartrees

1	1	0	-0.172539	-0.123125	0.090147
2	6	0	0.081178	-0.201710	1.141662
3	7	0	1.357837	-0.019373	1.467549
4	6	0	-0.546043	-0.563473	3.443240
5	6	0	1.726829	-0.093269	2.783179
6	6	0	-0.904032	-0.479302	2.110329
7	6	0	0.803045	-0.368232	3.832147
8	6	0	3.123382	0.135702	3.028260
9	1	0	-1.932611	-0.620924	1.794259
10	1	0	0.609104	-0.631520	5.980577
11	1	0	-1.295813	-0.776292	4.201986
12	6	0	3.557948	0.073210	4.352770
13	1	0	4.608061	0.243587	4.569390
14	6	0	2.641732	-0.203987	5.392226
15	1	0	3.016626	-0.244278	6.412253
16	6	0	1.292094	-0.422411	5.162225
17	8	0	3.879668	0.382464	1.985388
18	1	0	8.174551	-2.108084	-4.396567
19	6	0	7.516294	-2.077554	-3.532354
20	1	0	8.596437	-3.540260	-2.383954
21	6	0	7.745639	-2.862816	-2.425187
22	7	0	5.543269	-1.114150	-2.520662
23	6	0	6.863270	-2.792635	-1.314833
24	6	0	6.391536	-1.214086	-3.526022
25	6	0	5.756988	-1.883788	-1.415642
26	6	0	7.041169	-3.572543	-0.141393
27	1	0	6.191217	-0.581729	-4.391371
28	6	0	6.142832	-3.449400	0.897971
29	1	0	7.884883	-4.255814	-0.077394
30	1	0	6.272848	-4.041511	1.801034
31	6	0	5.047026	-2.560526	0.816503
32	1	0	4.356065	-2.473524	1.649232
33	6	0	4.834236	-1.776214	-0.311104
34	8	0	3.784616	-0.963612	-0.433722
35	1	0	3.051007	4.830681	-0.519662
36	6	0	2.514435	4.144038	-1.167265
37	6	0	2.527993	2.784994	-0.878348
38	6	0	1.149867	3.775344	-3.178592
39	6	0	1.814814	1.910221	-1.758769
40	6	0	1.820655	4.618133	-2.308154
41	6	0	1.144122	2.378429	-2.921964
42	7	0	1.873871	0.596479	-1.406868
43	1	0	1.829953	5.686768	-2.508992
44	1	0	0.017768	1.676582	-4.640788
45	1	0	0.641897	4.165803	-4.056040
46	6	0	1.333926	-0.313810	-2.207065
47	1	0	1.457941	-1.352151	-1.914552
48	6	0	0.649085	0.048198	-3.387383
49	1	0	0.219326	-0.729049	-4.011445
50	6	0	0.544089	1.383300	-3.735096
51	8	0	3.159776	2.220253	0.140588
52	13	0	3.016614	0.414435	0.348804

Pt2 HF = -1672.34962035 Hartrees

1	1	0	-0.172591	-0.123873	0.088808
2	6	0	0.080725	-0.202420	1.140412
3	7	0	1.357214	-0.019807	1.466804
4	6	0	-0.547310	-0.564352	3.441737
5	6	0	1.725719	-0.093645	2.782571
6	6	0	-0.904797	-0.480256	2.108688
7	6	0	0.801580	-0.368799	3.831175
8	6	0	3.122136	0.135575	3.028188
9	1	0	-1.933212	-0.622131	1.792217
10	1	0	0.606858	-0.632125	5.979526
11	1	0	-1.297325	-0.777364	4.200190
12	6	0	3.556193	0.073199	4.352867
13	1	0	4.606202	0.243792	4.569908
14	6	0	2.639620	-0.204167	5.391967
15	1	0	3.014126	-0.244366	6.412148
16	6	0	1.290118	-0.422874	5.161442
17	8	0	3.878782	0.382446	1.985591
18	1	0	8.177500	-2.106050	-4.393906
19	6	0	7.518638	-2.075952	-3.530140
20	1	0	8.598678	-3.538307	-2.381210
21	6	0	7.747601	-2.861252	-2.422926
22	7	0	5.544551	-1.113501	-2.519600
23	6	0	6.864482	-2.791581	-1.313138
24	6	0	6.393496	-1.212981	-3.524432
25	6	0	5.757904	-1.883154	-1.414523
26	6	0	7.041975	-3.571548	-0.139680
27	1	0	6.193458	-0.580601	-4.389846
28	6	0	6.142967	-3.448859	0.899157
29	1	0	7.885932	-4.254473	-0.075237
30	1	0	6.272672	-4.041011	1.802244
31	6	0	5.046895	-2.560370	0.817134
32	1	0	4.355423	-2.473686	1.649475
33	6	0	4.834492	-1.775993	-0.310496
34	8	0	3.784682	-0.963691	-0.433548
35	1	0	3.050164	4.830600	-0.519620
36	6	0	2.513993	4.143863	-1.167466
37	6	0	2.527694	2.784814	-0.878576
38	6	0	1.150359	3.774950	-3.179389
39	6	0	1.815022	1.909932	-1.759299
40	6	0	1.820607	4.617849	-2.308641
41	6	0	1.144760	2.378030	-2.922784
42	7	0	1.874153	0.596198	-1.407381
43	1	0	1.829790	5.686493	-2.509454
44	1	0	0.019390	1.675990	-4.642171
45	1	0	0.642714	4.165327	-4.057059
46	6	0	1.334756	-0.314182	-2.207843
47	1	0	1.458838	-1.352507	-1.915288
48	6	0	0.650413	0.047712	-3.388483
49	1	0	0.221133	-0.729612	-4.012781
50	6	0	0.545315	1.382798	-3.736222
51	8	0	3.159186	2.220161	0.140590
52	13	0	3.016296	0.414315	0.348704

Pt3 HF = -1672.34962039 Hartrees

1	1	0	-0.172706	-0.124054	0.088332
2	6	0	0.080518	-0.202605	1.140037
3	7	0	1.356969	-0.019950	1.466553
4	6	0	-0.547737	-0.564568	3.441296
5	6	0	1.725336	-0.093780	2.782357
6	6	0	-0.905093	-0.480471	2.108212
7	6	0	0.801107	-0.368982	3.830868
8	6	0	3.121733	0.135518	3.028105
9	1	0	-1.933519	-0.622373	1.791600
10	1	0	0.606133	-0.632346	5.979207
11	1	0	-1.297832	-0.777599	4.199640
12	6	0	3.555660	0.073135	4.352852
13	1	0	4.605409	0.243754	4.569959
14	6	0	2.638988	-0.204289	5.391855
15	1	0	3.013335	-0.244485	6.411996
16	6	0	1.289517	-0.423049	5.161186
17	8	0	3.878452	0.382449	1.985629
18	1	0	8.178473	-2.105270	-4.392987
19	6	0	7.519460	-2.075269	-3.529338
20	1	0	8.599366	-3.537757	-2.380356
21	6	0	7.748244	-2.860694	-2.422168
22	7	0	5.545137	-1.113043	-2.519064
23	6	0	6.864907	-2.791211	-1.312541
24	6	0	6.394285	-1.212334	-3.523753
25	6	0	5.758289	-1.882848	-1.414050
26	6	0	7.042172	-3.571343	-0.139155
27	1	0	6.194437	-0.579947	-4.388996
28	6	0	6.142905	-3.448894	0.899482
29	1	0	7.886170	-4.254244	-0.074600
30	1	0	6.272417	-4.041156	1.802463
31	6	0	5.046769	-2.560485	0.817326
32	1	0	4.355087	-2.474009	1.649481
33	6	0	4.834595	-1.775960	-0.310249
34	8	0	3.784716	-0.963749	-0.433468
35	1	0	3.049933	4.830486	-0.519722
36	6	0	2.513907	4.143773	-1.167591
37	6	0	2.527628	2.784725	-0.878713
38	6	0	1.150510	3.774809	-3.179669
39	6	0	1.815118	1.909809	-1.759531
40	6	0	1.820626	4.617734	-2.308844
41	6	0	1.144952	2.377885	-2.923080
42	7	0	1.874281	0.596070	-1.407623
43	1	0	1.829776	5.686353	-2.509649
44	1	0	0.019740	1.675809	-4.642568
45	1	0	0.642926	4.165171	-4.057403
46	6	0	1.334993	-0.314330	-2.208138
47	1	0	1.459077	-1.352605	-1.915590
48	6	0	0.650727	0.047549	-3.388833
49	1	0	0.221519	-0.729777	-4.013153
50	6	0	0.545614	1.382635	-3.736572
51	8	0	3.159015	2.220095	0.140538
52	13	0	3.016164	0.414241	0.348631

Pt4 HF = -1672.34962042 Hartrees

1	1	0	-0.172730	-0.124047	0.088283
2	6	0	0.080519	-0.202595	1.140055
3	7	0	1.356969	-0.019942	1.466558
4	6	0	-0.547732	-0.564548	3.441312
5	6	0	1.725346	-0.093771	2.782364
6	6	0	-0.905086	-0.480452	2.108230
7	6	0	0.801117	-0.368965	3.830879
8	6	0	3.121733	0.135510	3.028114
9	1	0	-1.933558	-0.622365	1.791630
10	1	0	0.606156	-0.632333	5.979251
11	1	0	-1.297805	-0.777577	4.199675
12	6	0	3.555660	0.073117	4.352847
13	1	0	4.605733	0.243760	4.569978
14	6	0	2.639003	-0.204297	5.391866
15	1	0	3.013389	-0.244501	6.412024
16	6	0	1.289528	-0.423039	5.161191
17	8	0	3.878468	0.382440	1.985613
18	1	0	8.178454	-2.105273	-4.393001
19	6	0	7.519442	-2.075300	-3.529355
20	1	0	8.599395	-3.537757	-2.380377
21	6	0	7.748234	-2.860704	-2.422181
22	7	0	5.545109	-1.113074	-2.519087
23	6	0	6.864898	-2.791220	-1.312557
24	6	0	6.394252	-1.212379	-3.523762
25	6	0	5.758276	-1.882865	-1.414066
26	6	0	7.042185	-3.571327	-0.139160
27	1	0	6.194366	-0.579927	-4.389132
28	6	0	6.142927	-3.448862	0.899488
29	1	0	7.886206	-4.254217	-0.074611
30	1	0	6.272463	-4.041102	1.802482
31	6	0	5.046787	-2.560461	0.817325
32	1	0	4.355120	-2.473969	1.649483
33	6	0	4.834587	-1.775951	-0.310254
34	8	0	3.784711	-0.963758	-0.433470
35	1	0	3.049948	4.830490	-0.519714
36	6	0	2.513910	4.143773	-1.167591
37	6	0	2.527633	2.784720	-0.878710
38	6	0	1.150508	3.774810	-3.179665
39	6	0	1.815113	1.909809	-1.759527
40	6	0	1.820627	4.617736	-2.308843
41	6	0	1.144945	2.377888	-2.923074
42	7	0	1.874270	0.596073	-1.407616
43	1	0	1.829784	5.686352	-2.509643
44	1	0	0.019732	1.675820	-4.642565
45	1	0	0.642922	4.165180	-4.057403
46	6	0	1.334983	-0.314328	-2.208132
47	1	0	1.459069	-1.352603	-1.915586
48	6	0	0.650719	0.047553	-3.388828
49	1	0	0.221517	-0.729770	-4.013150
50	6	0	0.545605	1.382638	-3.736566
51	8	0	3.159016	2.220092	0.140535
52	13	0	3.016165	0.414242	0.348629

Pt5 HF = -1672.34962040 Hartrees

1	1	0	-0.172668	-0.124139	0.088430
2	6	0	0.080430	-0.202666	1.139828
3	7	0	1.356865	-0.019995	1.466439
4	6	0	-0.547935	-0.564654	3.441073
5	6	0	1.725167	-0.093828	2.782261
6	6	0	-0.905236	-0.480556	2.107969
7	6	0	0.800884	-0.369050	3.830721
8	6	0	3.121540	0.135476	3.028095
9	1	0	-1.933458	-0.622451	1.791363
10	1	0	0.605881	-0.632414	5.978967
11	1	0	-1.298087	-0.777713	4.199415
12	6	0	3.555403	0.073084	4.352846
13	1	0	4.605184	0.243682	4.570027
14	6	0	2.638678	-0.204357	5.391786
15	1	0	3.013045	-0.244572	6.412107
16	6	0	1.289220	-0.423127	5.161067
17	8	0	3.878320	0.382426	1.985642
18	1	0	8.178996	-2.104849	-4.392529
19	6	0	7.519865	-2.074943	-3.528945
20	1	0	8.599646	-3.537331	-2.379923
21	6	0	7.748579	-2.860417	-2.421795
22	7	0	5.545364	-1.112888	-2.518852
23	6	0	6.865100	-2.791038	-1.312270
24	6	0	6.394641	-1.212085	-3.523436
25	6	0	5.758438	-1.882737	-1.413859
26	6	0	7.042298	-3.571205	-0.138897
27	1	0	6.194811	-0.579566	-4.388792
28	6	0	6.142912	-3.448837	0.899646
29	1	0	7.886289	-4.253998	-0.074286
30	1	0	6.272405	-4.041167	1.802728
31	6	0	5.046735	-2.560501	0.817410
32	1	0	4.354929	-2.474072	1.649563
33	6	0	4.834616	-1.775946	-0.310148
34	8	0	3.784701	-0.963800	-0.433432
35	1	0	3.049919	4.830538	-0.519680
36	6	0	2.513859	4.143717	-1.167667
37	6	0	2.527596	2.784676	-0.878776
38	6	0	1.150583	3.774733	-3.179813
39	6	0	1.815139	1.909747	-1.759626
40	6	0	1.820638	4.617665	-2.308949
41	6	0	1.145034	2.377809	-2.923215
42	7	0	1.874299	0.596012	-1.407706
43	1	0	1.829782	5.686351	-2.509768
44	1	0	0.019962	1.675703	-4.642756
45	1	0	0.643069	4.165066	-4.057536
46	6	0	1.335075	-0.314391	-2.208255
47	1	0	1.459176	-1.352778	-1.915663
48	6	0	0.650886	0.047465	-3.388991
49	1	0	0.221721	-0.729900	-4.013366
50	6	0	0.545765	1.382546	-3.736746
51	8	0	3.158941	2.220060	0.140505
52	13	0	3.016108	0.414207	0.348606

The optimized structure using the starting geometries obtained from IRC=forward calculation
¥RB3LYP¥6-31+G(d)¥C27H18Al1N3O3¥0,1
¥H,0.0523718505,0.1148575519,0.2380621213¥C,0.3633596176,0.1791064972,1.2759751951¥N,1.6656831693,0.1
103722938,1.5168462252¥C,-
0.1514559151,0.4046918315,3.6212081874¥C,2.1102253998,0.1829731998,2.8054120525¥C,-
0.5838276556,0.3280303806,2.3114198518¥C,1.2336126066,0.3332078669,3.9187246427¥C,3.5371209094,0.0926
334371,2.9607279578¥H,-
1.639377124,0.3802681847,2.0631211998¥H,1.1485514405,0.5124838746,6.0833517353¥H,-
0.8670069939,0.5196405683,4.4325847912¥C,4.0438387058,0.1602822881,4.2593179803¥H,5.1177758821,0.0949
950393,4.4067583747¥C,3.1729987244,0.3112677504,5.3613249036¥H,3.6055530751,0.3606746137,6.358183089
3¥C,1.7969214872,0.3976040404,5.2191066999¥O,4.2575554493,-
0.0474109669,1.872754014¥H,7.9386713977,0.3695405725,-2.1780598576¥C,7.1630501553,-0.306183163,-
1.8313385013¥H,8.1690503409,-2.0974271856,-2.4607838027¥C,7.2869098167,-1.6743860287,-
1.9848743623¥N,5.0368652563,-0.5604365151,-0.7702692693¥C,6.2649627287,-2.5407970159,-
1.5164257213¥C,6.0112295639,0.2239874464,-1.209469396¥C,5.145551301,-1.911966262,-
0.9046705363¥C,6.2751080606,-3.957767757,-1.6051366165¥H,5.8756707054,1.2903518075,-
1.0579715155¥C,5.2049264191,-4.6716449,-1.0905633538¥H,7.1176008939,-4.4647907976,-
2.0673768537¥H,5.214353783,-5.7574853411,-1.1540812968¥C,4.0945380698,-4.0458025459,-
0.4763428444¥H,3.278957167,-4.6398323596,-0.0739184995¥C,4.03979109,-2.6564527868,-
0.3675640188¥O,3.0569031775,-1.9678504517,0.1747022571¥H,3.4345297769,4.3128357941,-
0.8714620575¥C,2.8671678512,3.6014550818,-1.4644798428¥C,2.8589394714,2.257577921,-
1.08816296¥C,1.405627078,3.1582668685,-3.3909253923¥C,2.0895284516,1.3545340833,-
1.8976047908¥C,2.1437710525,4.0277201272,-2.6026724311¥C,1.3653460483,1.7822346522,-
3.04605949¥N,2.1167807626,0.0613781178,-1.4710647395¥H,2.1731626174,5.082648689,-
2.8660462952¥H,0.0904133493,1.0333705109,-4.636910641¥H,0.8622237154,3.5145415484,-
4.2617118206¥C,1.4493895199,-0.8629970032,-2.1513163696¥H,1.5085031844,-1.8759526658,-
1.7656999707¥C,0.7045694428,-0.5398234312,-3.3075627835¥H,0.1746336301,-1.3269090486,-
3.8351549166¥C,0.661364612,0.7699027929,-3.7490686605¥O,3.5008308528,1.7429472743,-
0.0638028422¥Al,3.3161190086,-0.1015600146,0.2696140441
¥HF= -1672.38182555 Hartrees

IRC Calculation
¥RB3LYP¥6-31+G(d) IRC=reverse¥C27H18Al1N3O3¥0,1
Pt1 HF = -1672.34961998 Hartrees

1	1	0	-0.170339	-0.125845	0.088173
2	6	0	0.082372	-0.204356	1.139933
3	7	0	1.358431	-0.020285	1.467215
4	6	0	-0.546782	-0.567594	3.440756
5	6	0	1.726103	-0.093983	2.783230
6	6	0	-0.903466	-0.483594	2.107484
7	6	0	0.801608	-0.370532	3.831143
8	6	0	3.122045	0.136939	3.029867
9	1	0	-1.931505	-0.626600	1.790283
10	1	0	0.605771	-0.634684	5.979297
11	1	0	-1.297057	-0.781674	4.198646
12	6	0	3.555317	0.074711	4.354806
13	1	0	4.604947	0.246576	4.572589
14	6	0	2.638400	-0.204083	5.393227
15	1	0	3.012271	-0.244114	6.413637
16	6	0	1.289329	-0.424372	5.161729
17	8	0	3.879088	0.384957	1.987828
18	1	0	8.164146	-2.126186	-4.405941
19	6	0	7.508821	-2.091080	-3.539674
20	1	0	8.591551	-3.549393	-2.388126
21	6	0	7.741213	-2.871389	-2.429644
22	7	0	5.540008	-1.121309	-2.525835
23	6	0	6.862691	-2.795226	-1.316637
24	6	0	6.384749	-1.226720	-3.533606
25	6	0	5.756945	-1.885772	-1.417849
26	6	0	7.043904	-3.569871	-0.140227
27	1	0	6.181933	-0.598367	-4.401290
28	6	0	6.149363	-3.440909	0.901701
29	1	0	7.887137	-4.253715	-0.076006
30	1	0	6.281924	-4.028948	1.807053
31	6	0	5.054276	-2.551173	0.820031
32	1	0	4.366578	-2.459367	1.654904
33	6	0	4.838313	-1.771887	-0.310481
34	8	0	3.789510	-0.958331	-0.433385
35	1	0	3.045849	4.833728	-0.514997
36	6	0	2.510918	4.146694	-1.163541
37	6	0	2.526314	2.787480	-0.875532
38	6	0	1.148760	3.777255	-3.176364
39	6	0	1.815322	1.912201	-1.757217
40	6	0	1.817442	4.620491	-2.304742
41	6	0	1.144980	2.380154	-2.920710
42	7	0	1.876205	0.598296	-1.406230
43	1	0	1.825274	5.689275	-2.504848
44	1	0	0.021346	1.677735	-4.641079
45	1	0	0.640995	4.167521	-4.054016
46	6	0	1.338591	-0.312294	-2.207646
47	1	0	1.464174	-1.350655	-1.915888
48	6	0	0.654210	0.049464	-3.388310
49	1	0	0.226352	-0.728034	-4.013363
50	6	0	0.547311	1.384646	-3.735119
51	8	0	3.158098	2.223019	0.143580
52	13	0	3.017677	0.416823	0.350356

Pt2 HF = -1672.34962030 Hartrees

1	1	0	-0.170245	-0.126785	0.086691
2	6	0	0.081994	-0.205253	1.138556
3	7	0	1.357840	-0.020787	1.466441
4	6	0	-0.548111	-0.568758	3.439074
5	6	0	1.724932	-0.094411	2.782620
6	6	0	-0.904203	-0.484845	2.105637
7	6	0	0.800033	-0.371261	3.830095
8	6	0	3.120696	0.136895	3.029903
9	1	0	-1.932037	-0.628192	1.787959
10	1	0	0.603282	-0.635508	5.978150
11	1	0	-1.298665	-0.783113	4.196609
12	6	0	3.553367	0.074798	4.355042
13	1	0	4.602852	0.246979	4.573326
14	6	0	2.636044	-0.204274	5.393033
15	1	0	3.009454	-0.244195	6.413623
16	6	0	1.287149	-0.424973	5.160906
17	8	0	3.878152	0.385109	1.988200
18	1	0	8.166443	-2.125337	-4.403913
19	6	0	7.510687	-2.090365	-3.537940
20	1	0	8.593475	-3.548048	-2.385653
21	6	0	7.742890	-2.870390	-2.427671
22	7	0	5.541094	-1.121121	-2.525109
23	6	0	6.863871	-2.794343	-1.315052
24	6	0	6.386283	-1.226436	-3.532517
25	6	0	5.757870	-1.885262	-1.416869
26	6	0	7.044891	-3.568703	-0.138426
27	1	0	6.183593	-0.598319	-4.400420
28	6	0	6.149927	-3.439811	0.903145
29	1	0	7.888331	-4.252245	-0.073748
30	1	0	6.282337	-4.027623	1.808667
31	6	0	5.054626	-2.550397	0.820905
32	1	0	4.366626	-2.458591	1.655535
33	6	0	4.838847	-1.771374	-0.309823
34	8	0	3.789912	-0.958053	-0.433183
35	1	0	3.044645	4.833849	-0.514641
36	6	0	2.510233	4.146697	-1.163491
37	6	0	2.525897	2.787467	-0.875570
38	6	0	1.149182	3.776988	-3.177015
39	6	0	1.815570	1.912042	-1.757647
40	6	0	1.817175	4.620364	-2.305001
41	6	0	1.145684	2.379869	-2.921453
42	7	0	1.876653	0.598135	-1.406706
43	1	0	1.824790	5.689165	-2.505034
44	1	0	0.023219	1.677217	-4.642488
45	1	0	0.641758	4.167158	-4.054905
46	6	0	1.339748	-0.312567	-2.208471
47	1	0	1.465506	-1.350912	-1.916721
48	6	0	0.655897	0.049058	-3.389482
49	1	0	0.228645	-0.728529	-4.014832
50	6	0	0.548766	1.384230	-3.736254
51	8	0	3.157386	2.223114	0.143787
52	13	0	3.017428	0.416863	0.350361

Pt3 HF = -1672.34961990 Hartrees

1	1	0	-0.170280	-0.127089	0.085957
2	6	0	0.081831	-0.205575	1.138065
3	7	0	1.357605	-0.020982	1.466148
4	6	0	-0.548606	-0.569193	3.438460
5	6	0	1.724478	-0.094596	2.782383
6	6	0	-0.904484	-0.485280	2.104977
7	6	0	0.799446	-0.371574	3.829703
8	6	0	3.120200	0.136883	3.029873
9	1	0	-1.932429	-0.628737	1.787033
10	1	0	0.602263	-0.635925	5.977785
11	1	0	-1.299318	-0.783640	4.195857
12	6	0	3.552663	0.074780	4.355122
13	1	0	4.601798	0.247022	4.573512
14	6	0	2.635196	-0.204429	5.392954
15	1	0	3.008358	-0.244347	6.413501
16	6	0	1.286362	-0.425265	5.160590
17	8	0	3.877764	0.385217	1.988358
18	1	0	8.166889	-2.125083	-4.402711
19	6	0	7.511330	-2.090208	-3.537395
20	1	0	8.594113	-3.547813	-2.384844
21	6	0	7.743424	-2.870149	-2.427027
22	7	0	5.541561	-1.121006	-2.524790
23	6	0	6.864302	-2.794079	-1.314498
24	6	0	6.386841	-1.226321	-3.532114
25	6	0	5.758260	-1.885056	-1.416477
26	6	0	7.045227	-3.568350	-0.137799
27	1	0	6.184308	-0.598473	-4.399747
28	6	0	6.150163	-3.439434	0.903671
29	1	0	7.888714	-4.251889	-0.072975
30	1	0	6.282487	-4.027176	1.809232
31	6	0	5.054806	-2.550074	0.821285
32	1	0	4.366831	-2.458266	1.655703
33	6	0	4.839134	-1.771153	-0.309542
34	8	0	3.790158	-0.957874	-0.433091
35	1	0	3.044173	4.833901	-0.514506
36	6	0	2.509969	4.146723	-1.163450
37	6	0	2.525742	2.787492	-0.875587
38	6	0	1.149289	3.776932	-3.177208
39	6	0	1.815689	1.912008	-1.757821
40	6	0	1.817041	4.620356	-2.305054
41	6	0	1.145928	2.379801	-2.921710
42	7	0	1.876892	0.598089	-1.406934
43	1	0	1.824550	5.689136	-2.505045
44	1	0	0.023760	1.677090	-4.642957
45	1	0	0.641929	4.167086	-4.055198
46	6	0	1.340218	-0.312650	-2.208816
47	1	0	1.466044	-1.350912	-1.917118
48	6	0	0.656484	0.048959	-3.389900
49	1	0	0.229361	-0.728726	-4.015389
50	6	0	0.549244	1.384127	-3.736632
51	8	0	3.157126	2.223171	0.143869
52	13	0	3.017335	0.416894	0.350352

Pt4 HF = -1672.34962032 Hartrees

1	1	0	-0.170250	-0.127025	0.086316
2	6	0	0.081881	-0.205481	1.138220
3	7	0	1.357676	-0.020920	1.466246
4	6	0	-0.548452	-0.569060	3.438666
5	6	0	1.724626	-0.094530	2.782466
6	6	0	-0.904402	-0.485153	2.105191
7	6	0	0.799635	-0.371472	3.829838
8	6	0	3.120339	0.136899	3.029911
9	1	0	-1.932198	-0.628580	1.787392
10	1	0	0.602665	-0.635783	5.977865
11	1	0	-1.299075	-0.783480	4.196113
12	6	0	3.552869	0.074796	4.355094
13	1	0	4.602363	0.247063	4.573503
14	6	0	2.635462	-0.204377	5.392981
15	1	0	3.008767	-0.244299	6.413617
16	6	0	1.286609	-0.425173	5.160700
17	8	0	3.877886	0.385212	1.988305
18	1	0	8.166753	-2.125674	-4.403880
19	6	0	7.510939	-2.090481	-3.537649
20	1	0	8.593746	-3.548035	-2.385216
21	6	0	7.743184	-2.870352	-2.427287
22	7	0	5.541408	-1.121062	-2.524902
23	6	0	6.864187	-2.794147	-1.314658
24	6	0	6.386570	-1.226516	-3.532312
25	6	0	5.758179	-1.885091	-1.416583
26	6	0	7.045177	-3.568405	-0.137960
27	1	0	6.183850	-0.598479	-4.400366
28	6	0	6.150157	-3.439460	0.903558
29	1	0	7.888623	-4.251931	-0.073193
30	1	0	6.282534	-4.027211	1.809125
31	6	0	5.054831	-2.550089	0.821199
32	1	0	4.366767	-2.458255	1.655793
33	6	0	4.839090	-1.771154	-0.309598
34	8	0	3.790130	-0.957890	-0.433109
35	1	0	3.044320	4.833905	-0.514534
36	6	0	2.510044	4.146725	-1.163467
37	6	0	2.525790	2.787490	-0.875578
38	6	0	1.149251	3.776952	-3.177151
39	6	0	1.815657	1.912023	-1.757769
40	6	0	1.817077	4.620363	-2.305043
41	6	0	1.145851	2.379826	-2.921630
42	7	0	1.876828	0.598109	-1.406864
43	1	0	1.824622	5.689170	-2.505047
44	1	0	0.023596	1.677129	-4.642783
45	1	0	0.641886	4.167101	-4.055084
46	6	0	1.340083	-0.312615	-2.208710
47	1	0	1.465905	-1.350962	-1.916981
48	6	0	0.656301	0.048987	-3.389768
49	1	0	0.229169	-0.728618	-4.015179
50	6	0	0.549089	1.384161	-3.736512
51	8	0	3.157195	2.223169	0.143848
52	13	0	3.017364	0.416903	0.350360

Pt5 HF = -1672.34962011 Hartrees

1	1	0	-0.170214	-0.127229	0.085938
2	6	0	0.081794	-0.205692	1.137870
3	7	0	1.357535	-0.021035	1.466055
4	6	0	-0.548785	-0.569376	3.438231
5	6	0	1.724330	-0.094644	2.782317
6	6	0	-0.904582	-0.485466	2.104717
7	6	0	0.799237	-0.371687	3.829570
8	6	0	3.119998	0.136900	3.029932
9	1	0	-1.932329	-0.628962	1.786786
10	1	0	0.602023	-0.636064	5.977567
11	1	0	-1.299488	-0.783873	4.195581
12	6	0	3.552374	0.074806	4.355172
13	1	0	4.601754	0.247153	4.573700
14	6	0	2.634862	-0.204470	5.392939
15	1	0	3.008036	-0.244381	6.413608
16	6	0	1.286056	-0.425377	5.160491
17	8	0	3.877645	0.385298	1.988429
18	1	0	8.166617	-2.125747	-4.402759
19	6	0	7.511345	-2.090500	-3.537372
20	1	0	8.594077	-3.547919	-2.384687
21	6	0	7.743497	-2.870253	-2.426881
22	7	0	5.541684	-1.121060	-2.524758
23	6	0	6.864456	-2.793985	-1.314302
24	6	0	6.386912	-1.226580	-3.532108
25	6	0	5.758421	-1.884978	-1.416358
26	6	0	7.045430	-3.568122	-0.137521
27	1	0	6.184228	-0.598677	-4.400120
28	6	0	6.150374	-3.439102	0.903954
29	1	0	7.888897	-4.251616	-0.072657
30	1	0	6.282738	-4.026754	1.809586
31	6	0	5.055017	-2.549776	0.821469
32	1	0	4.366946	-2.457876	1.656015
33	6	0	4.839291	-1.770966	-0.309417
34	8	0	3.790308	-0.957741	-0.433046
35	1	0	3.043985	4.833971	-0.514433
36	6	0	2.509845	4.146757	-1.163439
37	6	0	2.525674	2.787519	-0.875575
38	6	0	1.149322	3.776905	-3.177291
39	6	0	1.815720	1.912007	-1.757865
40	6	0	1.816971	4.620357	-2.305087
41	6	0	1.146015	2.379773	-2.921798
42	7	0	1.876966	0.598091	-1.406980
43	1	0	1.824445	5.689166	-2.505070
44	1	0	0.024032	1.677011	-4.643104
45	1	0	0.642025	4.167027	-4.055279
46	6	0	1.340403	-0.312666	-2.208911
47	1	0	1.466282	-1.351000	-1.917192
48	6	0	0.656734	0.048901	-3.390045
49	1	0	0.229745	-0.728733	-4.015525
50	6	0	0.549443	1.384072	-3.736774
51	8	0	3.157013	2.223233	0.143914
52	13	0	3.017319	0.416950	0.350377

The optimized structure using the starting geometries obtained from IRC=reverse calculation

¥RB3LYP¥6-31+G(d)¥C27H18Al1N3O3¥0,1

¥H,0.5463616059,-0.331970625,-0.7452118907¥C,0.6557884191,-0.6144069801,0.2959322702¥N,1.7456529328,-0.1842784353,0.9247499404¥C,-0.1490589461,-1.7368296701,2.2742999383¥C,1.9280541434,-0.5107799962,2.2409547217¥C,-0.3185994274,-1.3991408832,0.9442017201¥C,0.9985016742,-1.2965143853,2.9799359142¥C,3.1344051537,0.0041650831,2.8238865636¥H,-1.1911316058,-1.7262935773,0.3877930468¥H,0.5927974577,-2.1711358449,4.9279114676¥H,-0.8937248829,-2.3406283204,2.788209034¥C,3.3741908922,-0.2940879711,4.1648126817¥H,4.2786343251,0.0812091272,4.6336327876¥C,2.4515306731,-1.0739813863,4.8983828599¥H,2.6716598821,-1.2865578744,5.9419494758¥C,1.2850963763,-1.5740948587,4.3411883146¥O,3.9171063861,0.7127486182,2.0431178863¥H,4.7497492833,-5.5089141588,-2.4474696787¥C,4.9604051983,-4.5407398953,-2.0014290787¥H,6.8869966056,-5.0779926297,-1.2133204859¥C,6.1338367322,-4.3001030848,-1.3225706141¥N,4.192432962,-2.2831811689,-1.6008583854¥C,6.3725406593,-3.0219195755,-0.7528279316¥C,4.0168524569,-3.4894347862,-2.1091168874¥C,5.3520918569,-2.0264564132,-0.925343115¥C,7.5577370932,-2.7097246976,-0.0365951388¥H,3.0794662621,-3.6598341675,-2.6398868217¥C,7.7184802725,-1.4453877617,0.4929845521¥H,8.322745538,-3.472600622,0.0868471558¥H,8.6219677457,-1.2004068678,1.0465966656¥C,6.7263332726,-0.453145809,0.3319782994¥H,6.8631439365,0.5355894976,0.7594085067¥C,5.5522892998,-0.7110564451,-0.3659922738¥O,4.6307000767,0.2261680719,-0.5725600304¥H,2.0239767365,5.3045278888,0.5016263435¥C,1.8345215275,4.7030272971,-0.3822442608¥C,2.2557762187,3.3792843189,-0.4098415341¥C,0.9399025174,4.5407831456,-2.6681012785¥C,1.9906619422,2.6238499057,-1.5967026366¥C,1.1785328072,5.2600481529,-1.5088292862¥C,1.3595025275,3.1853446065,-2.7390212813¥N,2.4348533207,1.3389280589,-1.5446500203¥H,0.8621227354,6.2991578134,-1.457583698¥H,0.7557138051,2.6927150623,-4.7661438494¥H,0.4486294132,5.0007588099,-3.5210828492¥C,2.333352899,0.5624898651,-2.6179014616¥H,2.7616442111,-0.4342414957,-2.5292413711¥C,1.7211316518,1.0311415983,-3.8021006098¥H,1.6508021228,0.3689035459,-4.6595020605¥C,1.2293619223,2.3237198199,-3.8588906777¥O,2.8990428511,2.7499195744,0.5643765727¥Al,3.3082105828,0.9853102296,0.3178300067

¥HF=-1672.35493121 Hartrees

INT

¥RB3LYP¥6-31+G(d)¥C27H18Al1N3O3¥0,1

¥H,0.5463616059,-0.331970625,-0.7452118907¥C,0.6557884191,-0.6144069801,0.2959322702¥N,1.7456529328,-0.1842784353,0.9247499404¥C,-0.1490589461,-1.7368296701,2.2742999383¥C,1.9280541434,-0.5107799962,2.2409547217¥C,-0.3185994274,-1.3991408832,0.9442017201¥C,0.9985016742,-

1.2965143853,2.9799359142¥C,3.1344051537,0.0041650831,2.8238865636¥H,-1.1911316058,-1.7262935773,0.3877930468¥H,0.5927974577,-2.1711358449,4.9279114676¥H,-0.8937248829,-2.3406283204,2.788209034¥C,3.3741908922,-0.2940879711,4.1648126817¥H,4.2786343251,0.0812091272,4.6336327876¥C,2.4515306731,-1.0739813863,4.8983828599¥H,2.6716598821,-1.2865578744,5.9419494758¥C,1.2850963763,-1.5740948587,4.3411883146¥O,3.9171063861,0.7127486182,2.0431178863¥H,4.7497492833,-5.5089141588,-2.4474696787¥C,4.9604051983,-4.5407398953,-2.0014290787¥H,6.8869966056,-5.0779926297,-1.2133204859¥C,6.1338367322,-4.3001030848,-1.3225706141¥N,4.192432962,-2.2831811689,-1.6008583854¥C,6.3725406593,-3.0219195755,-0.7528279316¥C,4.0168524569,-3.4894347862,-2.1091168874¥C,5.3520918569,-2.0264564132,-0.925343115¥C,7.5577370932,-2.7097246976,-0.0365951388¥H,3.0794662621,-3.6598341675,-2.6398868217¥C,7.7184802725,-1.4453877617,0.4929845521¥H,8.322745538,-3.472600622,0.0868471558¥H,8.6219677457,-1.2004068678,1.0465966656¥C,6.7263332726,-0.453145809,0.3319782994¥H,6.8631439365,0.5355894976,0.7594085067¥C,5.5522892998,-0.7110564451,-0.3659922738¥O,4.6307000767,0.2261680719,-0.5725600304¥H,2.0239767365,5.3045278888,0.5016263435¥C,1.8345215275,4.7030272971,-0.3822442608¥C,2.2557762187,3.3792843189,-0.4098415341¥C,0.9399025174,4.5407831456,-2.6681012785¥C,1.9906619422,2.6238499057,-1.5967026366¥C,1.1785328072,5.2600481529,-1.5088292862¥C,1.3595025275,3.1853446065,-2.7390212813¥N,2.4348533207,1.3389280589,-1.5446500203¥H,0.8621227354,6.2991578134,-1.457583698¥H,0.7557138051,2.6927150623,-4.7661438494¥H,0.4486294132,5.0007588099,-3.5210828492¥C,2.333352899,0.5624898651,-2.6179014616¥H,2.7616442111,-0.4342414957,-2.5292413711¥C,1.7211316518,1.0311415983,-3.8021006098¥H,1.6508021228,0.3689035459,-4.6595020605¥C,1.2293619223,2.3237198199,-3.8588906777¥O,2.8990428511,2.7499195744,0.5643765727¥Al,3.3082105828,0.9853102296,0.3178300067¥HF=-1672.3549312 Hartrees

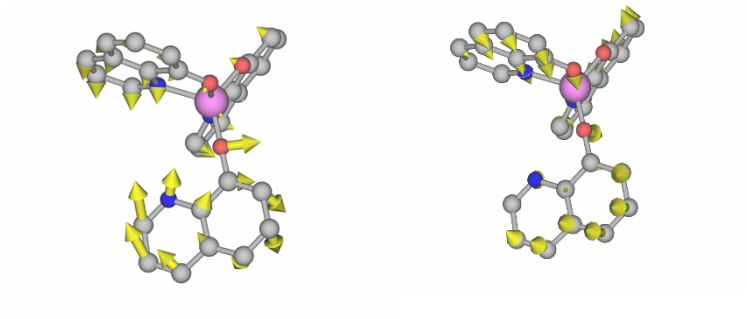
PCM : HF=-1672.37498219 Hartrees

TS2

¥RB3LYP¥6-31+G(d)¥C27H18Al1N3O3¥0,1¥H,-0.0608337357,0.0275716761,0.163487088¥C,-0.1549643424,0.1245309763,1.2388855759¥N,0.9736934345,0.169101359,1.9411183844¥C,-1.5060344066,0.3286423077,3.2274540595¥C,0.9049800957,0.3007837444,3.3014835978¥C,-1.4204664541,0.2018609695,1.8532992342¥C,-0.3268682729,0.3849859981,4.0114020421¥C,2.1782619017,0.3524088709,3.9622584665¥H,-2.3119870048,0.1606987551,1.2356413502¥H,-1.2076732417,0.583835881,5.9883523951¥H,-2.47629126,0.3886980754,3.715544566¥C,2.1725537123,0.4863519862,5.3510184524¥H,3.120378816,0.52847259

38,5.8787788459¥C,0.9501777844,0.5657687907,6.0552801317¥H,0.9847350563,0.6685578929,7.1373934599¥C,-0.2825401362,0.5190091823,5.4227625299¥O,3.2449260278,0.270499609,3.204409461¥H,1.0466784477,-6.8032606973,-0.0146323542¥C,1.7342870638,-5.987086195,0.1897068709¥H,3.5068271191,-7.2024289649,0.2346599017¥C,3.0870243072,-6.2028595355,0.3289577772¥N,2.012321779,-3.6156328231,0.5641783921¥C,3.9548911788,-5.1125271009,0.6024224708¥C,1.2470712528,-4.6623985171,0.3117701638¥C,3.3530262253,-3.8145374126,0.7250527614¥C,5.3573777035,-5.2674030887,0.7535261557¥H,0.1810566322,-4.4655949722,0.1934632121¥C,6.1361076288,-4.1595996959,1.0244705373¥H,5.7991952831,-6.2560216815,0.6560964925¥H,7.2117318387,-4.2695072073,1.1420920225¥C,5.5639040249,-2.8776105729,1.1645240923¥H,6.1868298274,-2.0185890501,1.3969378975¥C,4.1910563736,-2.6759745799,1.0301385218¥O,3.6536825338,-1.4891050899,1.184948919¥H,4.4266862008,4.0692945905,-0.0913127623¥C,3.9279820346,3.3811007238,-0.7669882599¥C,3.4844411818,2.1553314034,-0.2852071089¥C,3.1321759174,2.8582266951,-3.0335837474¥C,2.8347742174,1.2736998668,-1.2069225618¥C,3.740407145,3.7149322897,-2.1312753615¥C,2.6677359638,1.5942151624,-2.5819953454¥N,2.4269360615,0.0962314101,-0.6576703937¥H,4.1000146179,4.6804314105,-2.4790281949¥H,1.9031809386,0.7778165427,-4.4435311972¥H,3.0155894954,3.1354551744,-4.0776136631¥C,1.8853716051,-0.833854709,-1.4373611952¥H,1.6252366357,-1.7734026379,-0.9545028923¥C,1.6808341542,-0.6108954921,-2.8172381319¥H,1.2325742524,-1.3953935618,-3.4191154176¥C,2.0577390283,0.5943909833,-3.3824249821¥O,3.6206650481,1.7211809126,0.9593705573¥Al,2.9415204442,0.0834148309,1.3898766878¥HF=-1672.3516318 Hartrees

i=-27.4705 cm^{-1} i=-22.8073 cm^{-1}



PCM : HF=-1672.37220351 Hartrees

***fac*-Alq$_3$**

¥RB3LYP¥6-31+G(d)¥C27H18Al1N3O3¥0,1

¥H,-0.1643421899,-0.0528211896,0.0275936964¥C,-0.1285609175,-0.0357587398,1.1124545761¥N,1.0751731052,-0.0252617207,1.6720678067¥C,-1.2315821194,0.0007251755,3.2579551307¥C,1.1733445256,0.008180693,3.0333216605¥C,-1.3142514608,-0.0234122207,1.8790349609¥C,0.0363982444,0.0174376437,3.8942104538¥C,2.5184517659,0.0384742566,3.5412

217364¥H,-2.2746465904,-0.0300739067,1.3727931292¥H,-0.6005781652,0.0523759082,5.9716221982¥H,-2.1343967504,0.0107075899,3.8648902141¥C,2.6776193021,0.0597554361,4.9283696007¥H,3.6823567364,0.0847186651,5.3393435156¥C,1.5499501324,0.0623555761,5.7781477101¥H,1.7139528759,0.084579899,6.8531914644¥C,0.2499393126,0.0437647844,5.2956117846¥O,3.4967885508,0.0422656817,2.668679852¥H,1.7961975539,-5.0779271811,1.2891664014¥C,2.5442369111,-4.3436851554,1.0062939628¥H,4.062821615,-5.7828592562,0.5163695978¥C,3.8005212411,-4.7289405898,0.579359868¥C,4.7622133288,-3.7486108835,0.2232102771¥C,2.2272725681,-2.9697956504,1.0808734804¥C,4.347473582,-2.3888114357,0.3366669473¥C,6.0794626124,-4.0181837195,-0.2266745055¥H,1.2488885022,-2.6389486008,1.4152503702¥C,6.91533694,-2.9559624069,-0.5368253619¥H,6.418628507,-5.0461207372,-0.3201167989¥H,7.9266008155,-3.1624187466,-0.8800982472¥C,6.5098806572,-1.6084845354,-0.419280923¥H,7.1935646258,-0.8002146574,-0.6607429624¥C,5.2240830796,-1.2924809419,0.0242851312¥O,4.7543770947,-0.0780788234,0.1762724201¥H,2.6550972883,4.5089604386,-0.0095067007¥C,2.3716563346,3.7727141457,-0.7555906649¥C,2.4805542001,2.4171474745,-0.4385120843¥C,1.5526813591,3.2690315617,-3.0148481989¥C,2.0983869493,1.4712320124,-1.4520715167¥C,1.9131596634,4.1753009614,-2.0289862736¥C,1.6420030613,1.8810865979,-2.7395281405¥N,2.2112543369,0.1610307491,-1.0853582739¥H,1.8469765344,5.240163691,-2.2406363452¥H,0.963891751,1.0955541146,-4.6464460143¥H,1.2083656636,3.6055274814,-3.9888322746¥C,1.8973055749,-0.7838180735,-1.9634943611¥H,2.0088821362,-1.8131422652,-1.6368544157¥C,1.441291451,-0.4792571699,-3.2646445742¥H,1.2007382096,-1.2889083849,-3.9467555626¥C,1.3132306899,0.8420274296,-3.6478408987¥O,2.9006127871,1.9410631155,0.7084097797¥Al,3.0433799092,0.0990523949,0.8710303458¥N,3.0992490427,-2.02425822,0.7522309065

¥HF=-1672.3731588 Hartrees

PCM : HF=-1672.39838489 Hartrees

***mer*-Alq$_3$-H$_3$O$^+$**

¥RB3LYP¥6-31+G(d)¥C27H21Al1N3O4(1+)¥1,1

¥H,-0.1979003189,0.0341488844,0.0624721533¥C,-0.1706928334,0.0238531596,1.1479360504¥N,1.0354254823,-0.025229877,1.7087358149¥C,-1.2561743282,0.0364604937,3.304993393¥C,1.1431021588,-0.0350173156,3.0721009442¥C,-1.3472400644,0.056961339,1.9245005488¥C,0.0140958475,-0.0111648656,3.935720832¥C,2.4800389709,-0.0657472657,3.5713997708¥H,-2.3103126734,0.0988712581,1.4265918312¥H,-0.602995963,-0.015568256,6.0203972538¥H,-2.1558321279,0.0601247125,3.9151290962¥C,2.6617417327,-0.0881325813,4.9457584875¥H,3.6663420636,-0.1166882217,5.3582767976¥C,1.5389236797,-0.0721846803,5.8118833656¥H,1.7137978511,-0.0890480902,6.8840374496¥C,0.2408906407,-0.0322851628,5.3372550776¥O,3.4574222672,-0.062098687,2.6544178341¥H,3.9164705121,5.0122727782,1.9030650234¥C,3.5747432797,4.2865439419,1.17253

05983¥H,3.2675230775,5.7187549971,-0.3992801862¥C,3.2142995289,4.6731221217,-0.1058232993¥N,3.0931790686,1.991726643,0.6814612136¥C,2.7708485719,3.7058977515,-1.0433336843¥C,3.5031426941,2.9265175079,1.5349550759¥C,2.7285533134,2.3601903441,-0.5858065885¥C,2.3709200157,3.972746077,-2.3791910017¥H,3.7855450039,2.5916585057,2.5273304603¥C,1.956633769,2.9256531326,-3.1830835547¥H,2.3941232255,4.991213822,-2.7552950348¥H,1.6518798005,3.1296405693,-4.2060321274¥C,1.9132935478,1.5860901859,-2.7218020298¥H,1.5841303457,0.7867961002,-3.3791294354¥C,2.2956565074,1.285599484,-1.4218308768¥O,2.2865348097,0.0696966602,-0.874451462¥H,7.2037340756,-1.0899645639,-0.6821088032¥C,6.4421895474,-1.8536751882,-0.55445963¥C,5.2061755846,-1.5219476049,-0.0535784437¥C,5.7395357167,-4.1786340256,-0.7789715846¥C,4.194616758,-2.4983281039,0.1002503489¥C,6.7042744869,-3.2016834082,-0.9139332047¥C,4.4553607134,-3.8478293408,-0.267628043¥N,2.9925745262,-2.0833515259,0.6073743063¥H,7.682928949,-3.4568468632,-1.3086882558¥H,3.545315468,-5.8178024428,-0.3531886759¥H,5.9491017936,-5.2059754026,-1.062621846¥C,2.0281832029,-2.9820708148,0.7615826079¥H,1.0852299741,-2.6200279421,1.1574291347¥C,2.1919746886,-4.3435421649,0.4288239579¥H,1.3649259257,-5.0291619739,0.579465942¥C,3.3972624932,-4.7748624866,-0.0853281863¥Al,2.8817657143,-0.0333858465,0.8579806538¥O,4.846247544,-0.2362269245,0.3247140626¥O,6.0383674087,0.6418971967,2.4505523836¥H,5.2164437264,0.3498130279,2.9138123039¥H,6.8005609749,0.2359486589,2.8911860956¥H,5.4867214571,0.1370963452,1.0176197349

¥HF=-1749.2129518 Hartrees

PCM : HF=-1749.26977273 Hartrees

***mer*'-Alq$_3$-H$_3$O$^+$**

¥RB3LYP¥6-31+G(d)¥C27H21Al1N3O4(1+)¥1,1

¥C,0.0525006948,-0.4453436746,0.3666222226¥N,-0.0303101824,-0.1963969309,1.6680699944¥C,2.3199015808,-1.2410618911,0.5402894409¥C,1.0581202115,-0.4669394954,2.4535826588¥C,1.2122614177,-0.97411315,-0.2379554967¥C,2.2750730748,-0.9917432119,1.9356083491¥C,0.9402754006,-0.2081925274,3.8381505135¥C,1.9847886851,-0.4486581431,4.6970320489¥C,3.1982661777,-0.9729673857,4.1804171603¥C,3.3472472385,-1.2391148006,2.8349612596¥O,-0.2902520591,0.2978439333,4.243029274¥C,-4.2582132679,2.6453991749,5.5904074082¥C,-3.7571187295,3.9354079934,5.5823030946¥N,-2.6319876549,1.9388806544,3.9789824162¥C,-2.6611730314,4.2681223869,4.7465695592¥C,-3.6655628415,1.6645095132,4.7702272008¥C,-2.134679523,3.2129272398,3.9504245777¥C,-2.0627995308,5.5508484129,4.6389297056¥C,-1.0020964833,5.730637977,3.7685746067¥C,-0.4862681972,4.6785660963,2.9711171202¥C,-1.0438122894,3.4094319186,3.0481585882¥O,-0.6563441497,2.3495234226,2.3405915827¥C,-4.3312965006,-2.1860534805,2.3034563766¥C,-3.4953641107,-1.0822120602,2.2290722593¥C,-5.5377656853,-

1.4958305228,0.2820326216¥C,-3.6807696678,-0.1722618148,1.1448641403¥C,-5.3422746031,-
2.3792142673,1.327755565¥C,-4.697654848,-0.3568701339,0.1687050791¥N,-
2.8121970272,0.8839851398,1.1213883952¥C,-2.9184524592,1.7976076056,0.1593303402¥C,-
3.9021107144,1.7022684172,-0.8465162057¥C,-4.7812215674,0.6336832088,-0.8438497239¥O,-2.5209902785,-
0.7805143223,3.0982687429¥Al,-1.5351051125,0.7755504446,2.6968253904¥O,-1.5674752354,-
1.5444680507,5.5100882173¥H,-0.7191664837,-0.3163053942,4.9287246899¥H,-2.1755454248,-
1.5596891347,4.7330458495¥H,-2.1000062504,-1.5203474539,6.3195423854¥H,-0.8242940745,-0.2155437499,-
0.2294894239¥H,3.2271051297,-1.6419869539,0.0956908049¥H,1.2160717987,-1.157604666,-
1.307097566¥H,1.8802461466,-0.2400819763,5.7573526963¥H,4.0193182428,-
1.1626107124,4.8649085548¥H,4.2805850719,-1.6399673958,2.4502367627¥H,-
5.1018751112,2.3757745867,6.2173331839¥H,-4.2026880073,4.7015780464,6.2121639654¥H,-
4.0346708606,0.6438648523,4.7493937325¥H,-2.4423609326,6.3748993971,5.2356545049¥H,-
0.5438875202,6.7125787387,3.6862961344¥H,0.3459708585,4.8554854124,2.2963821646¥H,-4.2080795978,-
2.9043432399,3.1092035026¥H,-6.3221916584,-1.6625380399,-0.4500847572¥H,-5.9817371305,-
3.2533542157,1.4134490079¥H,-2.2051820666,2.6157080595,0.1909886351¥H,-3.9553991004,2.4704560537,-
1.6108466477¥H,-5.5422945602,0.5471538806,-1.6155286529
¥HF=-1749.2120841 Hartrees
PCM : HF=-1749.27169225 Hartrees

TS3

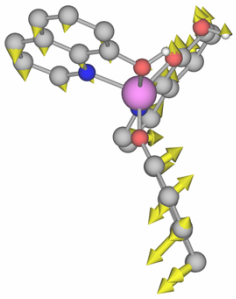
¥RB3LYP¥6-31+G(d)¥C27H21Al1N3O4(1+)¥1,1
¥C,-0.0034522681,0.0007168049,0.0015037407¥N,-0.0031363094,-
0.0004553623,1.3349843393¥C,2.4027874625,0.0082761059,-0.1110792501¥C,1.2052539163,-
0.0042294716,1.9903217521¥C,1.1816061989,0.0090393957,-0.7570670117¥C,2.4520261725,-
0.0045808037,1.3052034255¥C,1.1751978972,-0.0231681675,3.403065636¥C,2.3409168616,-
0.0514089871,4.1326560574¥C,3.5845699213,-0.0605537128,3.4495381393¥C,3.6482457977,-
0.0318539518,2.0715449631¥O,-0.0928419082,0.0093601255,3.9417643314¥C,-
6.0574056564,4.6029273594,2.8425154955¥C,-5.2507177036,5.149258221,3.8144213752¥N,-
4.4258798755,2.8826252705,2.3587440553¥C,-3.9865586497,4.5644167493,4.0911521516¥C,-
5.5922930834,3.4633610903,2.1406581364¥C,-3.617089235,3.4113239717,3.3232286218¥C,-
3.10491567,5.0751961582,5.0809062357¥C,-1.8919354405,4.45923092,5.3004075902¥C,-
1.5118985992,3.3194708837,4.5530566799¥C,-2.3470769316,2.7896464935,3.5821719955¥O,-
1.9854911237,1.7245138205,2.8511281795¥C,-3.5592139376,-3.4382860217,2.8150053381¥C,-3.05503878,-
2.1864432277,2.5188165159¥C,-5.1430300292,-3.2997276386,0.9470226568¥C,-3.5874553824,-
1.483670012,1.4035339884¥C,-4.5970933118,-3.9859231464,2.0149626333¥C,-4.6497502376,-
2.0073225893,0.6215893341¥N,-3.0290509582,-0.2551374626,1.1783489894¥C,-

3.5446421497,0.531083886,0.2355041658¥C,-4.6011966431,0.0964528524,-0.5899282317¥C,-5.1393507406,-1.1659425371,-0.4100408607¥O,-2.0910124317,-1.5416543183,3.216970288¥Al,-1.596238116,0.0865474095,2.5463120349¥O,-0.7572159503,-1.8319898485,5.573900194¥H,-0.2334743697,-0.635736366,4.7242386668¥H,-1.4598196509,-2.0542588013,4.9207614054¥H,-1.1838199645,-1.680273524,6.4322526993¥H,-0.9724378437,-0.008894897,-0.4845438138¥H,3.3290233258,0.0122915772,-0.6797674463¥H,1.1159237664,0.0130122467,-1.839658713¥H,2.3092279513,-0.0655448739,5.2178481743¥H,4.4994871787,-0.0848064438,4.0333408215¥H,4.6064735358,-0.033365475,1.5606934579¥H,-7.0298325763,5.025702562,2.608034516¥H,-5.5659958412,6.0250584204,4.3769239324¥H,-6.2172519607,3.017503738,1.3669349765¥H,-3.3989853071,5.9505219227,5.6541270653¥H,-1.2114272442,4.8486426399,6.0529916749¥H,-0.5497386456,2.847128745,4.7293684643¥H,-3.1693470679,-3.9984219037,3.6600083289¥H,-5.9502556736,-3.7305827483,0.3622554017¥H,-4.9767315982,-4.9720668364,2.2663557474¥H,-3.1252346847,1.5273087289,0.148225615¥H,-4.9842228462,0.7650726128,-1.3536549677¥H,-5.9520976099,-1.5122170618,-1.0437295486

¥HF=-1749.1719002 Hartrees

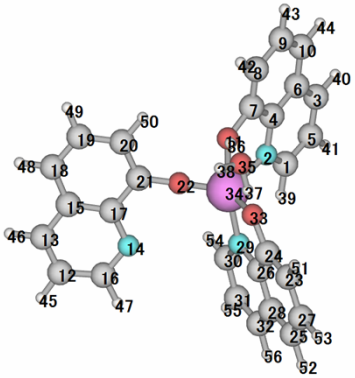
PCM : HF=-1749.23536367 Hartrees

i=-13.0199 cm^{-1}



IRC Calculation

Note that IRC calculations were carried out by applying perturbations to the TS geometries found in previous calculations, but not by performing full IRC calculations.



¥RB3LYP/6-31+G* IRC=forward ¥C27H21Al1N3O4(1+)¥1,1

Pt1 HF = -1749.17185436 Hartrees

1	6	0	0.158191	0.093785	0.112851
2	7	0	0.158639	-0.035403	1.440088
3	6	0	2.517864	-0.364222	-0.044514
4	6	0	1.342567	-0.339108	2.069264
5	6	0	1.321333	-0.059203	-0.664071
6	6	0	2.564013	-0.521783	1.363225
7	6	0	1.310111	-0.483524	3.474731
8	6	0	2.446886	-0.812397	4.175906
9	6	0	3.663103	-1.004941	3.470909
10	6	0	3.730938	-0.858971	2.100519
11	8	0	0.074973	-0.248040	4.038302
12	6	0	-5.000426	5.362568	3.637731
13	6	0	-4.084277	5.658931	4.620974
14	7	0	-3.693919	3.465482	2.895921
15	6	0	-2.927045	4.849801	4.771965
16	6	0	-4.753518	4.248385	2.797856
17	6	0	-2.778696	3.745523	3.869556
18	6	0	-1.941876	5.097394	5.765044
19	6	0	-0.841374	4.273267	5.857587
20	6	0	-0.679408	3.178506	4.975884
21	6	0	-1.621596	2.902411	3.997772
22	8	0	-1.463648	1.882661	3.139506
23	6	0	-3.949290	-2.893820	2.641296
24	6	0	-3.232493	-1.726442	2.461364
25	6	0	-5.486838	-2.290448	0.827978
26	6	0	-3.633108	-0.832155	1.431336
27	6	0	-5.068764	-3.166911	1.811033
28	6	0	-4.773485	-1.078530	0.623208
29	7	0	-2.866169	0.295229	1.318375
30	6	0	-3.238112	1.252473	0.470923
31	6	0	-4.357732	1.097378	-0.371037
32	6	0	-5.109812	-0.062869	-0.308119
33	8	0	-2.170386	-1.334102	3.203086
34	13	0	-1.388798	0.234924	2.681085
35	8	0	-0.933338	-2.062410	5.518728
36	1	0	-0.187877	-0.916910	4.767004
37	1	0	-1.659313	-2.096567	4.854414
38	1	0	-1.331826	-1.907078	6.389838
39	1	0	-0.793763	0.321949	-0.353059
40	1	0	3.426247	-0.489716	-0.627961
41	1	0	1.257781	0.061554	-1.740037
42	1	0	2.413611	-0.921824	5.255612
43	1	0	4.554858	-1.266115	4.032208
44	1	0	4.669392	-1.002590	1.573399
45	1	0	-5.895729	5.960864	3.496978
46	1	0	-4.231392	6.505894	5.287199
47	1	0	-5.467707	3.999384	2.013073
48	1	0	-2.068092	5.939360	6.440642
49	1	0	-0.081760	4.461161	6.611787
50	1	0	0.197000	2.541405	5.052229
51	1	0	-3.663424	-3.596041	3.419068
52	1	0	-6.358550	-2.511106	0.219201
53	1	0	-5.616245	-4.091424	1.970224
54	1	0	-2.649214	2.163176	0.474709
55	1	0	-4.619159	1.898031	-1.054877
56	1	0	-5.973021	-0.194034	-0.955972

Pt2 HF = -1749.17185510 Hartrees

1	6	0	0.156932	0.094550	0.111966
2	7	0	0.158151	-0.034801	1.439185
3	6	0	2.516678	-0.362600	-0.046738
4	6	0	1.342521	-0.338168	2.067689
5	6	0	1.319702	-0.057934	-0.665608
6	6	0	2.563646	-0.520320	1.360959
7	6	0	1.310884	-0.482717	3.473162
8	6	0	2.448175	-0.811217	4.173681
9	6	0	3.664080	-1.003235	3.467993
10	6	0	3.731103	-0.857126	2.097579
11	8	0	0.075966	-0.247707	4.037428
12	6	0	-5.001127	5.361705	3.639928
13	6	0	-4.084537	5.658166	4.622727
14	7	0	-3.694485	3.465108	2.897110
15	6	0	-2.927008	4.849330	4.772976
16	6	0	-4.754346	4.247740	2.799727
17	6	0	-2.778847	3.745217	3.870333
18	6	0	-1.941410	5.097015	5.765603
19	6	0	-0.840677	4.273128	5.857493
20	6	0	-0.678912	3.178506	4.975583
21	6	0	-1.621524	2.902317	3.997909
22	8	0	-1.463815	1.882652	3.139494
23	6	0	-3.948009	-2.894747	2.642067
24	6	0	-3.231779	-1.727054	2.461939
25	6	0	-5.486743	-2.291718	0.829645
26	6	0	-3.633263	-0.832787	1.432233
27	6	0	-5.067804	-3.168164	1.812349
28	6	0	-4.773972	-1.079490	0.624674
29	7	0	-2.866828	0.294918	1.319044
30	6	0	-3.239612	1.252157	0.471953
31	6	0	-4.359641	1.096762	-0.369413
32	6	0	-5.111220	-0.063800	-0.306287
33	8	0	-2.169474	-1.334393	3.203207
34	13	0	-1.388702	0.234952	2.680984
35	8	0	-0.930928	-2.062703	5.518069
36	1	0	-0.186267	-0.916790	4.766149
37	1	0	-1.657280	-2.096968	4.854176
38	1	0	-1.328932	-1.907737	6.389462
39	1	0	-0.795350	0.322461	-0.353396
40	1	0	3.424784	-0.487657	-0.630711
41	1	0	1.255511	0.062960	-1.741521
42	1	0	2.415563	-0.920711	5.253400
43	1	0	4.556269	-1.264064	4.028760
44	1	0	4.669320	-1.000289	1.569912
45	1	0	-5.896716	5.959724	3.499813
46	1	0	-4.231559	6.504945	5.289207
47	1	0	-5.468903	3.998648	2.015308
48	1	0	-2.067489	5.938849	6.441390
49	1	0	-0.080722	4.461103	6.611331
50	1	0	0.197668	2.541582	5.051421
51	1	0	-3.661446	-3.596968	3.419585
52	1	0	-6.358707	-2.512633	0.221322
53	1	0	-5.614825	-4.092922	1.971702
54	1	0	-2.651101	2.163109	0.475610
55	1	0	-4.621812	1.897449	-1.052927
56	1	0	-5.974766	-0.195189	-0.953645

Pt3 HF=-1749.17185590 Hartrees

1	6	0	0.155615	0.095461	0.110915
2	7	0	0.157626	-0.034017	1.438122
3	6	0	2.515443	-0.360813	-0.049152
4	6	0	1.342464	-0.337000	2.065930
5	6	0	1.318008	-0.056532	-0.667323
6	6	0	2.563264	-0.518630	1.358503
7	6	0	1.311663	-0.481749	3.471400
8	6	0	2.449454	-0.809928	4.171250
9	6	0	3.665036	-1.001418	3.464872
10	6	0	3.731249	-0.855111	2.094440
11	8	0	0.076969	-0.247314	4.036397
12	6	0	-5.001601	5.361148	3.642041
13	6	0	-4.084601	5.657608	4.624457
14	7	0	-3.695112	3.464737	2.898477
15	6	0	-2.926923	4.848873	4.774115
16	6	0	-4.755091	4.247277	2.801635
17	6	0	-2.779058	3.744858	3.871305
18	6	0	-1.940876	5.096589	5.766289
19	6	0	-0.839996	4.272829	5.857578
20	6	0	-0.678513	3.178309	4.975486
21	6	0	-1.621559	2.902097	3.998236
22	8	0	-1.464158	1.882549	3.139628
23	6	0	-3.946661	-2.895839	2.642909
24	6	0	-3.231019	-1.727813	2.462583
25	6	0	-5.486634	-2.293160	0.831420
26	6	0	-3.633466	-0.833534	1.433265
27	6	0	-5.066792	-3.169591	1.813750
28	6	0	-4.774503	-1.080587	0.626281
29	7	0	-2.867576	0.294516	1.319845
30	6	0	-3.241215	1.251739	0.473115
31	6	0	-4.361623	1.095999	-0.367682
32	6	0	-5.112671	-0.064895	-0.304349
33	8	0	-2.168447	-1.334828	3.203302
34	13	0	-1.388619	0.234938	2.680873
35	8	0	-0.928324	-2.063008	5.517277
36	1	0	-0.184593	-0.916630	4.765151
37	1	0	-1.655013	-2.097459	4.853757
38	1	0	-1.325942	-1.908373	6.388902
39	1	0	-0.797010	0.323065	-0.353896
40	1	0	3.423266	-0.485522	-0.633638
41	1	0	1.253173	0.064409	-1.743192
42	1	0	2.417457	-0.919609	5.250970
43	1	0	4.557612	-1.262039	4.025120
44	1	0	4.669223	-0.997917	1.566244
45	1	0	-5.897272	5.959136	3.502329
46	1	0	-4.231384	6.504347	5.291040
47	1	0	-5.469950	3.998214	2.017484
48	1	0	-2.066730	5.938353	6.442205
49	1	0	-0.079711	4.460823	6.611077
50	1	0	0.198178	2.541482	5.050858
51	1	0	-3.659386	-3.598075	3.420150
52	1	0	-6.358816	-2.514351	0.223510
53	1	0	-5.613335	-4.094608	1.973234
54	1	0	-2.653080	2.162933	0.476610
55	1	0	-4.624463	1.896666	-1.050964
56	1	0	-5.976471	-0.196564	-0.951311

Pt4 HF=-1749.17185667 Hartrees

1	6	0	0.154305	0.096328	0.109962
2	7	0	0.157112	-0.033316	1.437150
3	6	0	2.514206	-0.359061	-0.051503
4	6	0	1.342413	-0.335946	2.064253
5	6	0	1.316309	-0.055146	-0.668954
6	6	0	2.562879	-0.517039	1.356110
7	6	0	1.312461	-0.480859	3.469725
8	6	0	2.450777	-0.808681	4.168897
9	6	0	3.666035	-0.999623	3.461800
10	6	0	3.731409	-0.853147	2.091345
11	8	0	0.077995	-0.246938	4.035446
12	6	0	-5.002134	5.360576	3.644187
13	6	0	-4.084680	5.657063	4.626176
14	7	0	-3.695741	3.464432	2.899768
15	6	0	-2.926820	4.848471	4.775177
16	6	0	-4.755883	4.246832	2.803535
17	6	0	-2.779254	3.744567	3.872187
18	6	0	-1.940340	5.096200	5.766918
19	6	0	-0.839329	4.272550	5.857615
20	6	0	-0.678145	3.178127	4.975350
21	6	0	-1.621615	2.901910	3.998511
22	8	0	-1.464545	1.882444	3.139752
23	6	0	-3.945315	-2.896878	2.643722
24	6	0	-3.230262	-1.728524	2.463185
25	6	0	-5.486530	-2.294569	0.833170
26	6	0	-3.633625	-0.834269	1.434204
27	6	0	-5.065785	-3.170972	1.815140
28	6	0	-4.775004	-1.081675	0.627811
29	7	0	-2.868271	0.294121	1.320544
30	6	0	-3.242786	1.251328	0.474182
31	6	0	-4.363605	1.095256	-0.366010
32	6	0	-5.114123	-0.065968	-0.302454
33	8	0	-2.167476	-1.335202	3.203414
34	13	0	-1.388544	0.234922	2.680775
35	8	0	-0.925720	-2.063330	5.516500
36	1	0	-0.182909	-0.916466	4.764230
37	1	0	-1.653005	-2.097816	4.853666
38	1	0	-1.322486	-1.909686	6.388678
39	1	0	-0.798674	0.323665	-0.354287
40	1	0	3.421748	-0.483335	-0.636524
41	1	0	1.250818	0.065930	-1.744782
42	1	0	2.419437	-0.918475	5.248576
43	1	0	4.559035	-1.259924	4.021506
44	1	0	4.669151	-0.995495	1.562592
45	1	0	-5.897972	5.958422	3.505014
46	1	0	-4.231274	6.503690	5.292950
47	1	0	-5.471111	3.997743	2.019734
48	1	0	-2.065974	5.937876	6.442986
49	1	0	-0.078713	4.460556	6.610772
50	1	0	0.198640	2.541389	5.050259
51	1	0	-3.657315	-3.599116	3.420702
52	1	0	-6.358959	-2.516024	0.225727
53	1	0	-5.611858	-4.096244	1.974792
54	1	0	-2.655059	2.162779	0.477540
55	1	0	-4.627205	1.895949	-1.048970
56	1	0	-5.978258	-0.197879	-0.948924

Pt5 HF= -1749.17185676 Hartrees

1	6	0	0.153916	0.096698	0.109672
2	7	0	0.156964	-0.033059	1.436853
3	6	0	2.513853	-0.358399	-0.052206
4	6	0	1.342403	-0.335599	2.063737
5	6	0	1.315820	-0.054573	-0.669449
6	6	0	2.562775	-0.516479	1.355380
7	6	0	1.312698	-0.480654	3.469198
8	6	0	2.451160	-0.808408	4.168124
9	6	0	3.666316	-0.999146	3.460846
10	6	0	3.731470	-0.852531	2.090396
11	8	0	0.078295	-0.246943	4.035142
12	6	0	-5.002106	5.360579	3.644590
13	6	0	-4.084646	5.656974	4.626586
14	7	0	-3.695794	3.464449	2.900024
15	6	0	-2.926805	4.848334	4.775516
16	6	0	-4.755900	4.246893	2.803857
17	6	0	-2.779289	3.744482	3.872449
18	6	0	-1.940289	5.095978	5.767241
19	6	0	-0.839296	4.272296	5.857856
20	6	0	-0.678164	3.177923	4.975520
21	6	0	-1.621667	2.901783	3.998695
22	8	0	-1.464665	1.882352	3.139879
23	6	0	-3.944965	-2.897209	2.643968
24	6	0	-3.230056	-1.728775	2.463368
25	6	0	-5.486523	-2.294961	0.833690
26	6	0	-3.633696	-0.834493	1.434519
27	6	0	-5.065542	-3.171374	1.815545
28	6	0	-4.775174	-1.081980	0.628292
29	7	0	-2.868484	0.293987	1.320799
30	6	0	-3.243231	1.251191	0.474536
31	6	0	-4.364149	1.095036	-0.365502
32	6	0	-5.114535	-0.066272	-0.301889
33	8	0	-2.167165	-1.335390	3.203420
34	13	0	-1.388511	0.234881	2.680760
35	8	0	-0.925034	-2.063494	5.516334
36	1	0	-0.182425	-0.916563	4.763909
37	1	0	-1.652142	-2.098200	4.853106
38	1	0	-1.322444	-1.908781	6.388157
39	1	0	-0.799069	0.323927	-0.354364
40	1	0	3.421290	-0.482553	-0.637359
41	1	0	1.250147	0.066542	-1.745140
42	1	0	2.420024	-0.918353	5.248175
43	1	0	4.559476	-1.259452	4.020422
44	1	0	4.669059	-0.994763	1.561531
45	1	0	-5.897984	5.958522	3.505441
46	1	0	-4.231171	6.503566	5.293361
47	1	0	-5.471142	3.997881	2.019996
48	1	0	-2.065883	5.937615	6.443349
49	1	0	-0.078639	4.460239	6.611028
50	1	0	0.198652	2.541114	5.050380
51	1	0	-3.656787	-3.599425	3.420834
52	1	0	-6.359066	-2.516495	0.226313
53	1	0	-5.611478	-4.096676	1.975223
54	1	0	-2.655567	2.162738	0.477835
55	1	0	-4.627876	1.895693	-1.048434
56	1	0	-5.978703	-0.198265	-0.948278

The optimized structure using the starting geometries obtained from IRC=forward calculation

¥RB3LYP/6-31+G*¥C27H21Al1N3O4(1+)¥1,1

¥C,-0.6721443664,0.5861997093,0.1254534447¥N,-

0.3843336852,0.5312262816,1.4227539828¥C,1.635291163,0.3278174029,-

0.5211344674¥C,0.9251784103,0.3596016129,1.7913593569¥C,0.3123496036,0.492928921,-

0.8801760178¥C,1.9876053616,0.2493733586,0.850115145¥C,1.1989194696,0.2722362011,3.176460024¥C,2.481

7736026,0.0778406883,3.631922697¥C,3.5398221739,-

0.0352338401,2.6929715308¥C,3.3085661467,0.0518273989,1.3353367733¥O,0.0935558927,0.4082862414,3.9922

454489¥C,-1.2501620927,4.8991068068,2.5568224237¥C,-1.8545485556,5.3226378649,3.7269853905¥N,-

1.6476936659,2.5966295449,3.1089912156¥C,-2.3786154937,4.3737048095,4.6396590052¥C,-

1.1640015332,3.520723979,2.2802302966¥C,-2.2425015842,3.0026025456,4.2756165041¥C,-

3.0156586497,4.6839609738,5.8684917163¥C,-3.4799776663,3.6537246278,6.6677707378¥C,-

3.3390128608,2.2922665868,6.3065248538¥C,-2.7178902125,1.9454015016,5.1126890933¥O,-

2.5218496404,0.7054094255,4.6802891589¥C,-3.0820072424,-3.2005580674,2.2383841319¥C,-2.8046331606,-

1.8468867736,2.3663880499¥C,-5.1023710068,-2.7380531947,0.9296273368¥C,-3.6951544936,-

0.9170543869,1.745920321¥C,-4.225387467,-3.6293725537,1.5209057737¥C,-4.8520752128,-

1.3453639229,1.0342061377¥N,-3.3643478737,0.4053268575,1.8932777959¥C,-

4.1637897161,1.335169578,1.3749092155¥C,-5.3333347174,1.0050583374,0.6620536963¥C,-5.671864298,-

0.3248353537,0.4891908998¥O,-1.7669375455,-1.3327901711,3.0309564085¥Al,-

1.6916423395,0.5345035879,3.0492660811¥O,-0.4182822713,-1.6535488469,5.383759923¥H,0.0141744655,-

0.3459223591,4.6969836865¥H,-1.0504716328,-1.8920497406,4.663150034¥H,-0.9645496634,-

1.471854824,6.1664547711¥H,-1.7187649576,0.705723763,-0.1354923076¥H,2.4098945707,0.249410965,-

1.2796472617¥H,0.0128148254,0.546157271,-

1.9215127698¥H,2.6793503019,0.0084758216,4.6972745663¥H,4.5491124348,-

0.1918930194,3.061103061¥H,4.1272879443,-0.0357559728,0.6270806551¥H,-

0.8382703068,5.60963543,1.8477149906¥H,-1.928556508,6.3831660556,3.9550212928¥H,-

0.6908021858,3.1661753701,1.3701648403¥H,-3.131561389,5.7211143897,6.1683667449¥H,-

3.9693040268,3.8907200559,7.608633477¥H,-3.7146600742,1.5080730424,6.9569660586¥H,-2.4182039494,-

3.9278457212,2.6967262843¥H,-5.9781725281,-3.0884438626,0.3917734391¥H,-4.4162266272,-

4.6960839238,1.4421828462¥H,-3.8743719002,2.3702884418,1.5284046876¥H,-

5.9531833471,1.8001417238,0.2610785602¥H,-6.5701256201,-0.596572624,-0.0597671887

¥HF = -1749.20773150 Hartrees

IRC Calculation
¥RB3LYP/6-31+G* IRC=reverse ¥C27H21Al1N3O4(1+)¥1,1
Pt1 HF=-1749.17185437 Hartrees

1	6	0	0.159755	0.091472	0.112461
2	7	0	0.160026	-0.036679	1.439792
3	6	0	2.519231	-0.367702	-0.044352
4	6	0	1.343746	-0.340498	2.069302
5	6	0	1.322886	-0.062659	-0.664252
6	6	0	2.565179	-0.524223	1.363508
7	6	0	1.311087	-0.483911	3.474877
8	6	0	2.447669	-0.812757	4.176383
9	6	0	3.663870	-1.006320	3.471639
10	6	0	3.731892	-0.861380	2.101150
11	8	0	0.076015	-0.247574	4.038144
12	6	0	-5.009510	5.349026	3.641674
13	6	0	-4.092103	5.650600	4.622163
14	7	0	-3.696579	3.456856	2.898675
15	6	0	-2.930889	4.846803	4.771038
16	6	0	-4.759937	4.234892	2.802530
17	6	0	-2.779947	3.742203	3.869431
18	6	0	-1.944216	5.099926	5.761217
19	6	0	-0.839701	4.280942	5.851637
20	6	0	-0.675037	3.186111	4.970525
21	6	0	-1.618564	2.904662	3.995243
22	8	0	-1.457386	1.885012	3.137363
23	6	0	-3.951898	-2.888787	2.644077
24	6	0	-3.233559	-1.722542	2.462956
25	6	0	-5.488402	-2.285417	0.829876
26	6	0	-3.632836	-0.828882	1.431872
27	6	0	-5.071605	-3.161343	1.813951
28	6	0	-4.773428	-1.074662	0.623857
29	7	0	-2.864296	0.297275	1.317669
30	6	0	-3.234815	1.253995	0.469027
31	6	0	-4.354543	1.099500	-0.372886
32	6	0	-5.108255	-0.059623	-0.308680
33	8	0	-2.171002	-1.330799	3.204321
34	13	0	-1.387121	0.236501	2.680555
35	8	0	-0.934072	-2.060001	5.519814
36	1	0	-0.187289	-0.915809	4.767222
37	1	0	-1.660392	-2.093255	4.855841
38	1	0	-1.331930	-1.903703	6.391038
39	1	0	-0.792041	0.319745	-0.353710
40	1	0	3.427618	-0.494022	-0.627616
41	1	0	1.259477	0.057286	-1.740318
42	1	0	2.414244	-0.921385	5.256165
43	1	0	4.555462	-1.267468	4.033208
44	1	0	4.670330	-1.005796	1.574216
45	1	0	-5.907804	5.943208	3.502566
46	1	0	-4.241216	6.497684	5.287793
47	1	0	-5.475146	3.981672	2.020028
48	1	0	-2.072472	5.942032	6.436257
49	1	0	-0.078929	4.473086	6.603593
50	1	0	0.204574	2.553204	5.044973
51	1	0	-3.667049	-3.590529	3.422654
52	1	0	-6.360308	-2.505612	0.221209
53	1	0	-5.620301	-4.084976	1.974071
54	1	0	-2.644451	2.163756	0.471499
55	1	0	-4.614737	1.899697	-1.057731
56	1	0	-5.971550	-0.190362	-0.956507

Pt2 HF = -1749.17185511 Hartrees

1	6	0	0.158611	0.092075	0.111569
2	7	0	0.159632	-0.036170	1.438888
3	6	0	2.518146	-0.366327	-0.046532
4	6	0	1.343776	-0.339662	2.067756
5	6	0	1.321374	-0.061631	-0.665775
6	6	0	2.564890	-0.522940	1.361294
7	6	0	1.311912	-0.483140	3.473343
8	6	0	2.448993	-0.811621	4.174221
9	6	0	3.664884	-1.004729	3.468811
10	6	0	3.732115	-0.859717	2.098291
11	8	0	0.077062	-0.247215	4.037278
12	6	0	-5.010777	5.347311	3.644096
13	6	0	-4.092857	5.649313	4.623971
14	7	0	-3.697299	3.455944	2.900016
15	6	0	-2.931095	4.846149	4.771974
16	6	0	-4.761154	4.233400	2.804671
17	6	0	-2.780172	3.741694	3.870183
18	6	0	-1.943907	5.099712	5.761524
19	6	0	-0.838913	4.281290	5.851166
20	6	0	-0.674279	3.186591	4.969887
21	6	0	-1.618301	2.904715	3.995211
22	8	0	-1.457153	1.885157	3.137208
23	6	0	-3.950798	-2.889381	2.645009
24	6	0	-3.232923	-1.722895	2.463623
25	6	0	-5.488407	-2.286348	0.831638
26	6	0	-3.632971	-0.829294	1.432789
27	6	0	-5.070836	-3.162224	1.815428
28	6	0	-4.773904	-1.075360	0.625341
29	7	0	-2.864827	0.297103	1.318281
30	6	0	-3.236085	1.253785	0.469921
31	6	0	-4.356225	1.099032	-0.371401
32	6	0	-5.109546	-0.060329	-0.306909
33	8	0	-2.170143	-1.330872	3.204521
34	13	0	-1.386919	0.236630	2.680424
35	8	0	-0.931743	-2.060142	5.519232
36	1	0	-0.185663	-0.915624	4.766395
37	1	0	-1.658457	-2.093439	4.855697
38	1	0	-1.329081	-1.904154	6.390745
39	1	0	-0.793501	0.320108	-0.354077
40	1	0	3.426258	-0.492265	-0.630306
41	1	0	1.257341	0.058401	-1.741794
42	1	0	2.416214	-0.920265	5.254020
43	1	0	4.556897	-1.265533	4.029870
44	1	0	4.670317	-1.003728	1.570826
45	1	0	-5.909544	5.940950	3.505733
46	1	0	-4.242010	6.496215	5.289823
47	1	0	-5.476789	3.979821	2.022677
48	1	0	-2.072159	5.941694	6.436719
49	1	0	-0.077737	4.473780	6.602624
50	1	0	0.205700	2.554122	5.043715
51	1	0	-3.665321	-3.591094	3.423384
52	1	0	-6.360575	-2.506766	0.223428
53	1	0	-5.619152	-4.086044	1.975767
54	1	0	-2.646012	2.163734	0.472184
55	1	0	-4.617080	1.899238	-1.055985
56	1	0	-5.973183	-0.191261	-0.954241

Pt3 HF = -1749.17185588 Hartrees

1	6	0	0.157540	0.092734	0.110498
2	7	0	0.159288	-0.035562	1.437809
3	6	0	2.517143	-0.364924	-0.048865
4	6	0	1.343863	-0.338706	2.066037
5	6	0	1.319945	-0.060587	-0.667461
6	6	0	2.564669	-0.521567	1.358935
7	6	0	1.312776	-0.482295	3.471629
8	6	0	2.450311	-0.810509	4.171888
9	6	0	3.665908	-1.003187	3.465855
10	6	0	3.732388	-0.858035	2.095309
11	8	0	0.078151	-0.246840	4.036232
12	6	0	-5.012307	5.345141	3.646657
13	6	0	-4.093797	5.647796	4.625782
14	7	0	-3.698262	3.454499	2.901736
15	6	0	-2.931422	4.845364	4.772945
16	6	0	-4.762683	4.231275	2.807169
17	6	0	-2.780511	3.740940	3.871114
18	6	0	-1.943609	5.099636	5.761687
19	6	0	-0.838011	4.281938	5.850499
20	6	0	-0.673352	3.187312	4.969132
21	6	0	-1.617962	2.904767	3.995217
22	8	0	-1.456734	1.885324	3.137085
23	6	0	-3.949851	-2.889821	2.646192
24	6	0	-3.232379	-1.723132	2.464496
25	6	0	-5.488549	-2.287109	0.833636
26	6	0	-3.633200	-0.829586	1.433918
27	6	0	-5.070243	-3.162925	1.817168
28	6	0	-4.774472	-1.075921	0.627035
29	7	0	-2.865332	0.296952	1.318975
30	6	0	-3.237177	1.253500	0.470731
31	6	0	-4.357703	1.098500	-0.370030
32	6	0	-5.110776	-0.061000	-0.305105
33	8	0	-2.169266	-1.330885	3.204798
34	13	0	-1.386637	0.236791	2.680256
35	8	0	-0.929319	-2.060135	5.518578
36	1	0	-0.183995	-0.915410	4.765443
37	1	0	-1.656468	-2.093455	4.855462
38	1	0	-1.326126	-1.904250	6.390521
39	1	0	-0.794902	0.320549	-0.354683
40	1	0	3.424981	-0.490559	-0.633109
41	1	0	1.255311	0.059553	-1.743484
42	1	0	2.418070	-0.919378	5.251745
43	1	0	4.558245	-1.263836	4.026445
44	1	0	4.670374	-1.001677	1.567329
45	1	0	-5.911532	5.938236	3.508921
46	1	0	-4.242941	6.494690	5.291629
47	1	0	-5.478884	3.977115	2.025828
48	1	0	-2.071865	5.941592	6.436910
49	1	0	-0.076363	4.474959	6.601348
50	1	0	0.207115	2.555432	5.042280
51	1	0	-3.663747	-3.591542	3.424364
52	1	0	-6.360932	-2.507738	0.225810
53	1	0	-5.618207	-4.086922	1.977719
54	1	0	-2.647110	2.163486	0.472448
55	1	0	-4.618901	1.898538	-1.054684
56	1	0	-5.974642	-0.192167	-0.952068

Pt4 HF = -1749.17185588 Hartrees

1	6	0	0.157385	0.092692	0.110406
2	7	0	0.159250	-0.035508	1.437732
3	6	0	2.516968	-0.364970	-0.049091
4	6	0	1.343865	-0.338607	2.065901
5	6	0	1.319729	-0.060688	-0.667634
6	6	0	2.564618	-0.521500	1.358711
7	6	0	1.312885	-0.482122	3.471507
8	6	0	2.450488	-0.810210	4.171718
9	6	0	3.666012	-1.002924	3.465576
10	6	0	3.732383	-0.857907	2.095017
11	8	0	0.078283	-0.246683	4.036192
12	6	0	-5.012461	5.344944	3.646839
13	6	0	-4.093993	5.647594	4.625999
14	7	0	-3.698259	3.454476	2.901768
15	6	0	-2.931553	4.845246	4.773099
16	6	0	-4.762726	4.231196	2.807234
17	6	0	-2.780564	3.740890	3.871199
18	6	0	-1.943727	5.099547	5.761823
19	6	0	-0.838042	4.281957	5.850533
20	6	0	-0.673321	3.187384	4.969111
21	6	0	-1.617958	2.904786	3.995241
22	8	0	-1.456699	1.885377	3.137071
23	6	0	-3.949631	-2.889918	2.646221
24	6	0	-3.232177	-1.723231	2.464448
25	6	0	-5.488431	-2.287265	0.833732
26	6	0	-3.633088	-0.829693	1.433896
27	6	0	-5.070062	-3.163047	1.817265
28	6	0	-4.774407	-1.076057	0.627086
29	7	0	-2.865378	0.296962	1.319041
30	6	0	-3.237444	1.253616	0.471002
31	6	0	-4.358005	1.098563	-0.369702
32	6	0	-5.110897	-0.061062	-0.304895
33	8	0	-2.169062	-1.330932	3.204723
34	13	0	-1.386611	0.236844	2.680230
35	8	0	-0.929076	-2.060157	5.518598
36	1	0	-0.183763	-0.915242	4.765391
37	1	0	-1.655747	-2.093772	4.855061
38	1	0	-1.326553	-1.903790	6.389679
39	1	0	-0.795051	0.320374	-0.354645
40	1	0	3.424780	-0.490680	-0.633405
41	1	0	1.255013	0.059183	-1.743576
42	1	0	2.418398	-0.918821	5.251460
43	1	0	4.558456	-1.263435	4.026107
44	1	0	4.670303	-1.001705	1.567018
45	1	0	-5.911708	5.938002	3.509115
46	1	0	-4.243193	6.494430	5.291942
47	1	0	-5.478704	3.977158	2.025762
48	1	0	-2.072037	5.941439	6.437121
49	1	0	-0.076382	4.475025	6.601344
50	1	0	0.207198	2.555593	5.042181
51	1	0	-3.663554	-3.591549	3.424417
52	1	0	-6.360879	-2.507918	0.226013
53	1	0	-5.618044	-4.087014	1.977889
54	1	0	-2.647740	2.163762	0.473105
55	1	0	-4.619565	1.898769	-1.054005
56	1	0	-5.974857	-0.192220	-0.951768

Pt5 HF = -1749.17185602 Hartrees

1	6	0	0.157339	0.092712	0.110370
2	7	0	0.159227	-0.035495	1.437691
3	6	0	2.516928	-0.364917	-0.049188
4	6	0	1.343862	-0.338579	2.065830
5	6	0	1.319667	-0.060649	-0.667695
6	6	0	2.564603	-0.521454	1.358616
7	6	0	1.312913	-0.482088	3.471435
8	6	0	2.450540	-0.810164	4.171613
9	6	0	3.666063	-1.002856	3.465461
10	6	0	3.732397	-0.857837	2.094897
11	8	0	0.078325	-0.246668	4.036146
12	6	0	-5.012530	5.344859	3.646944
13	6	0	-4.094034	5.647531	4.626074
14	7	0	-3.698300	3.454426	2.901830
15	6	0	-2.931563	4.845219	4.773133
16	6	0	-4.762793	4.231113	2.807336
17	6	0	-2.780572	3.740869	3.871225
18	6	0	-1.943719	5.099542	5.761831
19	6	0	-0.838012	4.281977	5.850513
20	6	0	-0.673288	3.187410	4.969085
21	6	0	-1.617942	2.904795	3.995233
22	8	0	-1.456677	1.885393	3.137058
23	6	0	-3.949591	-2.889927	2.646266
24	6	0	-3.232171	-1.723217	2.464503
25	6	0	-5.488433	-2.287297	0.833805
26	6	0	-3.633111	-0.829689	1.433954
27	6	0	-5.070027	-3.163082	1.817323
28	6	0	-4.774437	-1.076071	0.627160
29	7	0	-2.865402	0.296965	1.319069
30	6	0	-3.237484	1.253598	0.471020
31	6	0	-4.358069	1.098543	-0.369653
32	6	0	-5.110956	-0.061083	-0.304824
33	8	0	-2.169072	-1.330892	3.204780
34	13	0	-1.386605	0.236852	2.680235
35	8	0	-0.928897	-2.060187	5.518461
36	1	0	-0.183719	-0.915266	4.765331
37	1	0	-1.656226	-2.093472	4.855595
38	1	0	-1.325441	-1.904829	6.390529
39	1	0	-0.795143	0.320438	-0.354700
40	1	0	3.424719	-0.490596	-0.633513
41	1	0	1.254927	0.059315	-1.743693
42	1	0	2.418441	-0.918850	5.251445
43	1	0	4.558493	-1.263380	4.025980
44	1	0	4.670324	-1.001561	1.566857
45	1	0	-5.911814	5.937878	3.509266
46	1	0	-4.243247	6.494354	5.292010
47	1	0	-5.478885	3.977011	2.025913
48	1	0	-2.072032	5.941436	6.437124
49	1	0	-0.076334	4.475056	6.601312
50	1	0	0.207250	2.555628	5.042140
51	1	0	-3.663455	-3.591590	3.424454
52	1	0	-6.360873	-2.507960	0.226075
53	1	0	-5.617971	-4.087076	1.977938
54	1	0	-2.647671	2.163722	0.472976
55	1	0	-4.619559	1.898702	-1.054050
56	1	0	-5.974902	-0.192261	-0.951691

The optimized structure using the starting geometries obtained from IRC=reverse calculation

¥RB3LYP/6-31+G*¥C27H21Al1N3O4(1+)¥1,1

¥C,0.0525006948,-0.4453436746,0.3666222226¥N,-0.0303101824,-0.1963969309,1.6680699944¥C,2.3199015808,-1.2410618911,0.5402894409¥C,1.0581202115,-0.4669394954,2.4535826588¥C,1.2122614177,-0.97411315,-0.2379554967¥C,2.2750730748,-0.9917432119,1.9356083491¥C,0.9402754006,-0.2081925274,3.8381505135¥C,1.9847886851,-0.4486581431,4.6970320489¥C,3.1982661777,-0.9729673857,4.1804171603¥C,3.3472472385,-1.2391148006,2.8349612596¥O,-0.2902520591,0.2978439333,4.243029274¥C,-4.2582132679,2.6453991749,5.5904074082¥C,-3.7571187295,3.9354079934,5.5823030946¥N,-2.6319876549,1.9388806544,3.9789824162¥C,-2.6611730314,4.2681223869,4.7465695592¥C,-3.6655628415,1.6645095132,4.7702272008¥C,-2.134679523,3.2129272398,3.9504245777¥C,-2.0627995308,5.5508484129,4.6389297056¥C,-1.0020964833,5.730637977,3.7685746067¥C,-0.4862681972,4.6785660963,2.9711171202¥C,-1.0438122894,3.4094319186,3.0481585882¥O,-0.6563441497,2.3495234226,2.3405915827¥C,-4.3312965006,-2.1860534805,2.3034563766¥C,-3.4953641107,-1.0822120602,2.2290722593¥C,-5.5377656853,-1.4958305228,0.2820326216¥C,-3.6807696678,-0.1722618148,1.1448641403¥C,-5.3422746031,-2.3792142673,1.327755565¥C,-4.697654848,-0.3568701339,0.1687050791¥N,-2.8121970272,0.8839851398,1.1213883952¥C,-2.9184524592,1.7976076056,0.1593303402¥C,-3.9021107144,1.7022684172,-0.8465162057¥C,-4.7812215674,0.6336832088,-0.8438497239¥O,-2.5209902785,-0.7805143223,3.0982687429¥Al,-1.5351051125,0.7755504446,2.6968253904¥O,-1.5674752354,-1.5444680507,5.5100882173¥H,-0.7191664837,-0.3163053942,4.9287246899¥H,-2.1755454248,-1.5596891347,4.7330458495¥H,-2.1000062504,-1.5203474539,6.3195423854¥H,-0.8242940745,-0.2155437499,-0.2294894239¥H,3.2271051297,-1.6419869539,0.0956908049¥H,1.2160717987,-1.157604666,-1.307097566¥H,1.8802461466,-0.2400819763,5.7573526963¥H,4.0193182428,-1.1626107124,4.8649085548¥H,4.2805850719,-1.6399673958,2.4502367627¥H,-5.1018751112,2.3757745867,6.2173331839¥H,-4.2026880073,4.7015780464,6.2121639654¥H,-4.0346708606,0.6438648523,4.7493937325¥H,-2.4423609326,6.3748993971,5.2356545049¥H,-0.5438875202,6.7125787387,3.6862961344¥H,0.3459708585,4.8554854124,2.2963821646¥H,-4.2080795978,-2.9043432399,3.1092035026¥H,-6.3221916584,-1.6625380399,-0.4500847572¥H,-5.9817371305,-3.2533542157,1.4134490079¥H,-2.2051820666,2.6157080595,0.1909886351¥H,-3.9553991004,2.4704560537,-1.6108466477¥H,-5.5422945602,0.5471538806,-1.6155286529

HF=-1749.21208412 Hartrees

***fac*-Alq_3-H_3O^+**

¥RB3LYP¥6-31+G(d)¥C27H21Al1N3O4(1+)¥1,1

¥H,0.0538579072,-0.0638106829,-0.0290051961¥C,0.0493432047,-0.0422595852,1.0560693323¥N,1.236416167,-0.0322280625,1.6557687747¥C,-1.1434862693,0.0204657046,3.1493596083¥C,1.2725449696,0.014487029,3.0254939294¥C,-1.1670733588,-0.0226338601,1.7695011513¥C,0.0994375774,0.0462688316,3.8313506245¥C,2.5484048618,0.0508243648,3.6357181445¥H,-2.1031747814,-0.0341829222,1.2213202946¥H,-0.641781055,0.1466904698,5.8684328053¥H,-2.0688357846,0.0422359673,3.7192408718¥C,2.6750704051,0.1246908662,5.0029642542¥H,3.6592152769,0.1568293134,5.4604427782¥C,1.5050799493,0.1624445739,5.8052868045¥H,1.6143423708,0.2239342301,6.8837250536¥C,0.24565075,0.1191611099,5.2428901116¥O,3.609932525,-0.0058233967,2.7549302838¥H,1.7870227659,-5.0418796313,0.7663186437¥C,2.570823243,-4.3064364568,0.6175620113¥H,4.096809574,-5.7375616805,0.1266282295¥C,3.8531759632,-4.6868710845,0.2641229726¥C,4.8601456791,-3.7064536197,0.0819624167¥C,2.2754896748,-2.9401361106,0.7905480995¥C,4.4682374607,-2.3510671731,0.283040794¥C,6.2061135308,-3.9712996856,-0.2789280179¥H,1.2769352746,-2.6192474159,1.0694171676¥C,7.0877012621,-2.9139695929,-0.4225559444¥H,6.5294648132,-4.9955303166,-0.4383761643¥H,8.1184410419,-3.1161387363,-0.7010096476¥C,6.6973496493,-1.5687652565,-0.2171854182¥H,7.41464751,-0.762600329,-0.3385283369¥C,5.3892264831,-1.266491063,0.1412448213¥O,4.9167653004,-0.0464511348,0.3690921627¥H,2.9419834263,4.5869637441,0.4727366943¥C,2.6632236283,3.941963116,-0.3554730999¥C,2.7268298886,2.5644988267,-0.1993257501¥C,1.8897412825,3.7178356729,-2.6704616353¥C,2.3470311808,1.7444709264,-1.306479419¥C,2.2445251771,4.5014588251,-1.5873508568¥C,1.9367408918,2.3049058156,-2.5499777281¥N,2.4156129459,0.3920354906,-1.0907740615¥H,2.2092894842,5.5835812799,-1.6782613644¥H,1.2976864144,1.7608184308,-4.5511697882¥H,1.579829397,4.1678223808,-3.6088377417¥C,2.1108591534,-0.4388726795,-2.0854120426¥H,2.1935433298,-1.5015115992,-1.8786667167¥C,1.70260738,0.0252515157,-3.35143497¥H,1.4678365177,-0.6929511688,-4.130037482¥C,1.6122231721,1.3862899828,-3.5801465182¥O,3.1209507866,1.9327815333,0.9089201008¥Al,3.1310574223,0.0681162101,0.7901434899¥N,3.1917571062,-1.987316017,0.6258187821¥H,4.3160336968,0.7323358681,2.9228187112¥O,5.0950487269,2.054570625,2.7999923713¥H,4.5421853689,2.3787319536,2.0486903588¥H,5.9781813679,1.8954063276,2.4271840279

¥HF=-1749.2077183 Hartrees

PCM : HF=-1749.26894080 Hartrees

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Table S1. Theoretically determined Al-N and Al-O bond lengths of *mer*-Alq_3 and *fac*-Alq_3 obtained at DFT-B3LYP level calculations using various basis sets and corresponding crystallographic data. A number 1, 2, or 3 in parenthesis following O or N indicates a ligand it belongs L1, L2, or L3, respectively. See Scheme S1 for ligand labeling schemes.

isomer	Basis set used	Bond length (Å)					
		Al–O(1)	Al–O(2)	Al–O(3)	Al–N(1)	Al–N(2)	Al–N(3)
mer-Alq_3	LANL2DZ	1.888	1.917	1.918	2.082	2.110	2.055
	6-31 G*	1.856	1.881	1.884	2.083	2.123	2.063
	6-31 +G*	1.860	1.884	1.887	2.079	2.120	2.062
	(single crystal)[7]	(1.850)	(1.860)	(1.857)	(2.050)	(2.087)	(2.017)
fac-Alq_3	6-31 +G*	1.855	1.855	1.855	2.127	2.127	2.129
	(XRPD)[8]	(1.883)	(1.890)	(1.877)	(2.112)	(2.140)	(2.180)

7. M. Brinkmann, G. Gadret, M. Muccini, C. Taliani, N. Masciocchi, A. Sironi, *J. Am. Chem. Soc.*, **2000**, *122*, 5147-5157.
8. M. Cölle, R.E. Dinnebier, W. Brütting, *Chem. Commun*., **2002**, 2908-2909.

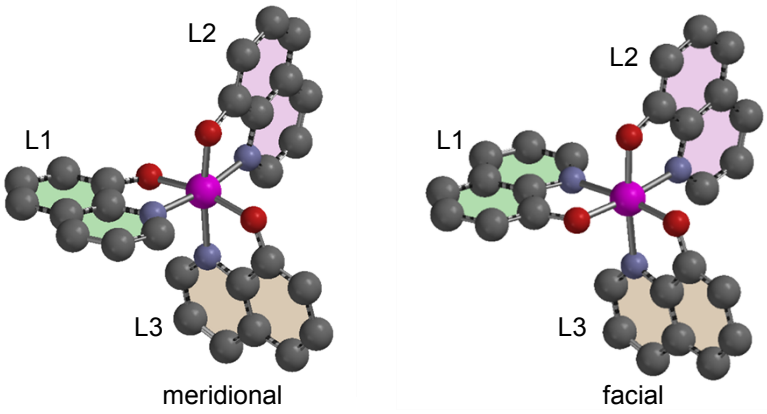

Figure S1. Labeling geometry of quinolinol ligands in *Δ*-*mer*-Alq3 (left) and *Δ*-*fac*-Alq3 (right). Color scheme: Al = purple, O = red, N = blue, C = gray. Hydrogen atoms were omitted for clarity.

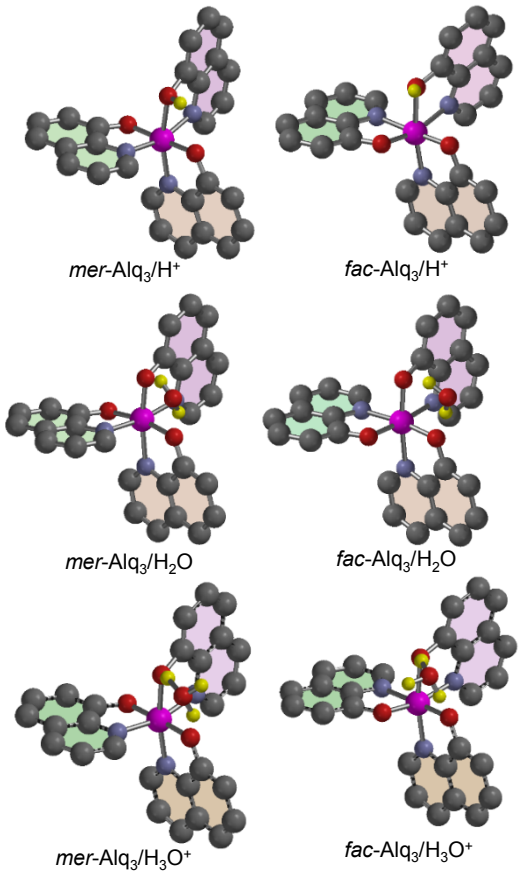

Figure S2. Optimized coordination geometry of H^+, H_2O, and H_3O^+ associated models of Alq_3 isomers. Color scheme: Al= purple, O = red, N = blue, C = grey, H = yellow. Hydrogen atoms on the ligands were omitted for clarity.

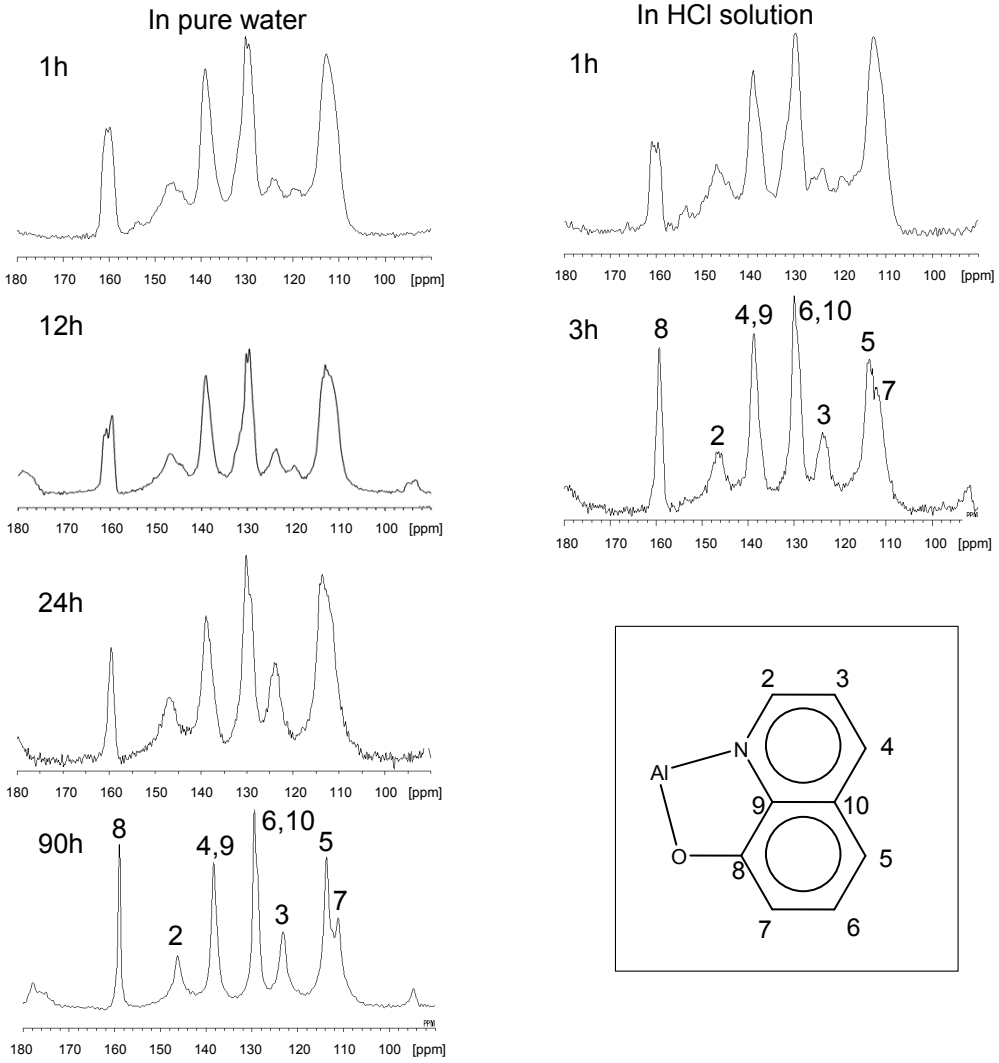

Figure S3. Solid-state ^{13}C NMR spectra of suspensions obtained from reactions in pure water and in an HCl solution. Inset shows the assignments of carbons.