

## Catalytic activity of $\gamma$ -Al<sub>2</sub>O<sub>3</sub>(110) in the NO+H<sub>2</sub> reaction: a DFT study

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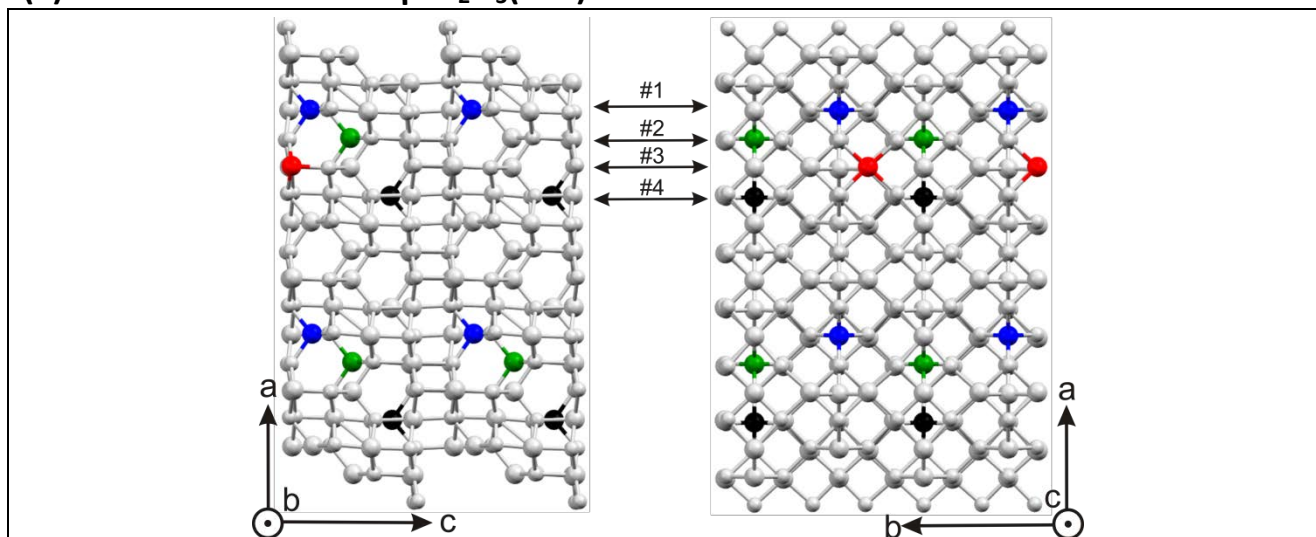
### Supplementary material

- (a) The terminations of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>(110); Figure S(a) and Table S(a)
- (b) Adsorbed states of NO (bound via O) on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>(110); Figure S(b)
- (c) Catalytic reaction of H<sub>2</sub> + O<sub>2</sub> on noble metals (from References 26, 27)
- (d) Absorption of NO and H<sub>2</sub> in bulk  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>; Table S(d)
- (e) Atomic coordinates of optimized configurations; Tables S1-S8 (the Table number in the supplementary material corresponds to the number of the Figure in the article)

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### (a) The terminations of $\gamma\text{-Al}_2\text{O}_3(110)$



**FIG. S(a).** Side views of the bulk (110)-oriented supercell  $\gamma\text{-Al}_{32}\text{O}_{48}\text{-}2\times 2\times 4$  (Al - large and O - small spheres); the colored Al atoms denote the corners of the  $1\times 1$   $\text{Al}_{32}\text{O}_{48}$  unit cell for the terminations #1-#4 faces (110) in Table S(a).1; atomic coordinates are given in Table S(a).2.

Table S(a).1 compares the surface energies obtained in this paper using a non-local plane wave basis set with the literature data. It is important to note that the surface energies calculated using localized basis sets are always much larger than those calculated using a non-localized plane wave basis.<sup>20-22,35</sup>

**Table S(a).1.** Surface energies for options #1 ÷ #4 of face selection (110) in Fig. S(a) (J/m<sup>2</sup>)

Configuration	#1 (used)	#2	#3	#4	Basis set
Non-optimized/optimized	2.561/1.548	3.064/1.753	3.525/1.948	3.064/1.753	Plane wave (this work)
Optimized	1.760				Plane wave <sup>21</sup>
Optimized	1.540				Plane wave <sup>20</sup>
Optimized	1.530				Plane wave <sup>35</sup>
Non-optimized/optimized	3.739/2.961	4.259/3.233	4.791/3.592		Localized <sup>22</sup>
Non-optimized/optimized	3.355/2.559				Localized <sup>21</sup>

**Table S(a).2. Bulk (110)-oriented  $\gamma$ -Al<sub>32</sub>O<sub>48</sub> in Fig. S(a)**

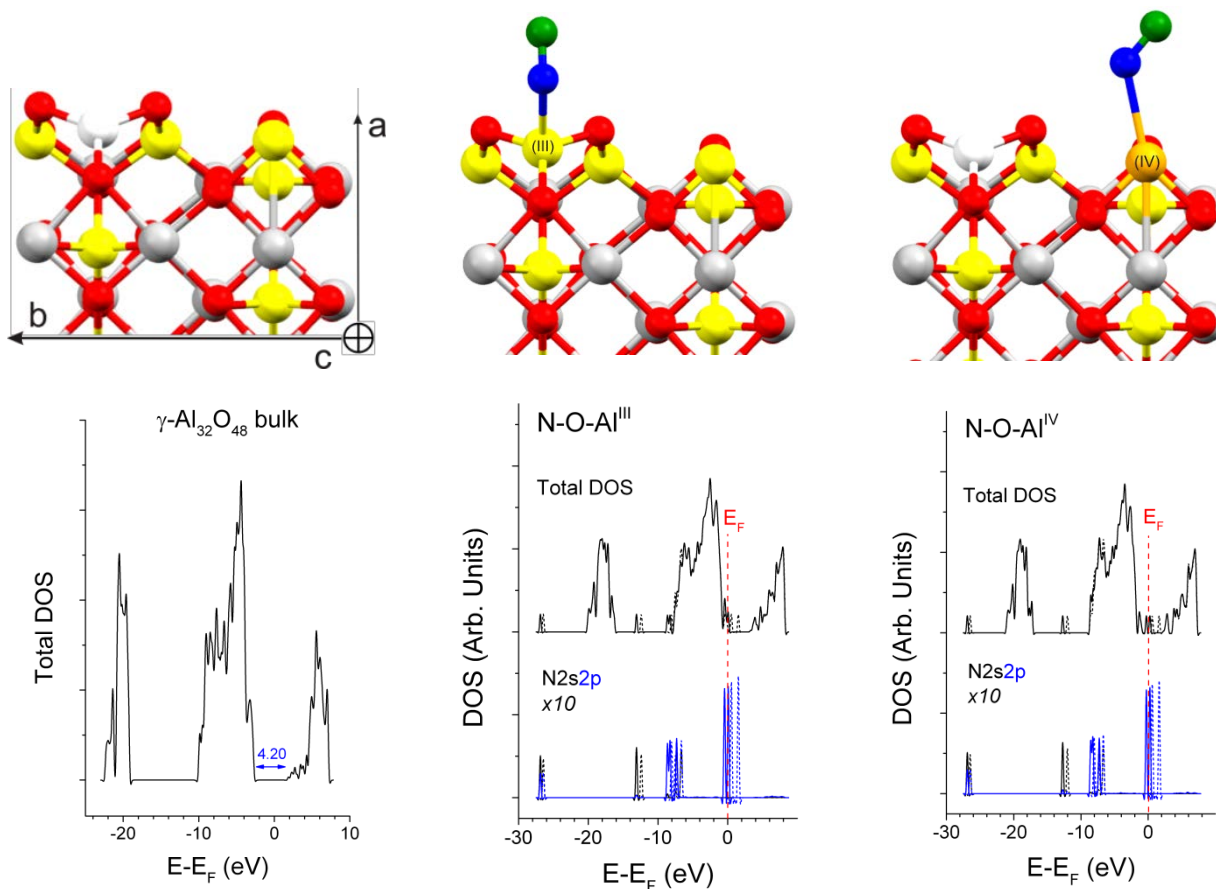
#		X	Y	Z	#		X	Y	Z
1	O	7.159796223	3.315816017	2.081512468	41	Al	3.880240318	2.005338711	7.555224472
2	O	7.159808249	0.694914971	2.081507542	42	Al	3.931214743	2.005340262	1.972116739
3	O	7.210770390	3.315817737	-3.501595074	43	Al	2.988301896	7.677560386	6.243020933
4	O	7.210782406	0.694916616	-3.501600044	44	Al	2.988318271	4.741396220	6.243023378
5	O	7.062991129	6.209507315	4.732841903	45	Al	3.039276280	7.677562120	0.659913298
6	O	7.113965680	6.209509033	-0.850265606	46	Al	3.039292886	4.741398027	0.659915920
7	O	6.974843983	6.209505856	2.050429277	47	O	2.995499542	3.417157318	4.912742715
8	O	7.025818355	6.209507538	-3.532678415	48	O	2.995514799	0.593509763	4.912736671
9	Al	6.951905681	2.005362668	3.401151896	49	O	3.046474212	3.417159168	-0.670364844
10	Al	7.002879955	2.005364294	-2.181955674	50	O	3.046489221	0.593511636	-0.670370952
11	Al	6.925097757	2.005366434	6.179281762	51	O	2.862210698	6.209477833	7.548936831
12	Al	6.976072317	2.005368190	0.596174155	52	O	2.913185037	6.209479620	1.965829230
13	Al	6.856197502	7.649893791	3.360148601	53	O	2.784099809	3.410578768	7.534455521
14	Al	6.856215157	4.769120873	3.360153851	54	O	2.784109249	0.600093213	7.534445495
15	Al	6.907171815	7.649895489	-2.222959172	55	O	2.835074375	3.410580471	1.951347952
16	Al	6.907189562	4.769122677	-2.222953692	56	O	2.835083529	0.600094917	1.951337836
17	O	6.773467112	3.316758633	4.702153508	57	O	2.778816169	6.209477725	4.870719253
18	O	6.773481642	0.693961804	4.702150376	58	O	2.829790711	6.209479544	-0.712388266
19	O	6.824441800	3.316760262	-0.880954068	59	Al	1.931147438	2.005327994	4.856191946
20	O	6.824455907	0.693963407	-0.880957216	60	Al	1.982121939	2.005329981	-0.726915647
21	Al	5.886081618	6.209497200	6.145776963	61	O	1.043745263	7.520869289	6.299817149
22	Al	5.937056138	6.209499037	0.562669369	62	O	1.043761497	4.898073580	6.299823399
23	O	5.038409926	2.005349095	6.131247142	63	O	1.094719738	7.520870993	0.716709460
24	O	5.089384471	2.005350713	0.548139558	64	O	1.094735997	4.898075304	0.716715857
25	O	5.033117204	7.614732346	3.467513568	65	Al	0.961018874	3.445718195	7.641821963
26	O	5.033134575	4.804244906	3.467512036	66	Al	0.961028993	0.564944135	7.641811183
27	O	5.084091608	7.614733982	-2.115593977	67	Al	1.011993423	3.445719913	2.058714410
28	O	5.084108981	4.804246642	-2.115595530	68	Al	1.012003359	0.564945822	2.058703491
29	O	4.955019551	2.005343758	3.453031085	69	Al	0.892128465	6.209474232	4.822690028
30	O	5.005994052	2.005345574	-2.130076500	70	Al	0.943103021	6.209475985	-0.760417547
31	O	4.821710952	7.621313145	6.089224169	71	Al	0.865331510	6.209473214	7.600822004
32	O	4.821726421	4.797669610	6.089219819	72	Al	0.916305787	6.209474922	2.017714399
33	O	4.872685335	7.621314916	0.506116692	73	O	0.842387396	2.005327947	8.951538925
34	O	4.872701057	4.797671343	0.506112243	74	O	0.893361684	2.005329683	3.368431315
35	Al	4.828909300	3.473426630	4.758941248	75	O	0.754236299	2.005329737	6.269126343
36	Al	4.828926724	0.537263592	4.758942016	76	O	0.805210810	2.005331547	0.686018695
37	Al	4.879883957	3.473428349	-0.824166265	77	O	0.657420050	7.519924688	8.920459445
38	Al	4.879901108	0.537265284	-0.824165512	78	O	0.657435491	4.899022420	8.920465426
39	Al	3.936990663	6.209481381	3.446743300	79	O	0.708394318	7.519926372	3.337351852
40	Al	3.987965048	6.209483118	-2.136364303	80	O	0.708409806	4.899024116	3.337357841
						<b>2a</b>	-0.101948677	-3.43800E-06	11.166215185
						<b>b</b>	-4.64020E-05	8.408287183	4.37540E-09
						<b>c</b>	8.077044348	4.25645E-05	3.78089E-09

## (b) Adsorbed states of NO (bound via O)

(a)  $\gamma\text{-Al}_2\text{O}_3(110)\text{-}1\times 1$

(b)  $Q_{\text{NO}} = 0.27 \text{ eV}$ ;  $d_{\text{AlO}} = 2.188 \text{ \AA}$   
 $d_{\text{NO}} = 1.171 \text{ \AA}$ ;  $\angle\text{AlON} = 125.7^\circ$

(c)  $Q_{\text{NO}} = 0.12 \text{ eV}$ ;  $d_{\text{AlO}} = 2.479 \text{ \AA}$   
 $d_{\text{NO}} = 1.164 \text{ \AA}$ ;  $\angle\text{AlON} = 127.7^\circ$



**FIG. S(b).** Views, total DOS and pDOS (solid lines for spin-up and dotted lines for spin-down) of (a) free  $\gamma\text{-Al}_2\text{O}_3(110)$ , (b)  $\text{NO}/\text{Al}^{\text{III}}$  and (c)  $\text{NO}/\text{Al}^{\text{IV}}$  states on  $\gamma\text{-Al}_2\text{O}_3(110)$ ; adsorption heats, bond lengths, bond angles and the primary coordination of the atom ( in parenthesis) are indicated. Color legends: white for  $\text{Al}^{\text{III}}$ , yellow for  $\text{Al}^{\text{IV}}$ , grey for  $\text{Al}^{\text{VI}}$ , green for N, red for O in oxide and blue for O in NO.

### (c) Catalytic reaction of H<sub>2</sub> + O<sub>2</sub> on noble metals (experimental data)

The reaction rate ( $w$ ) on Pt, Ir, Pd and Rh wires ( $P = 2 \cdot 10^{-5}$  Pa;  $T = 180-400$  K) is as follows:<sup>26</sup>

$$\text{Excess O}_2: w = k \cdot P_{\text{H}_2}^2 \cdot P_{\text{O}_2}^{-1}$$

$$\text{Excess H}_2: w = k \cdot P_{\text{H}_2}^0 \cdot P_{\text{O}_2}^1$$

The reaction rate on Pt single crystals ( $P = 10^{-6} - 10^{-4}$  Pa;  $T = 300 - 360$  K) is as follows:<sup>27</sup>

$$\text{Pt(111), excess O}_2: w = k \cdot P_{\text{H}_2}^{1.8} \cdot P_{\text{O}_2}^{-0.8}; \text{ excess H}_2: w = k \cdot P_{\text{H}_2}^0 \cdot P_{\text{O}_2}^1$$

$$\text{Pt(110), excess O}_2: w = k \cdot P_{\text{H}_2}^{1.9} \cdot P_{\text{O}_2}^{-0.9}; \text{ excess H}_2: w = k \cdot P_{\text{H}_2}^{-0.4} \cdot P_{\text{O}_2}^1$$

During the reaction, the surface is covered with either oxygen or hydrogen, depending on the H<sub>2</sub>/O<sub>2</sub> ratio in the reaction mixture.<sup>26, 27</sup>

With regard to the reaction of NO+H<sub>2</sub> on Pt/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub>(110), this means that an excess O<sub>2</sub> in the reaction mixture prevents the formation of H/Pt, excluding the flow of H atoms from Pt to  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>(110); and a highly stable NH<sub>2</sub>+H complex inhibiting the active center O<sup>II</sup>-Al<sup>III</sup>-O<sup>II</sup> is not formed, which ultimately increases the catalytic activity.

### (d) Absorption of NO and H<sub>2</sub> in bulk $\gamma$ -Al<sub>2</sub>O<sub>3</sub>

Table S(d). (i) Absorption of NO in bulk  $\gamma$ -Al<sub>32</sub>O<sub>48</sub>

#		X	Y	Z	#	X	Y	Z	
1	O	-3.636733978	0.646469708	7.197118771	43	O	4.712455593	6.201011548	7.139479633
2	O	-3.610119337	3.281834006	7.195634103	44	Al	6.095206270	2.009119694	7.003366421
3	O	-0.978378888	6.370367956	7.143371657	45	O	2.108486703	6.370155884	7.065759562
4	Al	0.479365283	1.904857309	7.005754327	46	Al	3.352940424	1.991014537	6.991487120
5	O	-3.591851540	6.161655854	6.999405722	47	Al	3.341520863	4.776612515	6.928812813
6	Al	-2.327436905	1.921018902	7.044866227	48	Al	3.396076551	7.675319730	6.932514854
7	Al	-2.241909303	4.726564081	6.913741042	49	O	4.648232557	0.690408790	6.832115741
8	Al	-2.353060940	7.626614526	6.883550122	50	O	4.673417842	3.301951218	6.833506467
9	O	-1.014501929	0.630126400	6.833067655	51	Al	6.102296664	6.170749673	5.953695666
10	O	-1.083979570	3.153430202	6.841455689	52	O	6.053576914	1.974098344	5.107037405
11	Al	0.571522442	6.482436518	6.114616469	53	O	3.454935508	4.813632369	5.103614073
12	O	0.430288174	1.853799772	5.110444602	54	O	3.428137114	7.614092965	5.088111722
13	O	-2.026386969	4.789421921	5.081494424	55	O	3.385584970	2.008819883	5.004331088
14	O	-2.203504807	7.574521524	5.050943424	56	O	6.081590703	4.754092273	4.897601910
15	O	-2.258750837	1.917691099	4.961927160	57	O	6.043805333	7.594524491	4.907211411
16	O	0.838794787	5.320397783	4.577617539	58	Al	4.704746939	0.522612238	4.878398069
17	O	0.448602897	7.707937116	4.874712911	59	Al	4.715994664	3.461078019	4.897170814
18	Al	-0.938719069	0.489954783	4.854586929	60	Al	3.385285953	6.211065048	3.982593676
19	Al	-1.002865476	3.268277577	4.858929072	61	Al	7.445541087	1.952931589	3.938490261
20	Al	-2.154814699	6.178199235	3.962012726	62	Al	6.215371908	4.711306664	3.065763435
21	Al	1.891799663	2.035519520	3.986157074	63	Al	6.206543990	7.625220685	3.079655542
22	Al	0.595854496	4.770837915	2.860654823	64	O	4.880844487	0.559481440	3.062917272
23	Al	0.657308305	7.720782732	3.043423358	65	O	4.885421919	3.390858865	3.067679908
24	O	-0.737888803	0.582498865	3.018673957	66	O	7.529926089	6.158963800	2.952193585
25	O	-0.686291807	3.419127564	3.059189888	67	O	7.476710201	0.547439645	2.872523255
26	O	2.012111510	6.320094570	2.822536847	68	O	7.511182932	3.375621627	2.872346358
27	O	1.905822464	0.656372218	2.866181655	69	O	4.859858681	6.175017290	2.866131143
28	O	1.898251717	3.443221807	2.854244037	70	Al	4.834972973	1.974125414	2.011133146
29	O	-0.738218970	6.223142346	2.788677014	71	O	6.292805547	4.860943819	1.127317920
30	Al	-0.759459456	1.995003823	1.964909536	72	O	6.281327884	7.474930527	1.130729891
31	O	0.727931240	4.948997685	1.048255286	73	Al	7.584566709	0.521815040	1.062376822
32	O	0.712757565	7.575249619	1.085968187	74	Al	7.612200081	3.418299385	1.043284832
33	Al	2.082559087	0.584924331	1.054759187	75	Al	7.592288284	6.167076129	0.952972965
34	Al	2.096427528	3.445373381	1.028327205	76	O	8.902317380	1.963223659	0.954636442
35	Al	2.056056895	6.269751975	0.932658068	77	Al	4.824705403	6.208446777	0.976209811
36	O	3.375066037	1.992378882	0.973101146	78	O	6.245796530	1.971465069	0.842361598
37	Al	-0.783500894	6.324719014	0.922973043	79	O	8.928200744	4.872103017	0.741646738
38	O	0.664851220	2.020274810	0.813977114	80	O	8.860226319	7.516125573	0.783222053
39	O	3.358124384	4.919684868	0.763953755	81	O	0.535157059	4.697703587	6.557513103
40	O	3.405350426	7.573247650	0.789119686	82	N	0.607634496	4.227960153	5.360979972
41	O	2.017870907	0.694275169	7.206533367	<b>2a</b>		11.166678380	-0.006741176	0.001911287
42	O	2.134670272	3.267257570	7.247660620	<b>b</b>		0.005073810	8.408285652	0.000007246
					<b>c</b>		-0.075123555	0.000036362	8.076694983

**Table S(d). (ii) Absorption of H<sub>2</sub> in bulk  $\gamma$ -Al<sub>32</sub>O<sub>48</sub>**

#	X	Y	Z	#	X	Y	Z		
1	O	-3.577602597	0.689411392	7.181371935	43	O	4.683861130	6.213852615	7.119707492
2	O	-3.574635681	3.310132082	7.184611107	44	Al	6.119467880	1.981299641	6.995443230
3	O	-0.922961673	6.213734015	7.105783044	45	O	1.993264466	6.203645572	6.982330688
4	Al	0.505509091	1.955154008	6.985549339	46	Al	3.347297570	1.997443456	6.989145122
5	O	-3.599164317	6.209320027	7.000875247	47	Al	3.344996770	4.782234092	6.912299410
6	Al	-2.256291105	2.000464943	6.986508231	48	Al	3.302975720	7.651914381	6.890122552
7	Al	-2.295821294	4.764214421	6.889337029	49	O	4.648774211	0.683972865	6.834810133
8	Al	-2.295120440	7.645780792	6.886777512	50	O	4.650304969	3.312403631	6.823464223
9	O	-0.965673660	0.676826840	6.827950082	51	Al	6.099784572	6.194628705	5.940834351
10	O	-0.951380740	3.309065359	6.808984326	52	O	6.099574607	1.993587620	5.105390948
11	Al	0.496624777	6.237200210	5.947879887	53	O	3.539080644	4.870358646	5.083292468
12	O	0.440100788	1.945488714	5.092471588	54	O	3.423697606	7.627017626	5.071183780
13	O	-2.215884995	4.786257222	5.067132979	55	O	3.465013290	1.961984889	4.978456270
14	O	-2.163850884	7.601021483	5.064716431	56	O	6.095222011	4.778864483	4.879987242
15	O	-2.194328644	1.994185684	4.990478564	57	O	6.049853220	7.607903452	4.880158207
16	O	0.338948432	4.871385887	4.844619726	58	Al	4.724044866	0.529364946	4.874809321
17	O	0.463531903	7.635325926	4.876395548	59	Al	4.773622362	3.458217384	4.886530841
18	Al	-0.888147836	0.529094540	4.862799763	60	Al	3.426416117	6.245755033	3.958052849
19	Al	-0.920454769	3.468391900	4.864061318	61	Al	7.515999633	1.996184308	3.946230696
20	Al	-2.168433411	6.193714278	3.971414827	62	Al	6.227139655	4.735891462	3.045883167
21	Al	1.938817148	2.039714058	3.976236779	63	Al	6.230721702	7.669663846	3.048897882
22	Al	0.592339321	4.750027585	3.015785544	64	O	4.896903971	0.581382255	3.039929797
23	Al	0.637252523	7.689923025	3.048637743	65	O	4.893039604	3.411352701	3.050810242
24	O	-0.718107818	0.580064943	3.028950107	66	O	7.529766676	6.201220797	2.929196757
25	O	-0.716879090	3.408133763	3.035693262	67	O	7.515107902	0.589337437	2.857484480
26	O	1.940625839	6.209730223	2.938435065	68	O	7.512499883	3.399359643	2.850633153
27	O	1.917317656	0.622789701	2.866468960	69	O	4.857936105	6.210960208	2.825205819
28	O	1.896157655	3.412826972	2.802802880	70	Al	4.837933711	1.998315491	1.983558184
29	O	-0.747213235	6.214655047	2.806144706	71	O	6.290787355	4.891983856	1.105714586
30	Al	-0.748687355	1.993313158	1.971485771	72	O	6.298018234	7.515997253	1.105381577
31	O	0.697065926	4.913804602	1.084499410	73	Al	7.633252941	0.555367822	1.036849478
32	O	0.717263559	7.529945407	1.103297340	74	Al	7.632170339	3.436812422	1.031701001
33	Al	2.053025023	0.571624461	1.044593646	75	Al	7.596424614	6.200045239	0.938195065
34	Al	2.041489890	3.447196696	1.009943806	76	O	8.939978393	1.994126704	0.922844162
35	Al	2.011751592	6.212623422	0.936394701	77	Al	4.825275023	6.219610982	0.944992691
36	O	3.365013703	1.999167091	0.926050307	78	O	6.262577785	1.996381398	0.821562788
37	Al	-0.772105030	6.225123322	0.928183034	79	O	8.913816567	4.888977193	0.738544719
38	O	0.667649945	1.993568172	0.801481289	80	O	8.914351041	7.512985436	0.741068445
39	O	3.338552856	4.906986263	0.745396642	81	H	2.236804645	3.725875766	4.819364847
40	O	3.334001182	7.521088721	0.743147208	82	H	1.678335727	3.432876731	5.207996484
41	O	2.015340918	0.693462125	7.178282534	<b>2a</b>		11.166678380	-0.006741176	0.001911287
42	O	2.028704540	3.315142409	7.197625889	<b>b</b>		0.005073810	8.408285652	0.000007246
					<b>c</b>		-0.075123555	0.000036362	8.076694983

## (e) Atomic coordinates of optimized configurations (Å)

Table S1. Bulk  $\gamma$ -Al<sub>32</sub>O<sub>48</sub> in Fig. 1(a)

#		X	Y	Z	#		X	Y	Z
1	O	2.016830371	3.314553908	7.178867572	41	Al	7.520016647	2.000776461	3.950355463
2	O	2.015243939	0.693653342	7.17886283	42	Al	1.936677317	2.004146881	3.949399904
3	O	-3.566508766	3.317924497	7.177911758	43	Al	6.219588405	7.673789586	3.046287171
4	O	-3.568095241	0.697023856	7.177907005	44	Al	6.217819081	4.737625953	3.046284835
5	O	4.670691003	6.206644912	7.106744807	45	Al	0.636249173	7.677160189	3.045331572
6	O	-0.912648104	6.210015499	7.105789377	46	Al	0.634480024	4.740996629	3.04532947
7	O	1.989214736	6.208262119	6.993652693	47	O	4.886730392	3.414189993	3.041084575
8	O	-3.594124554	6.21163267	6.992697082	48	O	4.885020481	0.590542955	3.04108176
9	Al	3.337555345	2.003304673	6.983251461	49	O	-0.696608766	3.417560712	3.040129263
10	Al	-2.245783822	2.006675168	6.982295753	50	O	-0.698318739	0.593913697	3.040126199
11	Al	6.115813879	2.001632105	6.98228373	51	O	7.525734529	6.204919394	2.932338219
12	Al	0.532474674	2.00500273	6.981328309	52	O	1.942395332	6.20829005	2.931382576
13	Al	3.300849784	7.647859583	6.887202067	53	O	7.510291554	3.406029636	2.854078162
14	Al	3.299116676	4.767087186	6.887201391	54	O	7.508585657	0.595544599	2.854069577
15	Al	-2.282489585	7.65123015	6.886246398	55	O	1.926952387	3.409400208	2.853122747
16	Al	-2.284222464	4.770457859	6.886245815	56	O	1.925246403	0.598915172	2.853113875
17	O	4.640951348	3.313915497	6.816929428	57	O	4.848408924	6.206535415	2.824037535
18	O	4.639365543	0.691119148	6.816927194	58	O	-0.734930193	6.209906103	2.823082095
19	O	-0.942387828	3.317285995	6.815974134	59	Al	4.83922962	2.002395867	1.976243529
20	O	-0.943973644	0.69448962	6.815971477	60	Al	-0.744109571	2.005766723	1.975288048
21	Al	6.094510973	6.205783121	5.943027732	61	O	6.294373689	7.517065739	1.102341903
22	Al	0.511171782	6.209153827	5.94207227	62	O	6.292797252	4.894270504	1.102341461
23	O	6.085329184	2.001645199	5.095230742	63	O	0.711034402	7.520436313	1.101386395
24	O	0.501990002	2.005015686	5.094275305	64	O	0.709458111	4.897641097	1.101385979
25	O	3.425145115	7.612634759	5.065198989	65	Al	7.634630784	3.44110567	1.032074909
26	O	3.423447636	4.802147832	5.065198413	66	Al	7.632881716	0.560332141	1.032066547
27	O	-2.158194027	7.616005264	5.064243412	67	Al	2.051291633	3.444476257	1.031119476
28	O	-2.159891527	4.805518437	5.064242838	68	Al	2.049542427	0.563702697	1.031110931
29	O	3.408005058	2.003255991	4.986934226	69	Al	4.817929631	6.206562353	0.936984723
30	O	-2.175334125	2.006626676	4.985978745	70	Al	-0.765409542	6.209932975	0.936029298
31	O	6.048712074	7.617633751	4.878186122	71	Al	7.596190171	6.204885	0.936027981
32	O	6.047003856	4.793990732	4.878183534	72	Al	2.012850969	6.208255577	0.935072277
33	O	0.465372999	7.621004391	4.877230523	73	O	8.944525135	1.999925478	0.925620884
34	O	0.463664681	4.797361334	4.877228188	74	O	3.361185928	2.003296083	0.92466519
35	Al	4.715917241	3.470550692	4.872984901	75	O	6.263048949	2.001545934	0.81252482
36	Al	4.714146233	0.534388188	4.872983598	76	O	0.679709704	2.004916613	0.811569349
37	Al	-0.867421871	3.47392128	4.872029577	77	O	8.918494747	7.514540112	0.740407656
38	Al	-0.869192893	0.537758749	4.872028001	78	O	8.91691919	4.893638317	0.74040643
39	Al	3.413722789	6.207397425	3.968917713	79	O	3.335155559	7.517910665	0.739451942
40	Al	-2.169616411	6.210768031	3.967962115	80	O	3.333580009	4.897008882	0.739450764
						<b>2a</b>	11.166678377	-0.006741176	0.001911287
						<b>b</b>	0.005073810	8.408285652	7.24600E-06
						<b>c</b>	-0.075123555	3.63620E-05	8.076694983



**Table S2.**  $\gamma$ -Al<sub>32</sub>O<sub>48</sub>(110)-(1×1) unit cell in **Fig. 2(a)**

The atoms are listed in descending order Z; the lower half is a mirror image of the upper one; the charges and fillings of the states of the atoms are indicated.

#	Charge	State filling	X	Y	Z	#	X	Y	Z	
1	-0.84	O <sup>II</sup> 2s <sup>1.67</sup> 2p <sup>5.17</sup>	3.12621313	11.80336365	16.46196191	41	O	2.954182723	11.81867747	10.51250426
2	-0.84	O <sup>II</sup> 2s <sup>1.67</sup> 2p <sup>5.17</sup>	3.126226487	9.023887706	16.46195507	42	O	2.954199679	9.008571009	10.51249754
3	-0.84	O <sup>II</sup> 2s <sup>1.66</sup> 2p <sup>5.18</sup>	2.562966536	6.209476899	16.01031068	43	Al	1.882530913	10.41361774	10.42987002
4	1.42	Al <sup>III</sup> 3s <sup>0.52</sup> 3p <sup>1.05</sup>	2.26632668	10.41362231	15.95090033	44	O	2.730334019	6.209479587	10.42915086
5	-0.83	O <sup>III</sup> 2s <sup>1.65</sup> 2p <sup>5.18</sup>	6.488829769	9.013058014	15.877472	45	O	6.738233459	9.087481946	10.37808239
6	-0.83	O <sup>III</sup> 2s <sup>1.65</sup> 2p <sup>5.18</sup>	6.488818264	11.81423271	15.87744843	46	O	6.738210262	11.73980167	10.37807734
7	-0.82	O <sup>III</sup> 2s <sup>1.66</sup> 2p <sup>5.17</sup>	7.187841946	6.209504967	15.84615398	47	Al	4.792123074	11.86725484	10.35097019
8	1.39	Al <sup>IV</sup> 3s <sup>0.49</sup> 3p <sup>1.12</sup>	4.671210488	11.92038167	15.69307044	48	Al	4.79213822	8.960013644	10.35096937
9	1.39	Al <sup>IV</sup> 3s <sup>0.49</sup> 3p <sup>1.12</sup>	4.671220181	8.906890597	15.69306385	49	O	6.990294469	6.209497722	10.26645974
10	1.41	Al <sup>VI</sup> 3s <sup>0.51</sup> 3p <sup>1.08</sup>	0.903451658	6.209470143	15.65507609	50	Al	0.862037955	6.209464884	10.26064129
11	1.29	Al <sup>VI</sup> 3s <sup>0.50</sup> 3p <sup>1.21</sup>	7.031533076	10.41364576	14.84820299	51	Al	6.973319174	10.41364306	9.127182787
12	-0.78	O <sup>IV</sup> 2s <sup>1.65</sup> 2p <sup>5.13</sup>	0.891122813	10.41362167	14.76332609	52	Al	3.9402884	6.209485036	9.105290195
13	1.37	Al <sup>IV</sup> 3s <sup>0.49</sup> 3p <sup>1.13</sup>	3.680860126	6.209485737	14.68403784	53	O	4.932952275	10.41363316	9.086996142
14	-0.84	O <sup>III</sup> 2s <sup>1.62</sup> 2p <sup>5.22</sup>	4.887236501	7.511494942	14.66082839	54	O	4.998234335	7.631005724	9.030072255
15	-0.84	O <sup>III</sup> 2s <sup>1.62</sup> 2p <sup>5.22</sup>	4.887249488	4.907486706	14.66082692	55	O	4.99824922	4.787974466	9.030070862
16	1.69	Al <sup>VI</sup> 3s <sup>0.49</sup> 3p <sup>1.22</sup>	6.753558141	7.603045496	14.64294422	56	O	0.840113181	10.41361037	8.970680568
17	1.69	Al <sup>VI</sup> 3s <sup>0.49</sup> 3p <sup>1.22</sup>	6.753568696	4.815961658	14.64294034	57	Al	6.823626558	4.750994291	8.969014702
18	-0.82	O <sup>IV</sup> 2s <sup>1.64</sup> 2p <sup>5.19</sup>	4.658915965	10.41363706	14.61313755	58	Al	6.823608804	7.668003439	8.969010749
19	-0.80	O <sup>IV</sup> 2s <sup>1.63</sup> 2p <sup>5.17</sup>	0.653328813	7.546851888	14.38947367	59	O	0.624588949	7.473243098	8.811931342
20	-0.80	O <sup>IV</sup> 2s <sup>1.63</sup> 2p <sup>5.17</sup>	0.653334566	4.872082966	14.38946572	60	O	0.624620721	4.945690377	8.811917655
21	-0.79	O <sup>IV</sup> 2s <sup>1.65</sup> 2p <sup>5.14</sup>	7.090609944	9.149865117	13.3563149	61	O	7.061903279	11.75103323	7.778706126
22	-0.79	O <sup>IV</sup> 2s <sup>1.65</sup> 2p <sup>5.14</sup>	7.090620619	11.67742446	13.35625127	62	O	7.061904517	9.076256393	7.778691724
23	1.27	Al <sup>VI</sup> 3s <sup>0.49</sup> 3p <sup>1.24</sup>	0.891625692	8.955105715	13.19916935	63	O	3.056288727	6.209480396	7.555067663
24	1.27	Al <sup>VI</sup> 3s <sup>0.49</sup> 3p <sup>1.24</sup>	0.891610675	11.87212345	13.19916556	64	Al	0.961660076	11.80714999	7.525240262
25	-0.78	O <sup>IV</sup> 2s <sup>1.63</sup> 2p <sup>5.15</sup>	6.875136651	6.209500401	13.19747857	65	Al	0.96167366	9.020069544	7.525234382
26	-0.82	O <sup>III</sup> 2s <sup>1.63</sup> 2p <sup>5.19</sup>	2.717002653	8.992110426	13.13810389	66	O	2.827980675	11.7156281	7.507368575
27	-0.82	O <sup>III</sup> 2s <sup>1.63</sup> 2p <sup>5.19</sup>	2.716983923	11.83514786	13.13810378	67	O	2.827995736	9.111617238	7.507358691
28	-0.79	O <sup>IV</sup> 2s <sup>1.63</sup> 2p <sup>5.16</sup>	2.782285994	6.20947877	13.08117687	68	Al	4.034373339	10.41362861	7.484141773
29	1.35	Al <sup>IV</sup> 3s <sup>0.50</sup> 3p <sup>1.15</sup>	3.774946867	10.41363375	13.06289824	69	O	6.824123947	6.20949736	7.404861763
30	1.24	Al <sup>VI</sup> 3s <sup>0.48</sup> 3p <sup>1.28</sup>	0.741922737	6.209468685	13.04100102	70	Al	0.683712368	6.209465021	7.319994373
31	1.27	Al <sup>VI</sup> 3s <sup>0.50</sup> 3p <sup>1.23</sup>	6.85319406	10.41364233	11.90754445	71	Al	6.811773245	10.4136437	6.513104196
32	-0.77	O <sup>IV</sup> 2s <sup>1.63</sup> 2p <sup>5.14</sup>	0.72493575	10.41360857	11.90172066	72	Al	3.044028456	4.702737698	6.475126328
33	1.26	Al <sup>VI</sup> 3s <sup>0.48</sup> 3p <sup>1.26</sup>	2.923114367	4.755861801	11.8172076	73	Al	3.044010771	7.716218517	6.475123376
34	1.26	Al <sup>VI</sup> 3s <sup>0.48</sup> 3p <sup>1.26</sup>	2.923098055	7.663103445	11.81720752	74	O	0.527380793	10.41361096	6.322009349
35	-0.78	O <sup>IV</sup> 2s <sup>1.64</sup> 2p <sup>5.14</sup>	0.977014706	7.535624978	11.79009955	75	O	1.226392068	7.610053848	6.290727903
36	-0.78	O <sup>IV</sup> 2s <sup>1.64</sup> 2p <sup>5.14</sup>	0.97702176	4.883322852	11.79009405	76	O	1.226418645	4.808883509	6.290724775
37	-0.78	O <sup>IV</sup> 2s <sup>1.62</sup> 2p <sup>5.16</sup>	4.984900137	10.41363422	11.73901942	77	Al	5.448917668	6.209494302	6.217295276
38	1.37	Al <sup>IV</sup> 3s <sup>0.51</sup> 3p <sup>1.12</sup>	5.832711059	6.209496153	11.7383139	78	O	5.152254507	10.41363912	6.157857554
39	-0.82	O <sup>III</sup> 2s <sup>1.62</sup> 2p <sup>5.20</sup>	4.76105501	4.804439206	11.65567184	79	O	4.589013188	7.599227782	5.706242391
40	-0.82	O <sup>III</sup> 2s <sup>1.62</sup> 2p <sup>5.20</sup>	4.761039989	7.614541908	11.65567117	80	O	4.58902529	4.819753304	5.706238185
						<b>T1</b>	8.077044348	4.25645E-05	0	
						<b>T2</b>	-4.64021E-05	8.408287183	0	

**Table S3(a).** The surface oxynitride  $\gamma\text{-Al}_{32}\text{O}_{47}\text{N}^{\text{IV}}(110)$  in Fig. 3(a)

#		X	Y	Z	#		X	Y	Z
1	O	3.200853628	9.046178659	16.64417502	41	O	2.952090713	9.012971093	10.47724542
2	O	3.200838285	11.78107613	16.64416929	42	O	2.952072922	11.81428454	10.47724169
3	O	2.559229209	6.209480501	16.00092772	43	Al	1.868840569	10.41361904	10.44658005
4	Al	2.334736644	10.41362189	15.96715948	44	O	2.731579387	6.209479823	10.38988618
5	O	6.48439857	9.015952267	15.885696	45	O	6.73399256	9.082087176	10.37199527
6	O	6.484383054	11.8113374	15.88569355	46	O	6.733975235	11.74520411	10.37198746
7	O	7.163964513	6.209504525	15.82061129	47	Al	4.788767321	8.962451672	10.3563798
8	Al	4.694555523	8.90251589	15.73877239	48	Al	4.788750673	11.86481727	10.35637378
9	Al	4.694541027	11.92475644	15.73876838	49	Al	0.860888225	6.209471559	10.26562089
10	Al	0.872191089	6.209471054	15.63009437	50	O	6.980335691	6.209501603	10.24778564
11	Al	7.172126325	10.41364614	14.94058042	51	Al	6.973077153	10.41364472	9.138423994
12	N	0.970586215	10.41361383	14.75936462	52	Al	3.957911609	6.209481919	9.095128638
13	O	4.45929599	10.41363409	14.71464498	53	O	4.937489003	10.41363015	9.083448
14	O	4.866194889	7.523896648	14.67549806	54	O	5.000012225	7.640974866	9.010216839
15	O	4.866209198	4.895088644	14.67549705	55	O	5.000030154	4.777997818	9.010196227
16	Al	3.683785929	6.209487734	14.63713603	56	Al	6.820677497	7.682379925	8.989119998
17	Al	6.744543442	7.618881599	14.60834603	57	Al	6.820694365	4.736623707	8.98911004
18	Al	6.744558774	4.80012419	14.6083438	58	O	0.83758325	10.41361302	8.964115917
19	O	0.663274028	4.890219324	14.37667096	59	O	0.612235629	7.470354537	8.786634607
20	O	0.663253282	7.528719409	14.37666868	60	O	0.612249911	4.948586873	8.786626376
21	O	7.076920661	9.138719195	13.37450792	61	O	7.051236534	11.74887204	7.770555891
22	O	7.076911514	11.68857192	13.37450734	62	O	7.051244374	9.078412971	7.770554617
23	Al	0.931765685	11.80460177	13.30659282	63	Al	0.958166842	9.016119752	7.532737997
24	Al	0.93177471	9.022620265	13.30658148	64	Al	0.958149566	11.81110374	7.532733321
25	O	6.858353561	6.209500227	13.1866037	65	Al	4.022362941	10.41362823	7.507674344
26	O	2.745535074	8.965378959	13.09453739	66	O	3.144945982	6.209478268	7.502980057
27	O	2.745523173	11.86186947	13.09453541	67	O	2.828104673	9.109080897	7.486956673
28	Al	3.760834409	10.41362738	13.0750333	68	O	2.828087121	11.71815582	7.486952711
29	O	2.782414078	6.209482431	13.05826811	69	O	6.803681047	6.209497851	7.364794538
30	Al	0.7380126	6.209472281	13.00508676	70	Al	0.625750755	6.209466153	7.29449719
31	Al	6.863336517	10.41364468	11.95602756	71	Al	6.821535825	10.41364063	6.521733209
32	O	0.716259142	10.41361014	11.89952251	72	Al	3.03093257	7.717567486	6.453113032
33	Al	2.898943955	7.665997374	11.78232039	73	Al	3.030945815	4.70138934	6.453112424
34	Al	2.898959488	4.752969635	11.78231852	74	O	0.530478042	10.41360995	6.319765323
35	O	4.989222612	10.413635	11.75485052	75	O	1.22286565	7.602741356	6.284056783
36	O	0.974211181	7.523791404	11.7535089	76	O	1.222880865	4.816198471	6.284049989
37	O	0.974227962	4.895165317	11.75349784	77	Al	5.413574521	6.209484964	6.227771975
38	Al	5.824659306	6.209498442	11.72277314	78	O	5.143327529	10.41363829	6.152195005
39	O	4.750406334	7.606965545	11.63263298	79	O	4.572806685	7.600316836	5.645910062
40	O	4.75042162	4.812020778	11.63261967	80	O	4.572816694	4.818641768	5.64590874

**Table S3(b).** The surface oxynitride  $\gamma\text{-Al}_{32}\text{O}_{47}\text{N}^{\text{II}}(110)$  in **Fig. 3(b)**

#	X	Y	Z	#	X	Y	Z		
1	N	3.140365039	9.01405522	16.67859437	41	O	2.953468701	9.009755133	10.51451188
2	O	3.122331165	11.7304856	16.43843921	42	O	2.953482783	11.82156629	10.5117927
3	O	2.566648327	6.289632842	16.01108609	43	O	2.730592716	6.209379298	10.43154295
4	Al	2.183986327	10.36526682	15.95450912	44	Al	1.883421007	10.41651904	10.42456994
5	O	6.489022236	11.81720569	15.87375177	45	O	6.737344187	11.739708	10.37394148
6	O	6.528081602	9.007868418	15.87041747	46	O	6.738002938	9.088724193	10.37194282
7	O	7.185955325	6.215965482	15.84236057	47	Al	4.792286435	8.961500089	10.3493534
8	Al	4.709317982	8.902390074	15.73325907	48	Al	4.790500895	11.86738183	10.34857747
9	Al	4.671952078	11.89906523	15.67851811	49	O	6.991604577	6.209093433	10.26637686
10	Al	0.897607862	6.229334487	15.65381886	50	Al	0.862789489	6.208466154	10.25690735
11	Al	6.990581946	10.41593627	14.8145225	51	Al	6.971157606	10.41408018	9.120258169
12	O	0.861546486	10.4200637	14.72659271	52	Al	3.937905942	6.209924649	9.10356915
13	O	4.874831507	4.911237836	14.67761438	53	O	4.930916722	10.41442407	9.084312766
14	Al	3.690231256	6.22966936	14.67712315	54	O	4.997376348	4.789399301	9.031027465
15	O	4.894029488	7.526272061	14.6586903	55	O	4.997299796	7.630655856	9.03090702
16	Al	6.751712482	4.820364344	14.64804476	56	O	0.839067597	10.41423718	8.9672506
17	Al	6.760399141	7.609312071	14.62915194	57	Al	6.822709285	7.669057894	8.965497466
18	O	4.726276123	10.39826509	14.59772033	58	Al	6.822150715	4.752761892	8.962781429
19	O	0.667438587	4.877048971	14.40180892	59	O	0.623497467	4.945466987	8.811722639
20	O	0.651698381	7.554250679	14.38086031	60	O	0.623419206	7.473130118	8.810790155
21	O	7.086807278	11.69161585	13.34536832	61	O	7.061067176	11.75173033	7.77486562
22	O	7.082977817	9.148557699	13.33158119	62	O	7.061536994	9.075944589	7.773972889
23	Al	0.895655343	11.8662081	13.20978226	63	O	3.0514634	6.209709735	7.556046779
24	O	6.875749938	6.205796613	13.19861851	64	Al	0.960469012	11.80622398	7.521298016
25	Al	0.883745189	8.958889018	13.17956333	65	Al	0.960302613	9.021283412	7.520980126
26	O	2.726407661	11.82700715	13.14569087	66	O	2.826526532	9.111694127	7.506894059
27	O	2.714345416	8.989494103	13.14348052	67	O	2.826579937	11.71563078	7.506791465
28	O	2.784646447	6.209891587	13.08407167	68	Al	4.033481559	10.41367789	7.479321761
29	Al	3.785661939	10.40208835	13.07293212	69	O	6.822562763	6.208743923	7.404648298
30	Al	0.745587802	6.206870144	13.04011761	70	Al	0.68469827	6.209931052	7.319241731
31	O	0.725697213	10.41722584	11.89434974	71	Al	6.809695212	10.4139037	6.506956923
32	Al	6.853247843	10.42240779	11.89372682	72	Al	3.043030813	4.703040803	6.474073576
33	Al	2.925527271	4.75029688	11.82155344	73	Al	3.043098189	7.716230802	6.473740974
34	Al	2.924054467	7.662444493	11.81474724	74	O	0.526214134	10.41408606	6.318591573
35	O	0.981976506	4.879055572	11.7971988	75	O	1.225194412	4.809146145	6.29012091
36	O	0.977367744	7.533346383	11.78811713	76	O	1.22531788	7.610218504	6.289372712
37	Al	5.834518546	6.208674207	11.73493731	77	Al	5.448174762	6.209445591	6.213186025
38	O	4.982962466	10.41428654	11.73452308	78	O	5.151163698	10.41379985	6.155664722
39	O	4.762359469	4.803824638	11.65772636	79	O	4.587244723	4.819647435	5.70649772
40	O	4.761757502	7.614176806	11.65595474	80	O	4.58747763	7.599400489	5.706490435

**Table S3(c).** Adsorption of NO on the surface oxynitride  $\gamma\text{-Al}_{32}\text{O}_{47}\text{N}^{\text{IV}}$  (110) in **Fig. 3(c)**

#	X	Y	Z	#	X	Y	Z		
1	O	3.138005017	9.002238418	16.635427605	41	O	2.892887067	9.018707338	10.492383773
2	O	3.137611988	11.827232851	16.635113398	42	O	2.892898752	11.808729710	10.492498699
3	O	2.463911523	6.210957622	16.019497733	43	Al	1.802458225	10.413730547	10.447762059
4	Al	2.304427955	10.414033231	16.002449108	44	O	2.672043232	6.209518770	10.411560210
5	O	6.418949212	9.014510933	15.894162954	45	O	6.673248235	9.083807897	10.389011187
6	O	6.418762023	11.813576122	15.894043550	46	O	6.673242259	11.743585900	10.389007419
7	O	7.048479029	6.209828485	15.826762878	47	Al	4.733540688	8.963956773	10.361715418
8	Al	4.623862674	8.925355875	15.745216228	48	Al	4.733527140	11.863475917	10.361770267
9	Al	4.623875393	11.902485986	15.744469678	49	Al	0.796772298	6.209569535	10.255310570
10	Al	0.721196415	6.209494089	15.609123046	50	O	6.921567785	6.209559218	10.253787277
11	Al	7.136030883	10.414004616	14.959882042	51	Al	6.910945483	10.413696336	9.143640028
12	N	0.928297503	10.413983694	14.780885850	52	Al	3.884195493	6.209569505	9.091702391
13	O	4.397849060	10.414058052	14.712363010	53	O	4.874305784	10.413687629	9.097733552
14	O	4.795378138	7.528745187	14.694863231	54	O	4.935738836	7.634784778	9.033929586
15	O	4.794955661	4.891724280	14.695460846	55	O	4.935746048	4.784322381	9.033974464
16	Al	3.661627143	6.210520788	14.564700370	56	Al	6.758038692	7.674474553	8.971764420
17	Al	6.664824004	7.640024895	14.586336131	57	Al	6.758071333	4.744685174	8.971746766
18	Al	6.664786561	4.779781855	14.586222212	58	O	0.772484846	10.413677285	8.977562764
19	O	0.608293875	4.899956699	14.394152613	59	O	0.555486734	7.470566738	8.800493506
20	O	0.608743630	7.519121854	14.394029803	60	O	0.555558490	4.948529245	8.800531124
21	O	7.021253721	9.136078147	13.392179563	61	O	6.994909135	11.748688899	7.785431914
22	O	7.020969627	11.691538421	13.392131663	62	O	6.994897214	9.078723512	7.785420088
23	Al	0.885135886	11.787765087	13.345937234	63	Al	0.896739853	9.019106464	7.531213404
24	Al	0.885281421	9.040023074	13.346239952	64	Al	0.896717088	11.808236344	7.531197748
25	O	6.784244346	6.209719418	13.194087965	65	Al	3.967116347	10.413691339	7.498720402
26	O	2.691784423	8.954774763	13.110148181	66	O	3.021831957	6.209532403	7.534839287
27	O	2.691772322	11.872733728	13.110194481	67	O	2.762911953	9.109658549	7.505236992
28	Al	3.694927045	10.413755631	13.072378040	68	O	2.762885897	11.717699114	7.505264473
29	O	2.698773720	6.209642878	13.078886340	69	O	6.747267623	6.209530397	7.386731180
30	Al	0.659800850	6.209644775	12.990229793	70	Al	0.595728618	6.209541722	7.304297382
31	Al	6.809423704	10.413781004	11.949822801	71	Al	6.744903364	10.413678536	6.525317013
32	O	0.664509773	10.413722831	11.923887075	72	Al	2.977093835	7.719511607	6.464975211
33	Al	2.827979565	7.674602880	11.774499898	73	Al	2.977116801	4.699565468	6.464950336
34	Al	2.828110941	4.744629147	11.774642244	74	O	0.460964127	10.413658323	6.327304142
35	O	4.932117850	10.413685654	11.771059041	75	O	1.160610130	7.609597795	6.286895737
36	O	0.910610986	7.526182565	11.763974717	76	O	1.160616862	4.809454499	6.286909523
37	O	0.910648701	4.892870327	11.764196042	77	Al	5.367018945	6.209525523	6.206503694
38	Al	5.761330611	6.209641321	11.703259860	78	O	5.084384280	10.413676003	6.169187017
39	O	4.683904750	7.607456373	11.658017895	79	O	4.515303170	7.601324988	5.678961781
40	O	4.684019121	4.811683116	11.658158128	80	O	4.515334406	4.817701870	5.678944570
					81	N	2.845225620	6.191778145	17.678682130
					82	O	3.964941802	6.211427521	17.873541115

**Table S5(a). NO(1) in Fig. 5(a)**

#		X	Y	Z	#		X	Y	Z
1	O	3.1677392	11.79151283	16.458745	41	O	2.9862125	11.81892875	10.513454
2	O	3.1677168	9.034508607	16.458286	42	O	2.9861964	9.008318587	10.513546
3	O	2.5967865	6.208909679	16.018651	43	Al	1.9144431	10.41362908	10.434679
4	Al	2.2218998	10.41312675	16.052053	44	O	2.763228	6.20950044	10.432135
5	O	6.5228358	9.009624716	15.881177	45	O	6.771669	9.087443021	10.38004
6	O	6.5232744	11.81656443	15.881781	46	O	6.7716521	11.73995484	10.380099
7	O	7.22433	6.209055122	15.85206	47	Al	4.8238568	11.86621806	10.355312
8	Al	4.7013727	11.91123134	15.67846	48	Al	4.8238294	8.961144179	10.355293
9	Al	4.7012815	8.914918305	15.677813	49	O	7.0223926	6.209569027	10.270617
10	Al	0.9385875	6.209225012	15.648886	50	Al	0.8952276	6.209505501	10.265704
11	Al	7.0398835	10.41313403	14.833313	51	Al	7.0045919	10.41373722	9.1296671
12	O	0.9215817	10.41337945	14.751557	52	Al	3.9745613	6.209576469	9.1106221
13	Al	3.7149862	6.208861806	14.686323	53	O	4.9660935	10.41371643	9.0886894
14	O	4.9211964	7.509658806	14.660116	54	O	5.0310516	7.632185983	9.0330418
15	O	4.9213588	4.90812242	14.660596	55	O	5.0310769	4.786990086	9.0331024
16	Al	6.7877301	7.602462756	14.644277	56	O	0.8718603	10.41370467	8.9738393
17	Al	6.7878608	4.815632086	14.644342	57	Al	6.8556402	4.749414379	8.9757012
18	O	4.7416604	10.41327923	14.593168	58	Al	6.8556296	7.66976174	8.9756741
19	O	0.6887576	7.546917041	14.393941	59	O	0.6550486	7.4727728	8.8140722
20	O	0.6888003	4.871514073	14.393866	60	O	0.6550566	4.946350386	8.8140321
21	O	7.1235502	9.14593214	13.354944	61	O	7.0932276	11.75143136	7.7808942
22	O	7.1234616	11.68088324	13.355233	62	O	7.0932536	9.076075757	7.7808775
23	Al	0.9317168	8.965916949	13.217887	63	O	3.0976202	6.209598302	7.5566954
24	Al	0.9317424	11.86081226	13.218012	64	Al	0.9927878	11.8070402	7.5297962
25	O	6.9097652	6.209227588	13.202158	65	Al	0.9927968	9.020425533	7.5297865
26	O	2.7567605	8.990213244	13.141257	66	O	2.8593018	11.71565297	7.5100507
27	O	2.7567642	11.83679903	13.141201	67	O	2.8593213	9.111826503	7.5100711
28	O	2.8143199	6.209278801	13.08633	68	Al	4.0653048	10.41375006	7.488426
29	Al	3.8108317	10.41353169	13.069791	69	O	6.8527788	6.209621665	7.4049201
30	Al	0.7759395	6.209252447	13.039557	70	Al	0.7080055	6.209584403	7.322358
31	Al	6.8891004	10.41352434	11.908161	71	Al	6.8436391	10.41376386	6.5171707
32	O	0.7599987	10.41352206	11.906031	72	Al	3.0744473	4.703530207	6.4790378
33	Al	2.9541539	4.754416589	11.820262	73	Al	3.0744352	7.715669201	6.4790606
34	Al	2.9542315	7.664366558	11.820327	74	O	0.5590905	10.41373481	6.324847
35	O	1.0111037	7.536389097	11.793253	75	O	1.2577632	7.608858688	6.2949706
36	O	1.0110953	4.882317792	11.793135	76	O	1.2577777	4.810327885	6.2949583
37	O	5.0178152	10.41361165	11.738243	77	Al	5.4747776	6.209619524	6.2232306
38	Al	5.8651887	6.209469568	11.743023	78	O	5.1833482	10.41375316	6.1601659
39	O	4.7933225	4.805175776	11.657619	79	O	4.6167019	7.598828745	5.702601
40	O	4.7933598	7.613790048	11.657554	80	O	4.6167238	4.820387072	5.7026014
					81	O	0.8248796	10.40258222	17.735701
					82	N	1.1208527	10.4332603	18.868187

**Table S5(b). NO(2) in Fig. 5(b)**

#		X	Y	Z	#		X	Y	Z
1	O	3.131557015	11.80827868	16.48877695	41	O	2.944266145	11.81677802	10.50572473
2	O	3.131551015	9.01888158	16.48870091	42	O	2.94428288	9.010461629	10.50572454
3	O	2.577664696	6.209411733	15.9359803	43	Al	1.869747219	10.41361613	10.42910828
4	Al	2.286420732	10.41359525	15.95300196	44	O	2.715605204	6.209476432	10.41872122
5	O	6.475907808	9.014362185	15.8721437	45	O	6.729421314	9.086888728	10.37518863
6	O	6.475884629	11.81291716	15.87212992	46	O	6.729397092	11.74039749	10.3751807
7	O	7.125750466	6.209483445	15.80637958	47	Al	4.783684384	11.86683798	10.34660259
8	Al	4.662736306	11.92471605	15.68640013	48	Al	4.783699863	8.960423225	10.34660106
9	Al	4.662765496	8.902545473	15.68639222	49	O	6.979424319	6.209496826	10.25574156
10	Al	0.866717093	6.209411617	15.7298345	50	Al	0.846771345	6.209468112	10.26433813
11	Al	7.048253941	10.41364387	14.86084851	51	Al	6.96405412	10.41363839	9.125051642
12	O	0.898195759	10.41361019	14.77698679	52	Al	3.930481299	6.209478897	9.098802364
13	Al	3.702866183	6.209493896	14.62661319	53	O	4.924180508	10.41362496	9.084247395
14	O	4.879925253	7.527618528	14.62454945	54	O	4.988135514	7.632153658	9.023055936
15	O	4.879920531	4.891355159	14.62455459	55	O	4.988149999	4.786824044	9.02305997
16	Al	6.744864786	7.603748551	14.62217563	56	O	0.829874561	10.41360828	8.96814993
17	Al	6.744856726	4.815239974	14.62215685	57	Al	6.813001006	4.75064646	8.962327524
18	O	4.607523101	10.41363049	14.62339491	58	Al	6.812983867	7.668337945	8.962329905
19	O	0.643380545	7.544752421	14.40884478	59	O	0.613328244	7.473212505	8.807836854
20	O	0.643381761	4.874157981	14.40882767	60	O	0.613341466	4.945708166	8.807837231
21	O	7.088068473	9.153132379	13.3596605	61	O	7.051768015	11.75028414	7.774737408
22	O	7.088038793	11.67415723	13.35964491	62	O	7.051788321	9.076990677	7.774747952
23	Al	0.886199099	8.947493359	13.204112	63	O	3.052503431	6.209473675	7.546156913
24	Al	0.886175777	11.8797218	13.20409322	64	Al	0.951909932	11.80718196	7.522732179
25	O	6.873163982	6.20949769	13.17633829	65	Al	0.951916345	9.020020704	7.522739416
26	O	2.708174327	8.988421438	13.13114569	66	O	2.818405162	11.71607558	7.503262826
27	O	2.70815403	11.83883071	13.13114751	67	O	2.818415469	9.111133906	7.50328859
28	O	2.776333062	6.209481924	13.05935372	68	Al	4.024056629	10.41361039	7.481661205
29	Al	3.760586013	10.41363006	13.05708562	69	O	6.811881789	6.209494973	7.395463981
30	Al	0.743546408	6.209467597	13.06418234	70	Al	0.671478865	6.209456147	7.316488837
31	Al	6.848252541	10.41363739	11.908352	71	Al	6.801781369	10.41363456	6.51017024
32	O	0.717573205	10.41361143	11.90349057	72	Al	3.033637007	4.702221605	6.468695616
33	Al	2.909769324	4.754810259	11.80416304	73	Al	3.03360971	7.716719748	6.468688175
34	Al	2.909752731	7.664142832	11.80415359	74	O	0.517887252	10.41359903	6.318784293
35	O	0.966560297	7.533546659	11.79640191	75	O	1.216197122	7.609696092	6.287167626
36	O	0.966577168	4.885394541	11.79639432	76	O	1.2162239	4.809225136	6.287167536
37	O	4.977898046	10.41363082	11.73919367	77	Al	5.434779534	6.209484852	6.209296829
38	Al	5.825933001	6.209491312	11.72559952	78	O	5.141965856	10.41359902	6.155333793
39	O	4.749592045	4.806779516	11.64478926	79	O	4.57572044	7.599166968	5.693369524
40	O	4.749577756	7.612191062	11.64478003	80	O	4.575769739	4.819765477	5.693403331
					81	N	1.088508084	6.210605879	17.76531416
					82	O	1.442180394	6.20906646	18.87039236

**Table S5(c). NO(3) in Fig. 5(c)**

#		X	Y	Z	#		X	Y	Z
1	O	3.146985337	11.76790766	16.49273105	41	O	2.954173184	11.82121532	10.51107637
2	O	3.000432487	8.974497791	16.35287226	42	O	2.954817174	9.005901909	10.49888568
3	O	2.55884377	6.179557085	16.01413237	43	Al	1.886707775	10.41450092	10.42221102
4	Al	2.24705594	10.44158975	15.887316	44	O	2.732114185	6.208943625	10.42462772
5	O	6.550887067	9.025392802	15.84698832	45	O	6.736962768	9.087579025	10.36766302
6	O	6.494873242	11.82485429	15.86347877	46	O	6.736467945	11.73831897	10.36967219
7	O	7.189929605	6.219208927	15.84064976	47	Al	4.789579537	11.86628848	10.34779948
8	Al	4.676701209	11.92753458	15.69414744	48	Al	4.791880066	8.960016028	10.34628775
9	Al	4.692481572	8.903433267	15.81309713	49	O	6.990990565	6.207803615	10.26100997
10	Al	0.902387166	6.220084653	15.6429813	50	Al	0.864437653	6.207724632	10.25302853
11	Al	7.023013244	10.42735695	14.81449681	51	Al	6.972595406	10.41266337	9.117809221
12	O	0.881496779	10.44903004	14.70978741	52	Al	3.940002904	6.207124513	9.098980723
13	Al	3.682037673	6.22878926	14.6896673	53	O	4.931275968	10.41306492	9.082673699
14	O	4.888773833	7.528595503	14.72695444	54	O	4.999033649	7.627843821	9.027644654
15	O	4.880711199	4.915251187	14.65919778	55	O	4.997205893	4.785458768	9.02531803
16	Al	6.753951085	7.618313157	14.63520728	56	O	0.840517146	10.41267884	8.963200089
17	Al	6.751319105	4.829400706	14.63402452	57	Al	6.82163243	4.749111145	8.963739949
18	O	4.651410078	10.39558371	14.65505355	58	Al	6.823131773	7.668242283	8.964124469
19	O	0.657065226	7.553084401	14.3732782	59	O	0.622715395	7.47105444	8.804002527
20	O	0.649494891	4.878231754	14.3788898	60	O	0.62264791	4.944091661	8.806117217
21	O	7.087779118	9.154580343	13.32659923	61	O	7.061049539	11.74995469	7.771528295
22	O	7.079848768	11.68917375	13.33532493	62	O	7.060845516	9.074490389	7.770538136
23	Al	0.886836457	8.957502548	13.1730515	63	O	3.061407342	6.208695041	7.547050781
24	Al	0.89209309	11.87170603	13.19106052	64	Al	0.960677937	11.80470074	7.520178766
25	O	6.86812948	6.219843895	13.19418205	65	Al	0.960914016	9.018947227	7.519005698
26	O	2.712263257	8.994295558	13.12101485	66	O	2.827123144	11.7155321	7.503364302
27	O	2.726363675	11.82874159	13.14243153	67	O	2.827006277	9.110732674	7.498864063
28	O	2.788669802	6.215477317	13.08016792	68	Al	4.032786444	10.41298431	7.479728202
29	Al	3.78874709	10.40073335	13.08320384	69	O	6.820179455	6.207064424	7.395141934
30	Al	0.742641511	6.213047516	13.0334431	70	Al	0.677007479	6.207697472	7.312502061
31	Al	6.852825294	10.42006934	11.89164384	71	Al	6.811252311	10.41241115	6.50587756
32	O	0.724145042	10.41924559	11.8840039	72	Al	3.041904666	4.70167535	6.469463193
33	Al	2.929422475	4.754132142	11.82183891	73	Al	3.042324216	7.714723967	6.467543009
34	Al	2.923476982	7.663758738	11.80775926	74	O	0.527009843	10.41219826	6.31477012
35	O	0.975954938	7.533796037	11.7762641	75	O	1.225239104	7.607122362	6.28512948
36	O	0.98312428	4.883693375	11.78826667	76	O	1.225016839	4.807562249	6.286299425
37	O	4.982895383	10.41313148	11.74066226	77	Al	5.443477091	6.208319335	6.209539005
38	Al	5.832743435	6.211958626	11.73089865	78	O	5.151024606	10.41319731	6.153722291
39	O	4.764377864	4.805689993	11.65037269	79	O	4.585422192	7.598568809	5.694459389
40	O	4.761944277	7.617479544	11.65484065	80	O	4.583544987	4.819437712	5.694251536
					81	N	4.784249441	9.174515693	17.93447281
					82	O	4.649317182	8.572438239	18.92215855

**Table S6(a).  $^2\text{H}(1)$  in Fig. 6(a)**

#		X	Y	Z	#		X	Y	Z
1	O	3.15406151	11.8984066	16.446087	41	O	2.978531912	11.79795057	10.51962845
2	O	3.225234545	9.192527183	16.54401979	42	O	2.97692598	8.990571266	10.5107775
3	O	2.568589821	5.990848472	16.03466787	43	Al	1.902653103	10.39442001	10.43818808
4	Al	1.99196371	10.41076848	16.36306492	44	O	2.75445498	6.1917349	10.44053941
5	O	6.51133066	8.998400388	15.87628863	45	O	6.761022153	9.069465119	10.38969608
6	O	6.527154623	11.80246589	15.87292496	46	O	6.761495597	11.72273967	10.38907512
7	O	7.186191865	6.195444287	15.843611	47	Al	4.818301165	11.8466388	10.36641332
8	Al	4.747074512	11.85703741	15.62942707	48	Al	4.815693822	8.945791368	10.36280498
9	Al	4.691100186	8.935139579	15.70298383	49	O	7.012991965	6.192491129	10.27677982
10	Al	0.88747844	6.189201284	15.65330109	50	Al	0.883352937	6.19271011	10.2721404
11	Al	7.115598694	10.39145869	14.87432598	51	Al	6.994901208	10.39673376	9.138499564
12	O	0.944367403	10.39746278	14.71134575	52	Al	3.963636526	6.191782483	9.114044327
13	Al	3.703294388	6.187758641	14.66601224	53	O	4.957876479	10.39663036	9.096820946
14	O	4.871872055	7.501473354	14.71237419	54	O	5.021273522	7.613375548	9.043620917
15	O	4.905091278	4.891439794	14.66752939	55	O	5.021252833	4.770505416	9.044867598
16	Al	6.75579623	7.599716324	14.64540598	56	O	0.860602161	10.39675264	8.979232533
17	Al	6.782328265	4.796009089	14.62212866	57	Al	6.8460044	4.731073896	8.980712246
18	O	4.707617401	10.40067457	14.59500573	58	Al	6.845528895	7.651520872	8.977608833
19	O	0.715907614	7.522643777	14.4233166	59	O	0.645590987	7.45591377	8.82298511
20	O	0.670271106	4.855489882	14.39882386	60	O	0.645916709	4.929197604	8.822650905
21	O	7.126642248	9.11426363	13.37333041	61	O	7.083691787	11.7346291	7.788098769
22	O	7.115723092	11.66157734	13.3630199	62	O	7.083120696	9.059249147	7.788435482
23	Al	0.945101591	8.96919679	13.25913533	63	O	3.079241911	6.192605464	7.56593507
24	Al	0.932957358	11.82399951	13.23703937	64	Al	0.982653863	11.78936383	7.534776998
25	O	6.892106428	6.206417235	13.21141749	65	Al	0.982773232	9.00434939	7.535086567
26	O	2.759744727	8.959473766	13.13703654	66	O	2.849281008	11.69950502	7.517783746
27	O	2.755375457	11.83650834	13.14679234	67	O	2.849081609	9.09587721	7.518018648
28	O	2.79918584	6.194071532	13.09686814	68	Al	4.055745801	10.3975697	7.495436376
29	Al	3.785371943	10.39626323	13.07701468	69	O	6.844422324	6.193427472	7.414966212
30	Al	0.766465976	6.195581918	13.04011195	70	Al	0.703947046	6.192508868	7.331555555
31	Al	6.881807174	10.38751817	11.92446713	71	Al	6.832545437	10.39699956	6.523181085
32	O	0.754312729	10.39423442	11.91070936	72	Al	3.064348939	4.686402931	6.484772901
33	Al	2.940017248	4.735136355	11.81691825	73	Al	3.065128744	7.699743731	6.4867975
34	Al	2.938395227	7.651425873	11.81421142	74	O	0.548427792	10.3966963	6.331512158
35	O	1.001547583	7.519091357	11.80322735	75	O	1.247938254	7.592926425	6.302802624
36	O	1.000538282	4.86778193	11.80032582	76	O	1.247178888	4.792754982	6.301955115
37	O	5.007139609	10.39418106	11.75183091	77	Al	5.469770403	6.193871467	6.227038673
38	Al	5.854842787	6.195394473	11.73818354	78	O	5.17299213	10.39914666	6.168791007
39	O	4.782987517	4.79061906	11.66923713	79	O	4.610044537	7.584747195	5.718014179
40	O	4.781237685	7.596770024	11.66855009	80	O	4.607959813	4.805613426	5.714331571
					81	H	0.851609579	10.58232877	17.44598854
					82	H	2.818165189	12.86936636	16.43574069



**Table S6(b).  $2H(2)$  in Fig. 6(b)**

#		X	Y	Z	#		X	Y	Z
1	O	3.037098992	11.81340671	16.45394845	41	O	2.974372075	11.81755931	10.51602019
2	O	3.160691456	9.098386723	16.4625666	42	O	2.968468172	9.014191168	10.5061851
3	O	2.590009006	6.219499906	16.00127751	43	Al	1.893539103	10.41920747	10.43899718
4	Al	1.991094424	10.40393354	16.38195867	44	O	2.753568768	6.209997213	10.42656834
5	O	6.499640177	8.996942424	15.86762514	45	O	6.758521138	9.089036645	10.37040138
6	O	6.483859498	11.77646177	15.97386706	46	O	6.758742401	11.73901737	10.38284328
7	O	7.199827417	6.16341218	15.83562009	47	Al	4.811289112	11.86748007	10.35662838
8	Al	4.50232582	11.89302254	15.63093874	48	Al	4.805777215	8.965395775	10.34466606
9	Al	4.661356579	8.920638269	15.68115411	49	O	7.011097252	6.21264908	10.26136528
10	Al	0.928824516	6.20594113	15.65313879	50	Al	0.88536433	6.207910575	10.26467588
11	Al	7.025385591	10.34014134	14.77286371	51	Al	6.990869819	10.41757064	9.12198922
12	O	0.876891415	10.39638278	14.66873673	52	Al	3.959487225	6.212403524	9.101198775
13	Al	3.707431731	6.212160679	14.67912711	53	O	4.953691947	10.41836141	9.084923181
14	O	4.906427996	7.509521401	14.65645492	54	O	5.018347702	7.634247834	9.025583601
15	O	4.929349157	4.887820099	14.69377106	55	O	5.01898268	4.79093239	9.036802265
16	Al	6.766663237	7.593356867	14.64542869	56	O	0.857682188	10.41806808	8.972618709
17	Al	6.775511972	4.850132636	14.54318324	57	Al	6.843187187	4.754528093	8.96626127
18	O	4.805921572	10.43767456	14.58203493	58	Al	6.84423446	7.672081021	8.963819459
19	O	0.655944516	7.535445288	14.39557344	59	O	0.644044383	7.475028478	8.810089873
20	O	0.671408943	4.869137884	14.38982978	60	O	0.643304272	4.94784854	8.810429624
21	O	7.0939388	9.121477147	13.31775158	61	O	7.079244779	11.75485674	7.778096358
22	O	7.067508866	11.68975982	13.41684787	62	O	7.081864207	9.079725494	7.774055527
23	Al	0.936235352	8.98564285	13.25855439	63	O	3.079401349	6.213145735	7.550686509
24	Al	0.946496708	11.81179656	13.29018083	64	Al	0.981924264	11.81129986	7.527591125
25	O	6.886715678	6.204825461	13.18306019	65	Al	0.982179767	9.024572634	7.526169407
26	O	2.760416722	8.981162003	13.13718603	66	O	2.848179372	11.72142265	7.508384445
27	O	2.771815891	11.84002399	13.15634685	67	O	2.848163307	9.116088921	7.505422453
28	O	2.809256366	6.205089694	13.08459951	68	Al	4.053314292	10.41879977	7.483030723
29	Al	3.808069587	10.40297357	13.08022557	69	O	6.841515029	6.212095661	7.401907328
30	Al	0.781066217	6.207159927	13.03060569	70	Al	0.702137793	6.213657696	7.319286003
31	Al	6.879023591	10.40046494	11.88743979	71	Al	6.832062138	10.41790637	6.509837111
32	O	0.737541953	10.42870809	11.91194668	72	Al	3.062260397	4.706338238	6.471940903
33	Al	2.935329552	4.748102614	11.81815869	73	Al	3.063174286	7.720894994	6.472146845
34	Al	2.937549624	7.668033025	11.80920539	74	O	0.548347091	10.41930332	6.323206148
35	O	1.005004439	7.536721473	11.79348539	75	O	1.245864781	7.614155433	6.290294283
36	O	1.002832271	4.88045859	11.79315146	76	O	1.245183433	4.812891238	6.290723391
37	O	5.006375603	10.41258186	11.73686172	77	Al	5.46631562	6.213668149	6.213262017
38	Al	5.846570343	6.216642779	11.71488261	78	O	5.171898493	10.41842514	6.157186565
39	O	4.781507395	4.806251683	11.6626258	79	O	4.606695303	7.603337971	5.700376248
40	O	4.777574086	7.61807479	11.64618737	80	O	4.606862332	4.823084604	5.702248158
					81	H	0.714891117	10.48862636	17.36168169
					82	H	6.961962626	11.77524256	16.82766141

**Table S6(c). H(3) in Fig. 6(c)**

#		X	Y	Z	#		X	Y	Z
1	O	3.225812757	11.6177252	16.57921314	41	O	2.958706805	11.83491033	10.50801191
2	O	3.147034366	8.917958786	16.47878911	42	O	2.959879241	9.025659227	10.51470018
3	O	2.550918001	6.422107203	16.03254796	43	Al	1.885277053	10.43029623	10.43522293
4	Al	1.972953196	10.41731866	16.37270353	44	O	2.73701699	6.224645431	10.43732162
5	O	6.518127818	9.024445614	15.87298689	45	O	6.742651875	9.102919971	10.38567964
6	O	6.50054509	11.82594566	15.87603182	46	O	6.742593138	11.75616468	10.38723176
7	O	7.167705631	6.222817239	15.84133768	47	Al	4.797131615	11.8796378	10.36114569
8	Al	4.679707765	11.8886775	15.71446789	48	Al	4.799378532	8.978419245	10.36309481
9	Al	4.734353526	8.967372629	15.64305681	49	O	6.995587709	6.224733105	10.27341631
10	Al	0.869364172	6.228820876	15.65089711	50	Al	0.866505685	6.224853595	10.26806472
11	Al	7.095059771	10.43451327	14.86415118	51	Al	6.977057805	10.42927048	9.135801159
12	O	0.921636687	10.42663659	14.69887369	52	Al	3.946173263	6.225590774	9.110780932
13	Al	3.687011226	6.230810445	14.66492546	53	O	4.939512712	10.4293936	9.094935089
14	O	4.887739271	7.529607169	14.66910845	54	O	5.003395765	7.64720551	9.040575604
15	O	4.852323637	4.913210303	14.71938016	55	O	5.003691092	4.804054899	9.04171238
16	Al	6.7650754	7.621831086	14.6184889	56	O	0.843355047	10.42914645	8.975856314
17	Al	6.738658416	4.817986968	14.64383891	57	Al	6.8277847	4.765669209	8.97530741
18	O	4.685087848	10.42334933	14.60332839	58	Al	6.828090756	7.686382831	8.977645948
19	O	0.651071715	7.560132473	14.39245849	59	O	0.628270525	7.488231668	8.819299143
20	O	0.695267416	4.895309876	14.41821114	60	O	0.628202595	4.961464294	8.819466599
21	O	7.094001359	9.162829734	13.35735662	61	O	7.065549959	11.76664275	7.786108889
22	O	7.103977188	11.71187637	13.36816387	62	O	7.066048058	9.091530107	7.785527257
23	Al	0.913813247	9.000096959	13.23087328	63	O	3.0635689	6.225001926	7.561752712
24	Al	0.92462404	11.85869946	13.25094352	64	Al	0.965597855	11.82171403	7.532502026
25	O	6.871228934	6.210132434	13.20908158	65	Al	0.965303281	9.036498717	7.532373349
26	O	2.736885988	8.988838642	13.14216677	66	O	2.831860466	11.7306655	7.51420212
27	O	2.741041227	11.86523787	13.13535327	67	O	2.831864497	9.126636862	7.51561919
28	O	2.782920301	6.222952842	13.09456965	68	Al	4.038160289	10.42871434	7.493484337
29	Al	3.768118938	10.42853308	13.08024287	69	O	6.826463701	6.224233383	7.411161809
30	Al	0.747467799	6.221339232	13.03689598	70	Al	0.685070292	6.225089337	7.327325442
31	Al	6.862019352	10.43725213	11.919757	71	Al	6.815229381	10.42898019	6.520916553
32	O	0.734097839	10.43100263	11.90459692	72	Al	3.047631334	4.717999949	6.482125782
33	Al	2.921203377	4.765228626	11.81259603	73	Al	3.047426	7.73188467	6.482152005
34	Al	2.922557719	7.681544205	11.81389749	74	O	0.530892277	10.42927351	6.328595031
35	O	0.982397037	7.54824739	11.79594813	75	O	1.230128908	7.625164605	6.298976939
36	O	0.983462629	4.897560533	11.80011436	76	O	1.230177096	4.824973315	6.299190993
37	O	4.987349764	10.43071883	11.75114413	77	Al	5.451383541	6.224973069	6.223253162
38	Al	5.836864829	6.221335323	11.73458342	78	O	5.155624679	10.42816997	6.166904223
39	O	4.76347025	4.819790064	11.66714058	79	O	4.590735582	7.614114546	5.710286596
40	O	4.765020004	7.625674538	11.66481599	80	O	4.591994685	4.834539635	5.712021495
					81	H	2.806638591	7.947539002	16.45448189

**Table S7(b). NHOH(1) in Fig. 7(b)**

#		X	Y	Z	#		X	Y	Z
1	O	3.214172562	11.777429290	16.458243842	41	O	3.011044836	11.818348751	10.501753097
2	O	3.214205950	9.049845288	16.458261131	42	O	3.011064275	9.008906833	10.501748356
3	O	2.621020675	6.209494301	16.013700679	43	Al	1.938512690	10.413623377	10.427870173
4	Al	2.180633227	10.413626256	16.145155977	44	O	2.788966796	6.209481380	10.418568297
5	O	6.545127838	9.006970687	15.868008441	45	O	6.798161987	9.087125538	10.370323076
6	O	6.545108294	11.820332634	15.868011297	46	O	6.798147862	11.740160555	10.370321553
7	O	7.249964817	6.209513708	15.844655134	47	Al	4.848633331	11.864908727	10.345972922
8	Al	4.725292572	11.903468467	15.648514830	48	Al	4.848652691	8.962362597	10.345976131
9	Al	4.725317682	8.923814573	15.648519671	49	O	7.047431468	6.209503370	10.259530102
10	Al	0.964094011	6.209478515	15.631847034	50	Al	0.921529247	6.209471631	10.255292819
11	Al	7.063180642	10.413654977	14.8213111456	51	Al	7.030640132	10.413644747	9.121455742
12	O	0.942787476	10.413621086	14.751854495	52	Al	4.003593958	6.209486709	9.101294270
13	Al	3.738051375	6.209497456	14.675709585	53	O	4.992808234	10.413631296	9.077338844
14	O	4.944443562	7.508924166	14.644461384	54	O	5.057373278	7.633930779	9.022622238
15	O	4.944453108	4.910079756	14.644460954	55	O	5.057387012	4.785051852	9.022620860
16	Al	6.811667155	7.603503485	14.630850737	56	O	0.898275717	10.413608801	8.964262461
17	Al	6.811681359	4.815513179	14.630848489	57	Al	6.880866828	4.747207788	8.969021864
18	O	4.787311749	10.413640454	14.563888340	58	Al	6.880850440	7.671795609	8.969023472
19	O	0.714466463	7.545540373	14.382911677	59	O	0.678915450	7.470982870	8.799552265
20	O	0.714477910	4.873410765	14.382917614	60	O	0.678923309	4.947949755	8.799554874
21	O	7.150130729	9.144337011	13.343888874	61	O	7.119655115	11.751022729	7.772004880
22	O	7.150118180	11.682968834	13.343889191	62	O	7.119666321	9.076262299	7.772002700
23	Al	0.961292925	8.972750409	13.221482109	63	O	3.142159460	6.209477236	7.539425325
24	Al	0.961280276	11.854495483	13.221486830	64	Al	1.018531147	11.807519505	7.521146151
25	O	6.934536930	6.209511523	13.192133697	65	Al	1.018543200	9.019700311	7.521142917
26	O	2.784153019	8.988000806	13.131110952	66	O	2.884844342	11.715573020	7.497568506
27	O	2.784138178	11.839255381	13.131109511	67	O	2.884858105	9.111663716	7.497569668
28	O	2.837654972	6.209485912	13.076483012	68	Al	4.092045011	10.413622576	7.477150725
29	Al	3.833173833	10.413629043	13.058669881	69	O	6.871589646	6.209492926	7.387354198
30	Al	0.800481658	6.209477121	13.024398263	70	Al	0.720104224	6.209464597	7.306039539
31	Al	6.915657841	10.413651983	11.900854334	71	Al	6.867864505	10.413642354	6.511111808
32	O	0.787345492	10.413620502	11.900653180	72	Al	3.100498380	4.703081712	6.466749311
33	Al	2.977153955	4.753807588	11.809105646	73	Al	3.100476582	7.715868942	6.466742927
34	Al	2.977136584	7.665161062	11.809100914	74	O	0.583807103	10.413606239	6.313735513
35	O	1.036750270	7.536310061	11.780185235	75	O	1.283701467	7.607074024	6.283185721
36	O	1.036766064	4.882632791	11.780194806	76	O	1.283722609	4.811861373	6.283191123
37	O	5.042762131	10.413634856	11.725622581	77	Al	5.485683571	6.209487221	6.213357266
38	Al	5.889156734	6.209502125	11.732996097	78	O	5.209745060	10.413636520	6.148794244
39	O	4.817376420	4.805788149	11.645712234	79	O	4.635691495	7.599063420	5.676208591
40	O	4.817360609	7.613204201	11.645719544	80	O	4.635707408	4.819898343	5.676209399
					81	N	1.238085876	10.413560727	17.887928256
					82	H	1.858462015	10.413444957	18.708324313
					83	O	-0.063147875	10.413665824	18.231241914
					84	H	-0.141291501	10.413600248	19.209698289

**Table S7(c). NO+2H in Fig. 7(c)**

#		X	Y	Z	#		X	Y	Z
1	O	3.042428079	11.82974609	16.3969831	41	O	3.008177947	11.82796203	10.5218233
2	O	3.041974374	8.997686438	16.39695806	42	O	3.008178471	8.999146331	10.52176635
3	Al	1.90043435	10.41393351	16.2476505	43	O	2.793285342	6.209425649	10.46810843
4	O	2.561309928	6.208705961	16.10593619	44	Al	1.946019227	10.41355576	10.44142059
5	Al	4.851642229	9.05460455	15.88029241	45	O	6.791660024	11.7389263	10.38910868
6	Al	4.851557949	11.77264991	15.87983486	46	O	6.791673653	9.0882258	10.38909257
7	O	7.200232316	6.209481166	15.86335453	47	Al	4.84499296	11.86301065	10.37567162
8	O	6.679372364	9.008863992	15.85256481	48	Al	4.845007781	8.96412677	10.37562096
9	O	6.679220237	11.81842129	15.85242739	49	O	7.049969724	6.209437798	10.29472069
10	Al	0.879804479	6.209342982	15.65666726	50	Al	0.922092593	6.209429006	10.28427155
11	O	4.896250528	7.559699042	14.87624252	51	Al	7.025323786	10.4136102	9.137616071
12	O	4.896354941	4.859311079	14.87603741	52	Al	3.993001521	6.209450746	9.131094576
13	Al	7.114760784	10.4135996	14.80236006	53	O	4.987333787	10.41360292	9.103530704
14	Al	3.759076832	6.209479326	14.74294548	54	O	5.054199667	4.791379946	9.060552708
15	O	0.946951783	10.41368079	14.68953776	55	O	5.054189168	7.627536053	9.060471744
16	Al	6.774643537	7.612522761	14.6599883	56	Al	6.879434583	4.749128285	8.990532042
17	Al	6.774621152	4.806472166	14.65986423	57	Al	6.879422456	7.669781432	8.990497047
18	O	4.76337844	10.41347113	14.62955139	58	O	0.895985917	10.41358687	8.983517844
19	O	0.719895892	7.542290265	14.41312576	59	O	0.680896637	7.473297371	8.83788275
20	O	0.719974618	4.876575443	14.4129237	60	O	0.680893707	4.945578814	8.837805553
21	O	7.143802863	9.134652204	13.32915652	61	O	7.117111568	11.75314647	7.792938542
22	O	7.1439049	11.69235658	13.32891731	62	O	7.117133265	9.074072879	7.792890877
23	O	6.886196204	6.209497304	13.24876675	63	O	3.103891188	6.209489675	7.585221258
24	Al	0.955042249	11.85770027	13.21056146	64	Al	1.016755966	11.8046773	7.543714619
25	Al	0.955079953	8.969426065	13.21055205	65	Al	1.016769709	9.022586057	7.543707194
26	O	2.777698234	11.84083491	13.14710993	66	O	2.882990207	9.112382832	7.527614344
27	O	2.777698376	8.986181712	13.14707875	67	O	2.882965925	11.71489897	7.52759173
28	O	2.863024846	6.209417503	13.1450333	68	Al	4.089565672	10.41365291	7.501819124
29	Al	3.830638181	10.41349137	13.11802113	69	O	6.880240137	6.209504923	7.433906362
30	Al	0.800558611	6.20941263	13.06419905	70	Al	0.742471968	6.209473131	7.34762966
31	Al	6.906543076	10.41349874	11.9052895	71	Al	6.867500468	10.41364838	6.526633611
32	O	0.78483154	10.41350961	11.89819898	72	Al	3.098368935	7.714518355	6.500430069
33	Al	2.985030938	4.751029628	11.84476963	73	Al	3.098365098	4.704477908	6.50038425
34	Al	2.984988635	7.6677625	11.84468349	74	O	0.583142866	10.41363721	6.337951315
35	O	1.037500442	7.526312258	11.81962239	75	O	1.281214484	7.608785246	6.314897654
36	O	1.037520612	4.892479426	11.8195809	76	O	1.281237059	4.810201694	6.314838728
37	O	5.028593698	10.41351241	11.75683497	77	Al	5.508205188	6.209523951	6.243579338
38	Al	5.887491789	6.209414164	11.74921953	78	O	5.207367147	10.41367862	6.17541018
39	O	4.822218805	4.801445924	11.69216735	79	O	4.644958112	7.597956721	5.736050571
40	O	4.822164529	7.61730685	11.69202956	80	O	4.644927424	4.821122807	5.735981053
					81	N	0.722799151	10.41409173	17.64368215
					82	O	0.641672901	10.41702613	18.86662174
					83	H	2.713073415	12.76961004	16.46610359
					84	H	2.712637921	8.058152819	16.46757862

**Table S7(d). NHOH(2) in Fig. 7(d)**

#		X	Y	Z	#		X	Y	Z
1	O	3.17577714	11.81962865	16.56879816	41	O	2.964757189	11.81642937	10.49960787
2	O	3.175754908	9.007551408	16.56870835	42	O	2.964762264	9.010794882	10.49955418
3	O	2.619081858	6.209449634	15.90525622	43	Al	1.88882082	10.4136164	10.43182347
4	Al	2.391835763	10.41360964	15.94257377	44	O	2.730997181	6.209471991	10.40932801
5	O	6.49001568	9.02507577	15.86800797	45	O	6.7488829	9.086660181	10.38015615
6	O	6.490023827	11.80219245	15.86806056	46	O	6.748845763	11.74063186	10.38016959
7	O	7.114920202	6.209508331	15.78373056	47	Al	4.804621319	11.86719074	10.34802763
8	Al	4.681185861	11.94097624	15.7084999	48	Al	4.80463178	8.960084572	10.34800874
9	Al	4.681182787	8.886277675	15.70843238	49	O	6.99719833	6.209503116	10.25024427
10	Al	0.878957804	6.209467695	15.79641252	50	Al	0.861718642	6.20946539	10.27231671
11	Al	7.133790331	10.41364167	14.89230271	51	Al	6.985840682	10.413648	9.131609603
12	O	0.960862171	10.41361568	14.80000863	52	Al	3.952540303	6.209487257	9.097548096
13	Al	3.73020711	6.209472996	14.59844649	53	O	4.945362743	10.413644	9.087992093
14	O	4.898369642	7.539577174	14.60981925	54	O	5.007865918	7.634268509	9.019402822
15	O	4.898399282	4.879393593	14.60987541	55	O	5.007869464	4.784712251	9.019423879
16	Al	6.765259788	7.601228422	14.61485135	56	O	0.849738802	10.41361347	8.969517241
17	Al	6.765278907	4.817759993	14.61486718	57	Al	6.832173634	4.749921112	8.963428397
18	O	4.484103725	10.41363871	14.68534797	58	Al	6.832164303	7.66908453	8.963431089
19	O	0.664106945	7.544901502	14.42220073	59	O	0.631416652	7.472922207	8.806748708
20	O	0.664072146	4.87402199	14.42221943	60	O	0.631414339	4.946010162	8.806756064
21	O	7.117736725	9.16022726	13.37383119	61	O	7.071400298	11.74947838	7.778285853
22	O	7.117735889	11.66704054	13.37385351	62	O	7.071439555	9.077818791	7.778278536
23	Al	0.910275942	8.936697815	13.20450024	63	O	3.084583787	6.209475314	7.539740282
24	Al	0.910241771	11.89054184	13.204498	64	Al	0.971516602	11.80776029	7.525948346
25	O	6.897441215	6.209510362	13.1651698	65	Al	0.971528266	9.019465691	7.525937959
26	O	2.726097931	8.980803364	13.11895039	66	O	2.837658082	11.71573802	7.502160137
27	O	2.726068338	11.84647149	13.11897519	67	O	2.837670719	9.111509753	7.502158413
28	O	2.800274559	6.209488626	13.03928538	68	Al	4.044433225	10.41362836	7.484519238
29	Al	3.764949966	10.41364648	13.05915293	69	O	6.827581258	6.209487498	7.390399117
30	Al	0.773109845	6.209475776	13.08678804	70	Al	0.683677094	6.209465502	7.315733823
31	Al	6.87030733	10.41363649	11.92101235	71	Al	6.82053686	10.41364708	6.51658986
32	O	0.738210134	10.41362478	11.90604069	72	Al	3.053239445	4.701314747	6.467621903
33	Al	2.927424277	4.75719289	11.79450294	73	Al	3.053228674	7.717643809	6.467627223
34	Al	2.927410698	7.661781003	11.79449382	74	O	0.536692176	10.41361275	6.319987367
35	O	0.983300048	7.529982564	11.79940692	75	O	1.235130274	7.609020065	6.287683429
36	O	0.983322233	4.888964161	11.79936174	76	O	1.235131145	4.809911903	6.287689155
37	O	4.99920937	10.41362426	11.75636816	77	Al	5.44393065	6.209482646	6.211647876
38	Al	5.84813645	6.209499663	11.72156213	78	O	5.161975284	10.41364772	6.157065617
39	O	4.768998392	4.809149307	11.63765437	79	O	4.590802235	7.599228775	5.681440436
40	O	4.768981442	7.609833563	11.63762727	80	O	4.590803519	4.819745042	5.681418517
					81	N	1.037034873	6.209499255	17.7722104
					82	H	2.00199282	6.209517796	18.13014285
					83	O	0.097182363	6.209493307	18.74834528
					84	H	0.549957283	6.209515488	19.61843861

**Table S7(e). 2NHOH in Fig. 7(e)**

#		X	Y	Z	#		X	Y	Z
1	O	3.157808557	11.78299988	16.46132095	45	O	6.727415559	9.085324769	10.34353456
2	O	3.157939853	9.044468916	16.46147908	46	O	6.727401251	11.74199838	10.34354015
3	O	2.598046581	6.209552265	15.89061598	47	Al	4.777670563	11.86479873	10.31909989
4	Al	2.122591204	10.41367863	16.13334543	48	Al	4.777685228	8.962507994	10.31910046
5	O	6.46378459	9.006629841	15.84101159	49	O	6.973371253	6.209519777	10.22573724
6	O	6.463727208	11.82074933	15.84097052	50	Al	0.839948883	6.20948676	10.25327816
7	O	7.089605632	6.209543115	15.76447405	51	Al	6.95994645	10.41366102	9.09914847
8	Al	4.65266643	11.90846165	15.6072443	52	Al	3.932693744	6.20950476	9.079682676
9	Al	4.652718834	8.918900176	15.60729868	53	O	4.923694189	10.41365043	9.049825051
10	Al	0.845914617	6.209502362	15.75792231	54	O	4.985158227	7.635594567	8.988434769
11	Al	7.005937474	10.41369097	14.81158432	55	O	4.985171714	4.783420929	8.988420638
12	O	0.882553756	10.41365658	14.74528726	56	O	0.82609008	10.41363108	8.939877446
13	Al	3.707885362	6.209540969	14.56455633	57	Al	6.809491412	4.746189088	8.944849786
14	O	4.87302023	7.53331149	14.56295247	58	Al	6.809476344	7.672849096	8.944856333
15	O	4.873025262	4.885765293	14.56291647	59	O	0.60690127	7.472428678	8.777548765
16	Al	6.740792994	7.600030428	14.58807475	60	O	0.606914077	4.946535522	8.777551528
17	Al	6.740799008	4.819053684	14.5880641	61	O	7.047800567	11.75093877	7.745414408
18	O	4.686999006	10.41366188	14.54259233	62	O	7.047825381	9.076382438	7.745417328
19	O	0.644481414	7.542963628	14.40340013	63	O	3.07966525	6.209495056	7.511062826
20	O	0.644494853	4.876040209	14.40340745	64	Al	0.947373777	11.80840395	7.501527034
21	O	7.085464288	9.147409805	13.32636551	65	Al	0.947390834	9.018850729	7.501523162
22	O	7.085456125	11.67994731	13.32635814	66	O	2.814238399	11.71473328	7.471228383
23	Al	0.892864963	8.961122893	13.2167881	67	O	2.814252555	9.112539377	7.471234689
24	Al	0.892856322	11.86616177	13.21680313	68	Al	4.020853711	10.41364601	7.454403207
25	O	6.877499753	6.209530585	13.14211217	69	O	6.800744277	6.209514164	7.360225083
26	O	2.713163455	8.985382686	13.10261218	70	Al	0.648348962	6.209483153	7.289246767
27	O	2.713148334	11.8419108	13.10261143	71	Al	6.798824187	10.41366225	6.489619191
28	O	2.772259287	6.209507886	13.01656659	72	Al	3.028348584	4.703396322	6.443867223
29	Al	3.757284329	10.41365059	13.02737841	73	Al	3.028326336	7.715595539	6.443867786
30	Al	0.749142961	6.209500506	13.05356676	74	O	0.514586809	10.41362354	6.288921439
31	Al	6.851634132	10.41367767	11.88458115	75	O	1.212474094	7.605653899	6.260926904
32	O	0.717146871	10.41363585	11.88330007	76	O	1.212491568	4.813314549	6.260932023
33	Al	2.898187391	4.75128302	11.77177512	77	Al	5.408904703	6.209509032	6.198903704
34	Al	2.898169648	7.667725054	11.77177236	78	O	5.138677886	10.41364604	6.120687573
35	O	0.963166859	7.532570603	11.77563377	79	O	4.56177534	7.597583594	5.644556638
36	O	0.963183076	4.886419498	11.7756374	80	O	4.561793418	4.821419061	5.64455385
37	O	4.974294011	10.41365686	11.69925798	81	N	1.164218371	10.4131202	17.86352579
38	Al	5.822588378	6.209515891	11.70031097	82	H	1.767694085	10.41186036	18.69448397
39	O	4.742108128	4.810311798	11.60574174	83	O	-0.14945334	10.41436284	18.18585564
40	O	4.742094745	7.608714295	11.60575162	84	H	-0.24250556	10.41338981	19.16145252
41	O	2.937980196	11.81577804	10.47071407	85	N	1.073566318	6.209398468	17.73415811
42	O	2.937995166	9.011507726	10.47070839	86	H	2.06552526	6.209198839	18.00991153
43	Al	1.86054017	10.41364084	10.41100992	87	O	0.211390584	6.209450603	18.79708148
44	O	2.706759696	6.209504294	10.38281379	88	H	0.746675934	6.209197844	19.61710995

**Table S7(f). NHOH+NO in Fig. 7(f)**

#		X	Y	Z	#		X	Y	Z
1	O	3.197314487	11.805503856	16.626601703	41	O	2.970011134	11.818491744	10.490077267
2	O	3.038656512	8.950453641	16.513412708	42	O	2.970164161	9.007934572	10.484316366
3	O	2.613330879	6.179402374	15.900894644	43	Al	1.897017977	10.413990837	10.421784053
4	Al	2.443805220	10.447299908	15.852245486	44	O	2.736855422	6.207795202	10.401921881
5	O	6.530966287	9.045099018	15.823779376	45	O	6.750100279	9.087159916	10.372921024
6	O	6.490785302	11.799994401	15.844276137	46	O	6.749143214	11.739461473	10.373606075
7	O	7.112410369	6.219009944	15.769429578	47	Al	4.807297604	11.867995854	10.343084530
8	Al	4.684954253	11.960811928	15.737339480	48	Al	4.808408169	8.959255524	10.343899326
9	Al	4.696691701	8.865132232	15.842612831	49	O	7.001077383	6.207997374	10.241761890
10	Al	0.875289140	6.216256385	15.787434430	50	Al	0.866538078	6.206092344	10.264598115
11	Al	7.166966725	10.426639943	14.868678992	51	Al	6.989624992	10.412905852	9.124319180
12	O	0.981029347	10.447591649	14.742099464	52	Al	3.955804046	6.207816858	9.088774287
13	Al	3.729736463	6.222443124	14.600919658	53	O	4.948395061	10.413412928	9.085373701
14	O	4.890789271	7.557529395	14.671949706	54	O	5.011895067	7.632241492	9.014153653
15	O	4.893109406	4.881108617	14.610646918	55	O	5.011802673	4.784274392	9.009775290
16	Al	6.761049632	7.617993113	14.601673897	56	O	0.853524447	10.412650841	8.960797204
17	Al	6.761934316	4.826712927	14.598955705	57	Al	6.834562337	4.750179600	8.953415269
18	O	4.362393165	10.396561462	14.770348601	58	Al	6.835780049	7.668921015	8.957112392
19	O	0.667662243	7.549352035	14.404762188	59	O	0.634586898	7.471788584	8.798961054
20	O	0.659963335	4.876381460	14.409944551	60	O	0.634079690	4.944269224	8.799328978
21	O	7.122230390	9.164721902	13.345878085	61	O	7.073580661	11.748225841	7.771130267
22	O	7.115198128	11.673472167	13.355834456	62	O	7.073736882	9.076847905	7.770986256
23	Al	0.911828054	8.935090310	13.176945734	63	O	3.085128727	6.209116513	7.532767891
24	Al	0.918919751	11.886351531	13.197524921	64	Al	0.974673677	11.806889431	7.518800319
25	O	6.889475819	6.216468183	13.158815816	65	Al	0.974826978	9.018660921	7.518689785
26	O	2.725798666	8.976529489	13.096700414	66	O	2.841052004	11.715287181	7.495175785
27	O	2.739335168	11.844125148	13.110238097	67	O	2.841178535	9.110952206	7.494238707
28	O	2.809967018	6.212229021	13.032365683	68	Al	4.047026340	10.413084510	7.481438705
29	Al	3.771765574	10.401408433	13.075925224	69	O	6.831641284	6.207986178	7.381757558
30	Al	0.775490502	6.210146219	13.078759207	70	Al	0.687702180	6.209283358	7.308142641
31	Al	6.875117252	10.419264054	11.907756983	71	Al	6.823909459	10.412741231	6.509592039
32	O	0.743094888	10.417441859	11.887488869	72	Al	3.055903410	4.700742111	6.460653895
33	Al	2.934751404	4.755855647	11.790769925	73	Al	3.056262862	7.717155957	6.459997332
34	Al	2.931112303	7.658977104	11.781281682	74	O	0.539124125	10.412952092	6.312433714
35	O	0.984655684	7.525309147	11.783039154	75	O	1.239340253	7.608437264	6.279304517
36	O	0.989762740	4.888163831	11.791895785	76	O	1.238660762	4.809263271	6.280473712
37	O	5.001703876	10.413582045	11.768183244	77	Al	5.448835354	6.208678220	6.203509885
38	Al	5.851181474	6.210568304	11.709490536	78	O	5.163844065	10.413659392	6.153222195
39	O	4.774955582	4.810369237	11.628787341	79	O	4.594537404	7.598429653	5.675770057
40	O	4.774317185	7.612178491	11.635532722	80	O	4.593859974	4.819433974	5.675348202
					81	N	1.019627839	6.180946674	17.762908184
					82	H	1.978540520	6.118452317	18.130669240
					83	O	0.072407832	6.235832334	18.731543511
					84	H	0.516286743	6.207471834	19.605526308
					85	N	4.773050454	9.184720212	17.968229355
					86	O	4.574627005	8.651589047	18.990972672

**Table S8(a). NHOH+2H in Fig. 8(a)**

#		X	Y	Z	#		X	Y	Z
1	O	3.048797459	11.818724133	16.366002481	41	O	3.048084537	11.791798706	10.536959036
2	O	3.083747823	9.001346441	16.324766891	42	O	3.046203465	8.958648205	10.521555870
3	O	2.616792076	5.930682674	16.097906139	43	Al	1.986208600	10.375445156	10.455222432
4	Al	2.036173787	10.339380570	16.131529433	44	O	2.835431706	6.174000062	10.479213114
5	O	6.692359426	8.995950242	15.900866452	45	O	6.834042342	9.053206027	10.391402902
6	O	6.744438647	11.779743910	15.872234128	46	O	6.833665729	11.704635257	10.388792805
7	O	7.281237434	6.188104762	15.912027739	47	Al	4.883149787	11.828961324	10.387316166
8	Al	4.877916868	11.710305392	15.915092699	48	Al	4.880437536	8.928743065	10.381628489
9	Al	4.781675331	9.025224475	15.883959890	49	O	7.091154298	6.175003431	10.311071349
10	Al	0.965591255	6.178236243	15.665490760	50	Al	0.966570069	6.174033749	10.304420723
11	Al	7.049097022	10.385966041	14.738335236	51	Al	7.064826088	10.379347390	9.141697009
12	O	0.952273396	10.377160064	14.643067506	52	Al	4.038766693	6.176371690	9.150578763
13	Al	3.814091653	6.170778710	14.784907356	53	O	5.030133476	10.379360602	9.105654126
14	O	4.963373685	7.516474783	14.892938149	54	O	5.097946109	7.595294403	9.062499333
15	O	4.965687670	4.818515614	14.923474845	55	O	5.096126056	4.755833357	9.068875760
16	Al	6.818886172	7.580169463	14.703041953	56	O	0.938461470	10.379365546	8.988517370
17	Al	6.830581381	4.782446271	14.699728136	57	Al	6.921180386	4.710794772	9.011786127
18	O	4.901467572	10.390936857	14.597555329	58	Al	6.922115128	7.637195780	9.010154299
19	O	0.774892934	7.509080732	14.433712963	59	O	0.720707028	7.437738194	8.846683580
20	O	0.729845090	4.839903277	14.410433622	60	O	0.720309518	4.911388220	8.845783019
21	O	7.169076381	9.081079854	13.338512140	61	O	7.157121341	11.720097266	7.796172378
22	O	7.162075024	11.657995333	13.309876084	62	O	7.158070938	9.038260718	7.797810610
23	Al	1.001544569	8.946751800	13.243955750	63	O	3.167669354	6.175254972	7.591136333
24	Al	0.983693501	11.813915829	13.226416134	64	Al	1.057536894	11.770732968	7.555922340
25	O	6.925690583	6.182867757	13.276047712	65	Al	1.058080323	8.987417528	7.555664825
26	O	2.829350385	8.967829609	13.146091225	66	O	2.925131776	11.679484980	7.532736781
27	O	2.818690686	11.802026683	13.165558130	67	O	2.925018129	9.079102285	7.529124878
28	O	2.916560219	6.178150267	13.166193156	68	Al	4.130691382	10.379119528	7.511010708
29	Al	3.891287056	10.386893589	13.127544824	69	O	6.918045643	6.174891293	7.439260122
30	Al	0.835054906	6.175950851	13.079004813	70	Al	0.769974226	6.174492815	7.358336281
31	Al	6.952209544	10.370958903	11.900311442	71	Al	6.912417341	10.378963424	6.536543556
32	O	0.817567671	10.373905575	11.898352820	72	Al	3.138178095	4.672114411	6.512547992
33	Al	3.026642219	4.718284093	11.869512303	73	Al	3.137541207	7.677422170	6.510374353
34	Al	3.027618391	7.634553700	11.865097715	74	O	0.625981414	10.378949089	6.342899021
35	O	1.081572951	7.492222111	11.836100599	75	O	1.322337826	7.570384202	6.325842615
36	O	1.081443288	4.860861606	11.829044335	76	O	1.323253113	4.778970593	6.325834908
37	O	5.071781436	10.376538422	11.750612645	77	Al	5.538411750	6.174704793	6.266240976
38	Al	5.929599380	6.176075760	11.777212445	78	O	5.249129210	10.377513107	6.176667819
39	O	4.864812492	4.766308210	11.702677733	79	O	4.679618118	7.559811673	5.729626580
40	O	4.864370566	7.582663677	11.693146557	80	O	4.681475547	4.786878164	5.733738874
					81	N	0.586161446	10.253043599	17.419599055
					82	H	-0.294200358	9.742212010	17.161535717
					83	O	0.451130601	11.057083414	18.498099457
					84	H	-0.492602140	11.029373560	18.769863703
					85	H	5.001209668	10.446702346	17.092098062
					86	H	2.751687488	12.805191775	16.300839390



**Table S8(b). NH<sub>2</sub> in Fig. 8(b)**

#		X	Y	Z	#		X	Y	Z
1	O	3.204636511	11.744349093	16.452446012	41	O	3.010777007	11.822136311	10.512140034
2	O	3.198850426	9.077867298	16.468123563	42	O	3.010586724	9.011606369	10.514719716
3	O	2.626640219	6.206441462	16.035197961	43	Al	1.936109013	10.416931895	10.451573172
4	Al	2.068524195	10.412718325	16.274228274	44	O	2.789495579	6.213029121	10.436449242
5	O	6.536181249	9.007105498	15.881884006	45	O	6.798318200	9.090093283	10.383439325
6	O	6.550833418	11.806738200	15.895119572	46	O	6.798233966	11.745376902	10.384403891
7	O	7.242031764	6.205328593	15.861825473	47	Al	4.848194762	11.868795994	10.367104041
8	Al	4.726764864	11.887888713	15.666677936	48	Al	4.847816961	8.966026815	10.367061344
9	Al	4.714384324	8.929278705	15.664213247	49	O	7.046790458	6.213788739	10.279574360
10	Al	0.953644471	6.211796124	15.665565596	50	Al	0.921570368	6.213424518	10.286917757
11	Al	7.054011026	10.405457926	14.821289951	51	Al	7.029876153	10.418245015	9.138663235
12	O	0.940332294	10.417476725	14.713961663	52	Al	4.006462049	6.213853172	9.124906445
13	Al	3.745744128	6.201381507	14.685352388	53	O	4.996138585	10.417959932	9.093190398
14	O	4.937410957	7.507937740	14.667511238	54	O	5.059079705	7.638847124	9.036978116
15	O	4.947030508	4.901119849	14.671822289	55	O	5.059307493	4.789091105	9.037479252
16	Al	6.807711810	7.601483643	14.654781433	56	O	0.898753233	10.418402218	8.980665359
17	Al	6.814886912	4.809784810	14.653180814	57	Al	6.883437102	4.749435219	8.996026232
18	O	4.810944964	10.411269242	14.572145827	58	Al	6.883385163	7.678634478	8.995127582
19	O	0.718049921	7.545346598	14.411712348	59	O	0.680192147	7.477631477	8.821452822
20	O	0.720167439	4.874476360	14.411243876	60	O	0.680153927	4.951090967	8.820784777
21	O	7.145129653	9.136902353	13.353766338	61	O	7.117647229	11.756842572	7.786127730
22	O	7.143324084	11.690372689	13.359680210	62	O	7.117760173	9.080563175	7.785447630
23	Al	0.967981486	8.989250404	13.265247874	63	O	3.145771480	6.215021808	7.559067712
24	Al	0.969134989	11.837661307	13.267614115	64	Al	1.020309128	11.813719890	7.544289162
25	O	6.934167976	6.209433122	13.215569015	65	Al	1.020134209	9.024668615	7.544267501
26	O	2.790755930	8.987578736	13.144372711	66	O	2.888609552	11.721416811	7.514037525
27	O	2.791370760	11.843491150	13.141924269	67	O	2.888436448	9.117526285	7.514761917
28	O	2.840455112	6.209500226	13.096700093	68	Al	4.090194050	10.419406914	7.504916964
29	Al	3.835137332	10.415587415	13.082423012	69	O	6.879177732	6.215229860	7.408897319
30	Al	0.802247684	6.210317660	13.049288378	70	Al	0.723692716	6.215026034	7.332703836
31	Al	6.919855676	10.415689183	11.921010124	71	Al	6.877916456	10.419113605	6.528432410
32	O	0.784805675	10.416275481	11.914196403	72	Al	3.098446468	4.710883280	6.487856044
33	Al	2.971977086	4.753771602	11.825318319	73	Al	3.098613343	7.719699444	6.488771674
34	Al	2.973798086	7.669408804	11.827615791	74	O	0.590575413	10.419321307	6.334161602
35	O	1.038161682	7.535440029	11.802166144	75	O	1.285664650	7.611897126	6.306568944
36	O	1.036994404	4.888108704	11.800046067	76	O	1.285484788	4.818575610	6.306151127
37	O	5.042679327	10.416759889	11.739840283	77	Al	5.498828780	6.215730412	6.244570118
38	Al	5.890150140	6.212287626	11.756208668	78	O	5.210209108	10.419798136	6.165136800
39	O	4.815957953	4.810894712	11.661493388	79	O	4.642039895	7.603282085	5.703054821
40	O	4.816886950	7.614443381	11.661168828	80	O	4.641903243	4.828586482	5.702333590
					81	N	0.771847390	10.421508656	17.615935281
					82	H	0.932317629	10.056883821	18.554030064
					83	H	-0.172277377	10.804550296	17.532770769

**Table S8(c). NO/NH<sub>2</sub> in Fig. 8(c)**

#		X	Y	Z	#		X	Y	Z
1	O	3.150377212	9.129021831	16.452810138	41	O	3.000339652	11.857452073	10.514740679
2	O	3.206977160	11.837406776	16.452164385	42	O	3.000550612	9.047252515	10.513064021
3	Al	2.119995470	10.499767317	16.170201841	43	Al	1.927343559	10.452061553	10.438045365
4	O	2.620719601	6.258078916	16.022680032	44	O	2.778365911	6.248025609	10.434943443
5	O	6.557603096	11.842981482	15.897340783	45	O	6.787821475	11.778429207	10.377894966
6	O	6.520976107	9.058388049	15.887394732	46	O	6.787511321	9.126904594	10.377233744
7	O	7.239600511	6.244513339	15.863428571	47	Al	4.837870210	11.905097556	10.357456697
8	Al	4.679481247	8.968477008	15.675216231	48	Al	4.837550414	9.000354184	10.356790321
9	Al	4.724333462	11.945385692	15.663808459	49	O	7.037700001	6.249041430	10.274692778
10	Al	0.957550320	6.246733161	15.663476782	50	Al	0.910344034	6.249878104	10.274195301
11	Al	7.006334253	10.439364963	14.780151838	51	Al	7.018104224	10.452873625	9.126371967
12	O	0.924045287	10.455269209	14.706405818	52	Al	3.990870173	6.248482955	9.115659265
13	Al	3.735068804	6.243756818	14.687240455	53	O	4.982414227	10.452872895	9.087637449
14	O	4.929068599	7.553291794	14.674807706	54	O	5.047103540	4.825665182	9.034786328
15	O	4.954762701	4.949247518	14.665422421	55	O	5.046914701	7.671352520	9.034333327
16	Al	6.796425705	7.641817005	14.659955530	56	Al	6.871824749	4.787966259	8.979571336
17	Al	6.815991722	4.859169213	14.636099259	57	Al	6.871449495	7.709130623	8.978355724
18	O	4.804254670	10.459125245	14.573069406	58	O	0.886947424	10.452711353	8.973724217
19	O	0.699346506	7.586071884	14.406910296	59	O	0.670203088	4.985959051	8.816993186
20	O	0.705173575	4.908719668	14.405152976	60	O	0.670111271	7.511961610	8.816567564
21	O	7.125996848	11.728464563	13.349432224	61	O	7.108778745	11.791624366	7.779993062
22	O	7.129061957	9.175860876	13.344364925	62	O	7.108621106	9.114399804	7.779633425
23	Al	0.955338143	9.021739496	13.250137073	63	O	3.117900774	6.248853965	7.559103858
24	Al	0.952024069	11.884508226	13.237959508	64	Al	1.008622055	11.846288417	7.532837849
25	O	6.924273553	6.249540467	13.210342292	65	Al	1.008494678	9.059481749	7.532422896
26	O	2.779285519	11.880116008	13.145569948	66	O	2.875353516	11.754716456	7.511434701
27	O	2.781201492	9.028091562	13.143826497	67	O	2.875175627	9.151377427	7.510639777
28	O	2.832003166	6.247328165	13.092683884	68	Al	4.080964776	10.452963123	7.489450425
29	Al	3.827270857	10.454791134	13.071171906	69	O	6.867207221	6.249163439	7.407263694
30	Al	0.794349539	6.252003434	13.046282465	70	Al	0.721762909	6.248723364	7.326784616
31	O	0.773946418	10.453725168	11.906233078	71	Al	6.860251212	10.453144786	6.517305617
32	Al	6.909083192	10.450701763	11.895225867	72	Al	3.090079774	4.743390104	6.482360858
33	Al	2.966984320	7.706087585	11.823673721	73	Al	3.089975901	7.754073516	6.482132010
34	Al	2.966481401	4.792843248	11.822419260	74	O	0.575675158	10.453092061	6.324943604
35	O	1.026534729	4.922787113	11.801660334	75	O	1.273584463	4.850634059	6.298115226
36	O	1.029368933	7.575703813	11.800326990	76	O	1.273607596	7.646879791	6.297901330
37	Al	5.881147630	6.249266923	11.747192879	77	Al	5.487355891	6.248756552	6.228644674
38	O	5.033274060	10.452942235	11.734484133	78	O	5.199385879	10.453121336	6.159726416
39	O	4.808191589	7.652323976	11.659005378	79	O	4.630846777	4.859785675	5.702111122
40	O	4.808253560	4.845474854	11.658881844	80	O	4.630601437	7.637400422	5.701719835
					81	N	0.775655590	10.969517308	17.567405259
					82	H	0.710164512	10.371605045	18.399188656
					83	H	-0.172746932	11.168181111	17.184776851
					84	N	1.237266220	12.475833538	18.092353921
					85	O	1.726848675	12.444872565	19.152093113

**Table S8(d).  $\underline{2}\text{NH}_2$  in Fig. 8(d)**

#		X	Y	Z	#		X	Y	Z
1	O	3.181897067	11.66405418	16.47720347	41	O	2.943544287	11.77198705	10.49000365
2	O	3.135178115	9.023650793	16.45223243	42	O	2.942904408	8.966434613	10.48953323
3	O	2.597840003	6.009252907	15.93331732	43	Al	1.864281145	10.36965296	10.43995153
4	Al	1.994970668	10.37114431	16.26645171	44	O	2.71499986	6.166826277	10.40799208
5	O	6.462521504	8.948731588	15.85415977	45	O	6.733910572	9.043770768	10.36138902
6	O	6.485437531	11.74743379	15.87571811	46	O	6.733584296	11.70135235	10.36345655
7	O	7.094195124	6.150703726	15.78805059	47	Al	4.782809382	11.82273828	10.34654741
8	Al	4.677034887	11.83660065	15.633423	48	Al	4.782307946	8.920810158	10.34613256
9	Al	4.647418671	8.873690549	15.62303738	49	O	6.979097486	6.168279852	10.25353895
10	Al	0.849372432	6.26992278	15.8219289	50	Al	0.846705479	6.168187492	10.29273802
11	Al	6.994143922	10.35219238	14.80477842	51	Al	6.964074494	10.37340195	9.120213171
12	O	0.878800973	10.36645421	14.71279783	52	Al	3.941418838	6.168752606	9.108427949
13	Al	3.714762208	6.121523608	14.59683722	53	O	4.932061976	10.37293161	9.071147184
14	O	4.856022209	7.463874567	14.61153108	54	O	4.993190078	7.595200108	9.010967996
15	O	4.895751103	4.815948226	14.5940452	55	O	4.992957859	4.742129979	9.011508073
16	Al	6.73023285	7.541499005	14.60644725	56	O	0.83250844	10.37356145	8.962467557
17	Al	6.770004824	4.756882242	14.62490216	57	Al	6.818021669	4.703675579	8.979244774
18	O	4.732875345	10.35675735	14.54849559	58	Al	6.818219933	7.63447293	8.976445224
19	O	0.658830796	7.506851871	14.42531617	59	O	0.613776113	7.433936892	8.805570042
20	O	0.647837901	4.839685341	14.43256972	60	O	0.61339714	4.905856186	8.804391144
21	O	7.081107524	9.089372988	13.33511531	61	O	7.051235474	11.71269309	7.76558996
22	O	7.084203999	11.63672496	13.34418832	62	O	7.05144963	9.036373846	7.763542069
23	Al	0.903506195	8.933955244	13.25319198	63	O	3.09440207	6.17187312	7.533435149
24	Al	0.905436238	11.80760253	13.27516257	64	Al	0.955636255	11.7717196	7.530875957
25	O	6.879742494	6.172246411	13.17302243	65	Al	0.955321382	8.980014712	7.530266175
26	O	2.726358533	8.941798245	13.12080801	66	O	2.825004607	11.67839109	7.493572943
27	O	2.726277641	11.80036935	13.12508391	67	O	2.824498709	9.074936481	7.492604802
28	O	2.782652281	6.161718298	13.04993037	68	Al	4.024763391	10.3763371	7.487654674
29	Al	3.766788049	10.3711338	13.05581071	69	O	6.811995732	6.172454812	7.388879763
30	Al	0.757974031	6.159781519	13.08805421	70	Al	0.6548413	6.171480824	7.321319073
31	Al	6.861634295	10.37079237	11.90573391	71	Al	6.816522518	10.375874	6.511034821
32	O	0.721345717	10.36982139	11.90284385	72	Al	3.031190986	4.667843804	6.468483917
33	Al	2.897963104	4.705209825	11.79557989	73	Al	3.031136133	7.676410238	6.469015435
34	Al	2.903243131	7.624247855	11.8005911	74	O	0.528194145	10.37624317	6.316918005
35	O	0.973353427	7.484194727	11.80428415	75	O	1.21956749	7.566380219	6.290827198
36	O	0.970378341	4.84599074	11.79834635	76	O	1.219529737	4.77717742	6.29054503
37	O	4.980007385	10.37156347	11.71741437	77	Al	5.427365541	6.173458752	6.23480146
38	Al	5.828717272	6.166043244	11.72976733	78	O	5.145899402	10.37805154	6.143365653
39	O	4.746075579	4.768851233	11.62879752	79	O	4.573697564	7.55945951	5.675089184
40	O	4.748538711	7.565456116	11.62957393	80	O	4.574024678	4.787168574	5.675524844
					81	N	0.739609328	10.34202454	17.63922573
					82	H	1.021875964	10.55412476	18.59546423
					83	H	-0.246293201	10.57865338	17.51701044
					84	N	1.007464303	7.21248103	17.50567402
					85	H	1.672542738	6.907813438	18.22184428
					86	H	0.749303593	8.205123428	17.66285481

Table S8(e).  $\text{NH}_2+\text{H}$  in Fig. 8(e)

#		X	Y	Z	#		X	Y	Z
1	O	3.263880053	11.608539982	16.541826174	41	O	3.012326183	11.834125954	10.513599115
2	O	3.205138338	8.926819677	16.420235554	42	O	3.013266753	9.028345353	10.519102818
3	O	2.609240653	6.414755862	16.033683215	43	Al	1.936614101	10.431392773	10.440489719
4	Al	2.016329604	10.398850656	16.373638790	44	O	2.789741360	6.225921399	10.438760410
5	O	6.561268847	9.030330727	15.872114040	45	O	6.797949805	9.103974870	10.387054470
6	O	6.536069743	11.828014783	15.871491267	46	O	6.798149210	11.757259768	10.388412931
7	O	7.221715318	6.226222229	15.846568286	47	Al	4.851078508	11.880963145	10.363111281
8	Al	4.717945500	11.889641932	15.694650355	48	Al	4.852910164	8.979694636	10.364249452
9	Al	4.782907639	8.970028942	15.606649436	49	O	7.047891876	6.226004528	10.276187086
10	Al	0.925955085	6.228285889	15.662340682	50	Al	0.919009638	6.226344373	10.273186162
11	Al	7.131528175	10.442575308	14.852584316	51	Al	7.029610330	10.430589879	9.136687101
12	O	0.967633194	10.417581009	14.727956096	52	Al	4.000009919	6.227049073	9.113886331
13	Al	3.740027105	6.233357934	14.664825958	53	O	4.993514352	10.430662868	9.095456670
14	O	4.950099814	7.524892543	14.652676133	54	O	5.056599547	7.649248252	9.041778885
15	O	4.905103083	4.918000955	14.709475514	55	O	5.057035149	4.804914269	9.043788926
16	Al	6.824158365	7.620204706	14.620556911	56	O	0.896124995	10.430595341	8.979814789
17	Al	6.790035214	4.822069110	14.652075577	57	Al	6.881423657	4.766869313	8.978950775
18	O	4.761267355	10.428376135	14.575643328	58	Al	6.881353988	7.687550686	8.980025582
19	O	0.706793674	7.560198913	14.400698249	59	O	0.680968506	7.489576116	8.821663077
20	O	0.747201997	4.895119090	14.426365094	60	O	0.681181396	4.963456517	8.821862438
21	O	7.150090600	9.162728191	13.359625642	61	O	7.118772130	11.768489519	7.787735198
22	O	7.162749002	11.711946846	13.368404232	62	O	7.119209283	9.092936016	7.786846331
23	Al	0.970016410	9.002807603	13.246361113	63	O	3.119335284	6.226619592	7.563453235
24	Al	0.979707748	11.857900742	13.265440108	64	Al	1.018482655	11.823735344	7.535510960
25	O	6.929318015	6.209953214	13.211209608	65	Al	1.018066453	9.037931131	7.535215874
26	O	2.792185406	8.991130469	13.147116070	66	O	2.884902645	11.732739195	7.516719806
27	O	2.793399301	11.865990473	13.141505705	67	O	2.884629783	9.128635553	7.517562793
28	O	2.834613579	6.224576554	13.095873302	68	Al	4.091185420	10.430592019	7.494899137
29	Al	3.821018170	10.431493242	13.069194839	69	O	6.878349667	6.226181323	7.412794751
30	Al	0.802549552	6.221149499	13.042321446	70	Al	0.736263770	6.226747567	7.329766389
31	Al	6.920123239	10.436506272	11.918748785	71	Al	6.868335757	10.430873463	6.522848107
32	O	0.791368505	10.431379359	11.915632750	72	Al	3.100328159	4.720016761	6.484590178
33	Al	2.972808653	4.766758771	11.815842312	73	Al	3.100210439	7.733421703	6.484715861
34	Al	2.974344618	7.682803118	11.816451825	74	O	0.584276261	10.431201361	6.331320676
35	O	1.036371987	7.549580244	11.801312057	75	O	1.283111644	7.626336149	6.301556595
36	O	1.037671109	4.898447524	11.803713258	76	O	1.283197732	4.827108372	6.301746930
37	O	5.043845457	10.432038953	11.745878430	77	Al	5.502288213	6.226894426	6.226045555
38	Al	5.890330536	6.222328930	11.739788169	78	O	5.208705177	10.430772245	6.167889247
39	O	4.816097024	4.820756253	11.669011651	79	O	4.642998604	7.616462557	5.711292360
40	O	4.817821062	7.626578076	11.665216476	80	O	4.643311403	4.836897050	5.711739163
					81	N	0.810093220	10.155673140	17.667345034
					82	H	1.012154064	10.364270081	18.639807387
					83	H	-0.161870191	9.885475678	17.561348044
					84	H	2.861176568	7.965136137	16.447683831

**Table S8(f). NH in Fig. 8(f)**

#		X	Y	Z	#		X	Y	Z
1	O	3.201479820	11.770198576	16.457931907	41	O	3.024114283	11.823711991	10.522750457
2	O	3.209713117	9.082192424	16.477986542	42	O	3.025104184	9.012140799	10.523783737
3	O	2.641212833	6.221074359	16.041963439	43	Al	1.951039363	10.417448604	10.461562769
4	Al	2.103564792	10.422716081	16.257060799	44	O	2.803366716	6.213517319	10.447146877
5	O	6.558138737	9.020636472	15.908427605	45	O	6.811806509	9.089108385	10.396063875
6	O	6.556738978	11.822577165	15.897505678	46	O	6.811640652	11.744274981	10.394842687
7	O	7.256140809	6.218464102	15.870473498	47	Al	4.861651713	11.868298225	10.376731852
8	Al	4.731624951	11.904128831	15.680377811	48	Al	4.862841294	8.965625345	10.377937086
9	Al	4.731853797	8.939614536	15.685568928	49	O	7.060662949	6.212324502	10.289775228
10	Al	0.968366991	6.213854159	15.676866699	50	Al	0.935324689	6.212445453	10.295982697
11	Al	7.073573089	10.422637537	14.841075444	51	Al	7.044991781	10.415900155	9.150408106
12	O	0.960064383	10.424987745	14.719641778	52	Al	4.019916345	6.212079332	9.134864375
13	Al	3.760473163	6.217694771	14.694692488	53	O	5.009319930	10.416165745	9.104691275
14	O	4.956764759	7.522977619	14.683704897	54	O	5.072910409	7.636805427	9.048626174
15	O	4.956432500	4.913647098	14.678620418	55	O	5.072782923	4.787174152	9.046845823
16	Al	6.825605923	7.612643342	14.664060130	56	O	0.912776500	10.415419850	8.991816954
17	Al	6.824802062	4.821105202	14.665119580	57	Al	6.897036129	4.747806154	9.004466691
18	O	4.817344012	10.418420702	14.592018040	58	Al	6.897067488	7.676161567	9.005590027
19	O	0.733639203	7.552044154	14.421683781	59	O	0.694085391	7.474862482	8.832373380
20	O	0.732973567	4.880585508	14.421241681	60	O	0.694152647	4.948187636	8.832717578
21	O	7.158088985	9.144841530	13.374615687	61	O	7.132267073	11.753186092	7.796735409
22	O	7.158986808	11.695710891	13.368218200	62	O	7.131973209	9.077441088	7.797351350
23	Al	0.981305887	8.991926569	13.270358822	63	O	3.157251363	6.210580639	7.570295491
24	Al	0.981360523	11.848301198	13.269802434	64	Al	1.034067306	11.809076397	7.554496173
25	O	6.947973425	6.216605676	13.224976769	65	Al	1.034148473	9.020270918	7.554840304
26	O	2.804031813	8.991193133	13.153562080	66	O	2.901723206	11.715685786	7.525272564
27	O	2.804287498	11.846153138	13.151046204	67	O	2.901930363	9.112430760	7.525744569
28	O	2.855283999	6.215233883	13.105466700	68	Al	4.103839687	10.414173645	7.515894431
29	Al	3.849712851	10.418575038	13.095933120	69	O	6.893648933	6.210676431	7.419946935
30	Al	0.816116891	6.215978095	13.060504996	70	Al	0.738686354	6.210586584	7.343497780
31	Al	6.931991934	10.420537582	11.933884428	71	Al	6.892385293	10.414732490	6.538632381
32	O	0.797292954	10.417917650	11.923925228	72	Al	3.112223137	4.705519187	6.499611030
33	Al	2.988447165	4.756814485	11.836170870	73	Al	3.111689072	7.714967759	6.498743805
34	Al	2.987620823	7.671912470	11.836452390	74	O	0.604814122	10.414371499	6.345212219
35	O	1.051031294	7.538938439	11.811517081	75	O	1.298709082	7.607451063	6.317328556
36	O	1.051311534	4.891039674	11.812208266	76	O	1.299185888	4.813322790	6.317671532
37	O	5.056381850	10.418021365	11.752870818	77	Al	5.514070741	6.209789239	6.253700582
38	Al	5.904403447	6.213667905	11.765567177	78	O	5.224353431	10.413365895	6.177111582
39	O	4.831038410	4.811648124	11.670614984	79	O	4.655815350	7.597380849	5.715075869
40	O	4.830709192	7.615775516	11.672798195	80	O	4.656900436	4.821092225	5.716610821
					81	N	0.734590134	10.391269165	17.561792032
					82	H	-0.144737455	9.897702118	17.763051711