Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

R-VAPOL-Phosphoric Acid based ^{1}H and ^{13}C-NMR for Sensing of Chiral Amines and Acids

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***Simulation methods*:** The first-principles density functional theory (DFT) calculations were carried out using the Quantum Espresso software package.[1] The interatomic forces were derived within the framework of density functional theory (DFT) using the Perdew, Burke and Ernzerhof (PBE) - GGA approximation for the exchange-correlation energy functional.[2] The interaction between valence electrons and ionic cores was represented by the Troullier-Martin norm-conserving pseudopotentials.[3] The van der Waals dispersion corrections were treated using the Tkatchenko-Scheffler parameters.[4] The Brillouin zone was sampled at the gamma point. We performed the convergence test of the kinetic energy cutoff for the electronic wavefunctions and the charge density. The optimized values of kinetic energy cutoff of electronic wavefunctions and charge density are 70 and 280 Ry, respectively. The electronic kinetic energy convergence criteria used is 10^{-10}. A vacuum of at least 10 A in each direction was introduced to simulate an isolated system. Martyna-Tuckerman corrections to the total energy and SCF potential were included.[5] All energetics reported in the paper are in kcal/mol and coordinates/bond lengths in angstroms (Å). Snapshots of the optimized geometries were generated using CYLview. [6]

References

[1] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. Fabris, G. Fratesi, S. de Gironcoli, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, R. M. Wentzcovitch, *J. Phys.: Condens. Matter* 21, 395502 (2009)

[2] J. P. Perdew, K. Burke, M. Ernzerhof, Generalized gradient approximation made simple. *Phys. Rev. Lett.* **77**, 3865-3868 (1996)

[3] Troullier, N. & Martins, J. Efficient pseudopotentials for plane-wave calculations. *Phys. Rev. B* 43, 1993–2006 (1991)

[4] Tkatchenko, A.; Scheffler, M., Accurate molecular van der Waals interactions from ground-state electron density and free-atom reference data. *Phys. Rev. Lett.* **2009,** *102* (7), 073005

[5] G.J. Martyna, and M.E. Tuckerman, "A reciprocal space-based method for treating long-range interactions in ab-initio and force-field-based calculation in clusters", *J. Chem. Phys*. 110, 2810 (1999)

[6] CYLview, 1.0b; Legault, C. Y. Université de Sherbrooke, 2009. (http://www.cylview.org).

Table S1: Comparisons of the chemical shift difference

CSA	Analyte: 1-amino-indane ($\Delta\delta^{R/S}$)	
	^{1}H (Hz)	^{13}C (Hz)
R-BINOL	15.12 Hz (1), 17.57 Hz (3), 4.6 Hz (3'), 6.05 Hz (2), 28.08 Hz (2')	0 (No discrimination observed)
R-PA[1]	7.6 Hz (1), 50.4 Hz (3), 22.75 Hz (3'), 34.8 Hz (2), 38.2 Hz (2')	6.02 Hz (1), 9.4Hz (2), 4.2 Hz (3)
R-VAPOL-PA	39.34 Hz (1), 20.04 Hz (3), 34.80 Hz (3'), 152.82 Hz (2), 71.47 Hz (2')	15.71 Hz (1), 44.8 Hz (2), 3.6 Hz (3)

(Note: The chemical shift difference taken from the reference *Anal. Chem.* **2013**, 85, 10887−10894)

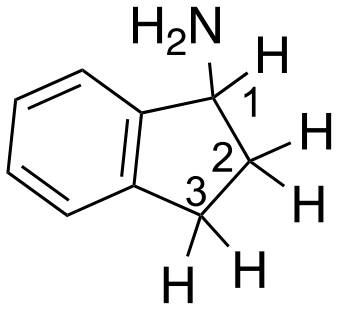


Table S2: Comparison of 1H and ^{13}C NMR Chemical shift values in the pure and complex state.

CSA	Analyte: α-methylbnenzylamine(1)		Analyte: Mandelic acid(6)	
	δ ^{1}H (ppm)	Δ (ppm)	δ ^{1}H (ppm)	Δ (ppm)
Pure	0.79 (CH_3) , 3.23 (CH)	0.62 (CH_3) , 0.9 (CH)	5.26 (CH)	0.19(CH)
R-VAPOL-PA:DMAP	1.41 (CH_3) , 4.13 (CH)		5.07 (CH)	

Figure S1: ^{1}H-NMR spectrum of racemic 1-aminoindane in $CDCl_3$ with 1 equivalent of *R*-VAPOL PA added.

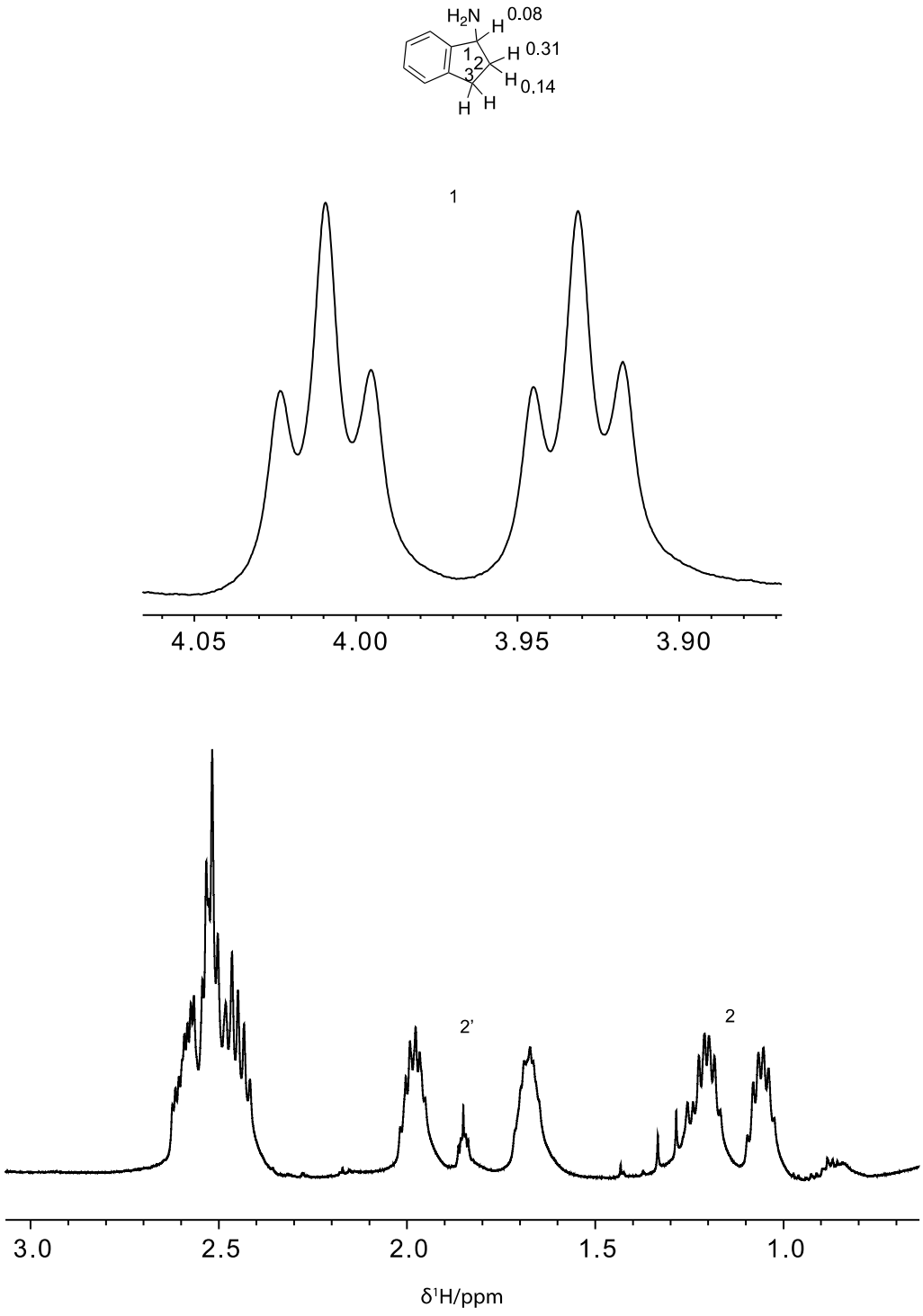


Figure S2: The ternary ion pair formation mechanism.

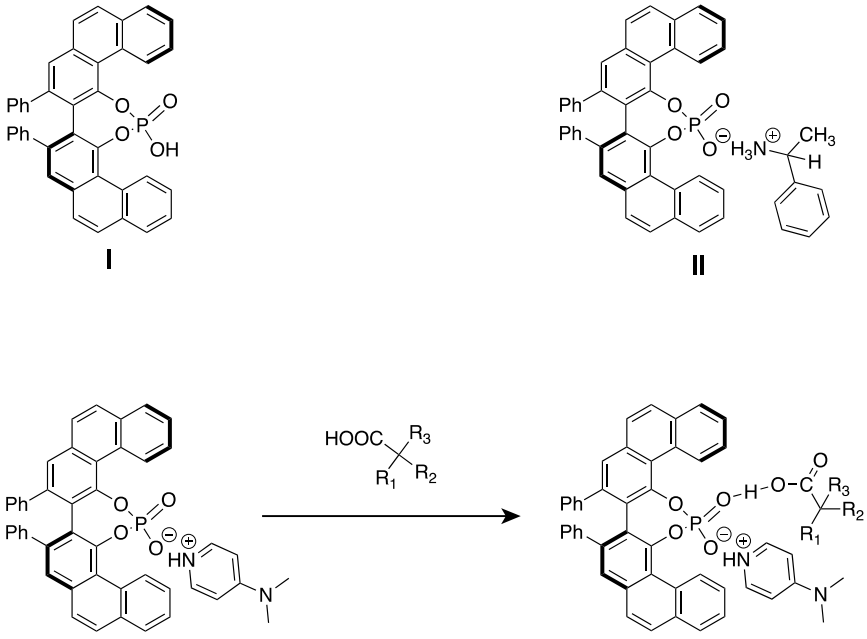
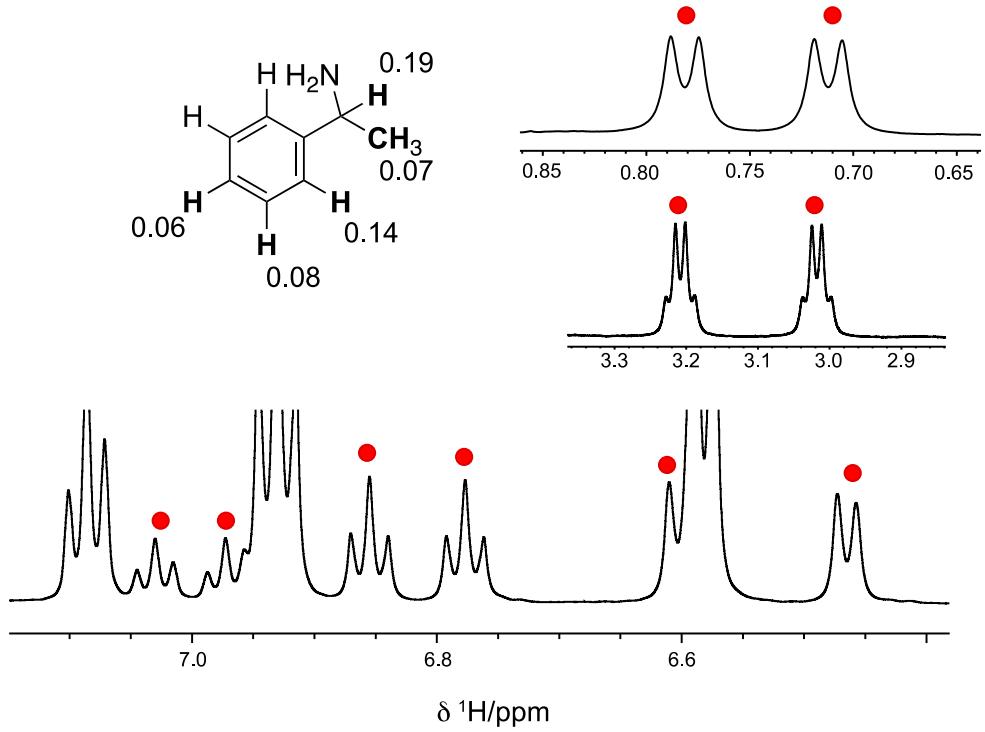


Figure S3: ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of racemic alphamethylbenzylamine**(1)** in $CDCl_3$ with 1 equivalent of *R*-VAPOL PA added.



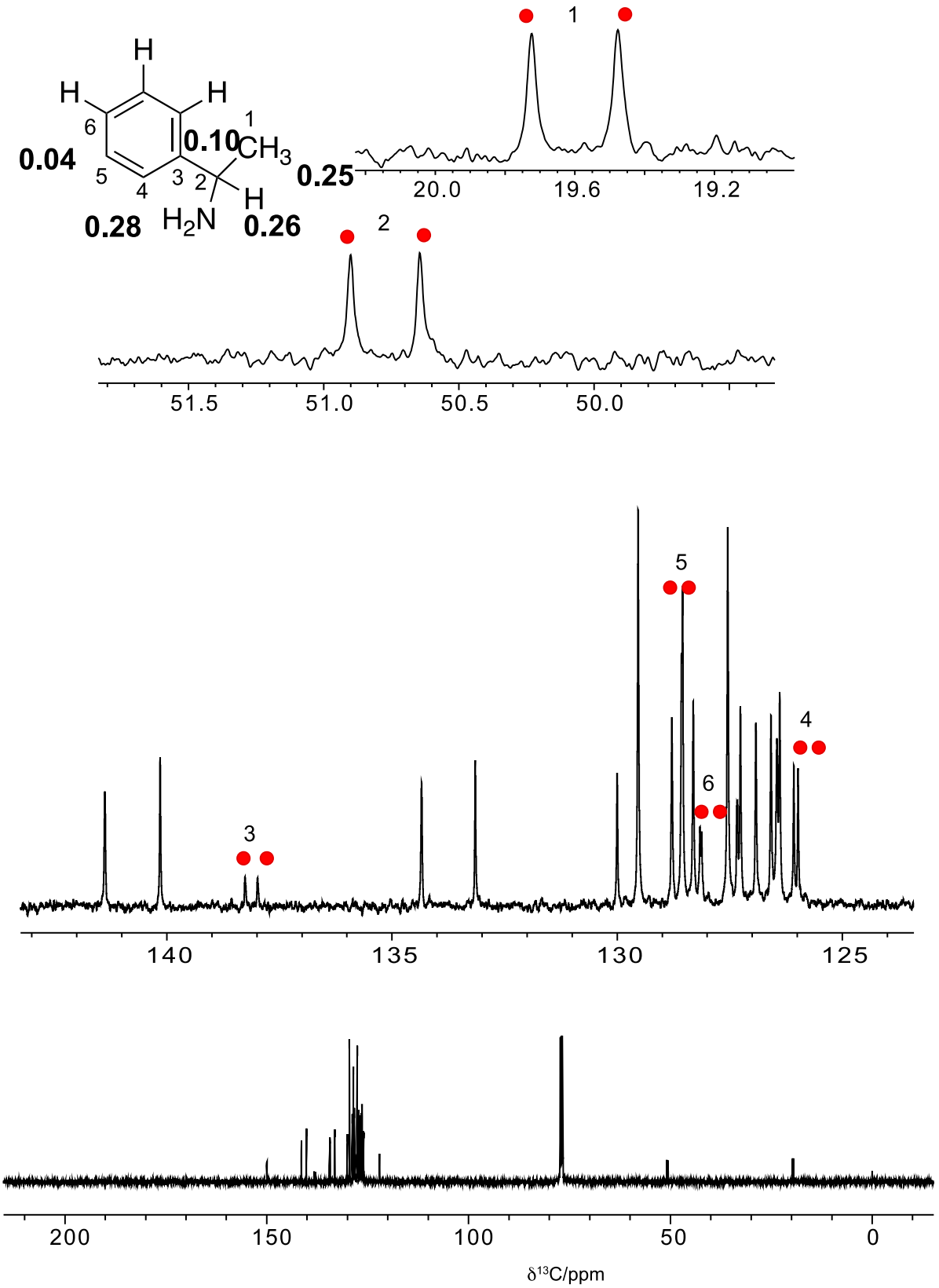
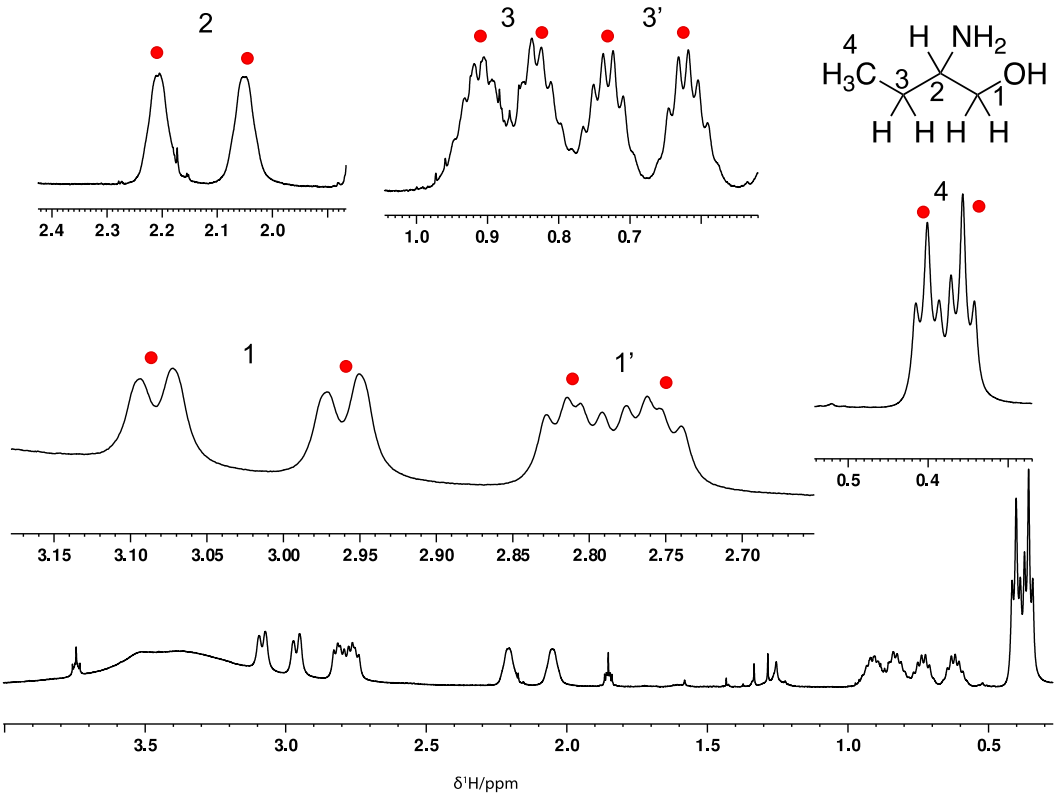

H
H
H
6
1
0.10
CH3
0.04
5
4
3
2
H
0.28
H2N
0.26
0.25
1
20.0
19.6
19.2
2
51.5
51.0
50.5
50.0
5
4
6
3
140
135
130
125
200
150
100
50
0
δ13C/ppm

Figure S4: ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of racemic 2-amino-1-butanol (1 equivalent) in $CDCl_3$ with 1 equivalent of R-VAPOL PA added.



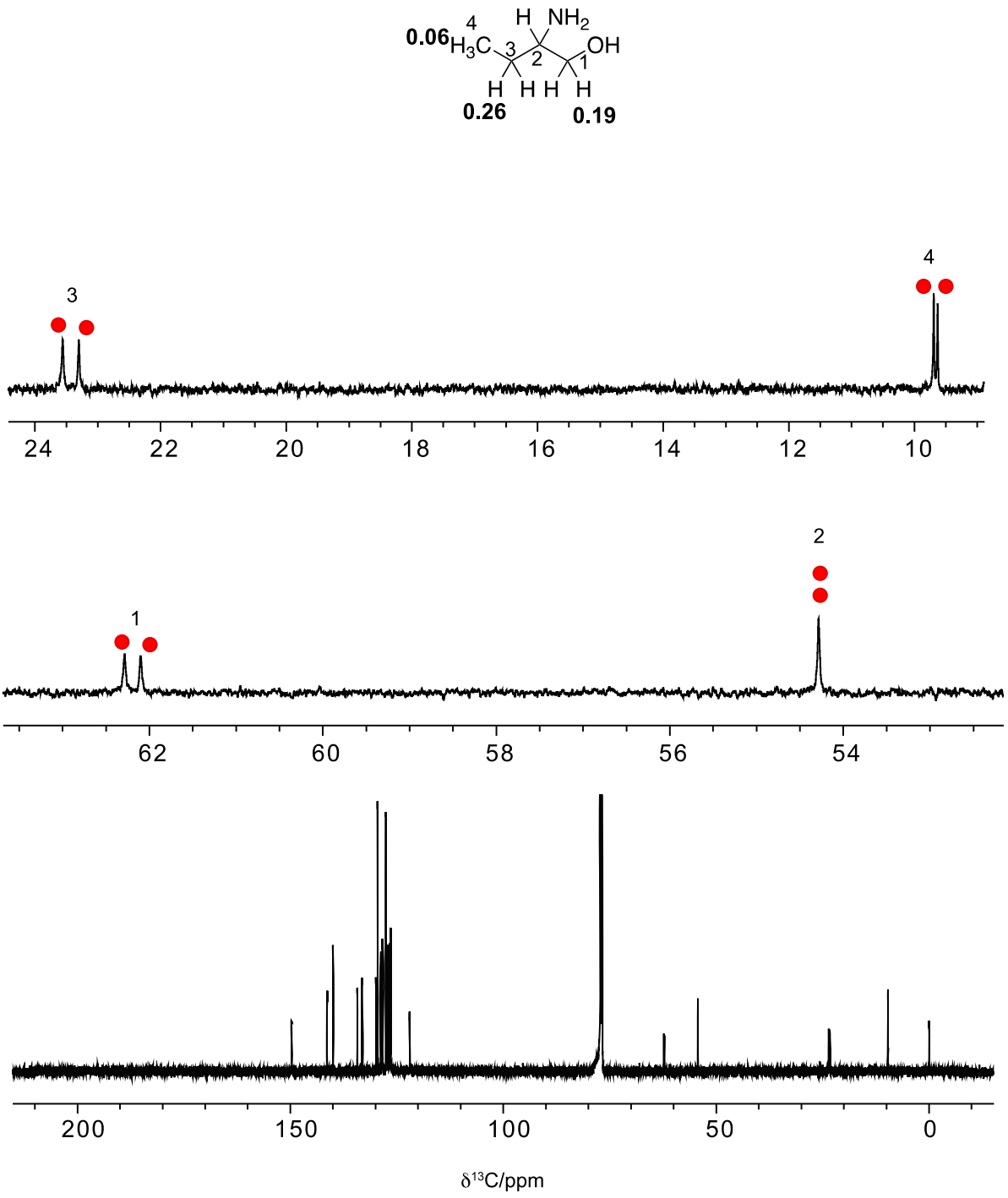
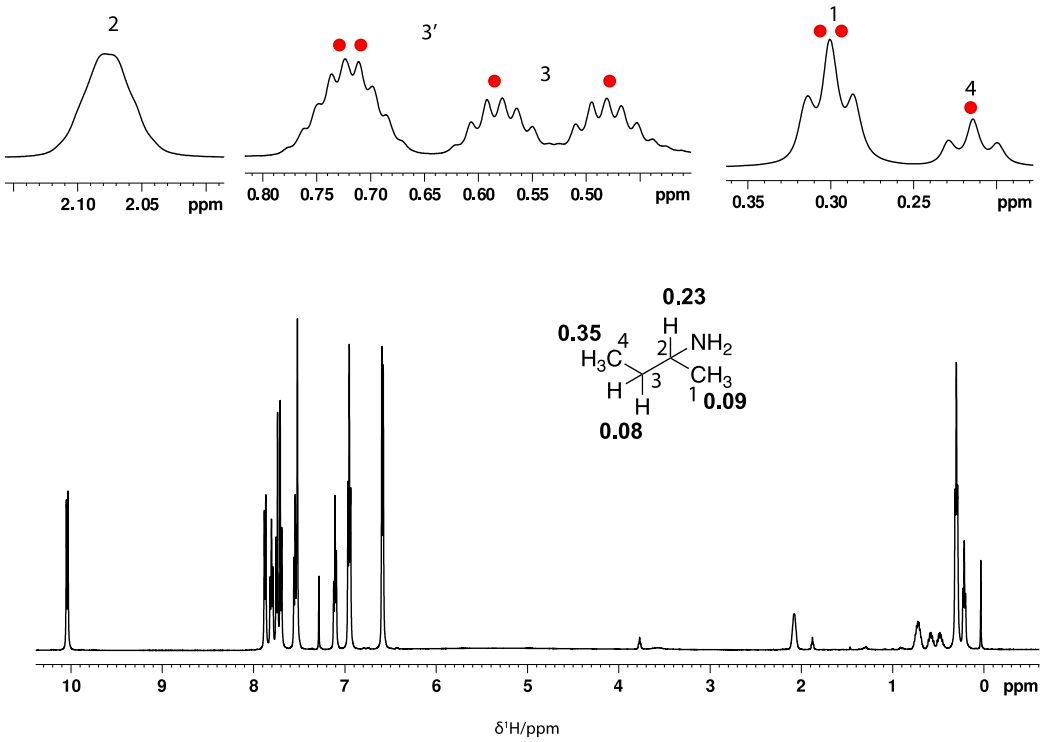

0.06
4
H3C
3
2
1
H
NH2
OH
H H H H
0.26
0.19
3
4
24
22
20
18
16
14
12
10
1
2
62
60
58
56
54
200
150
100
50
0
δ13C/ppm

Figure S5: ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of racemic 2-butylamine (1 equivalent) in $CDCl_3$ with 1 equivalent of R-VAPOL PA added.



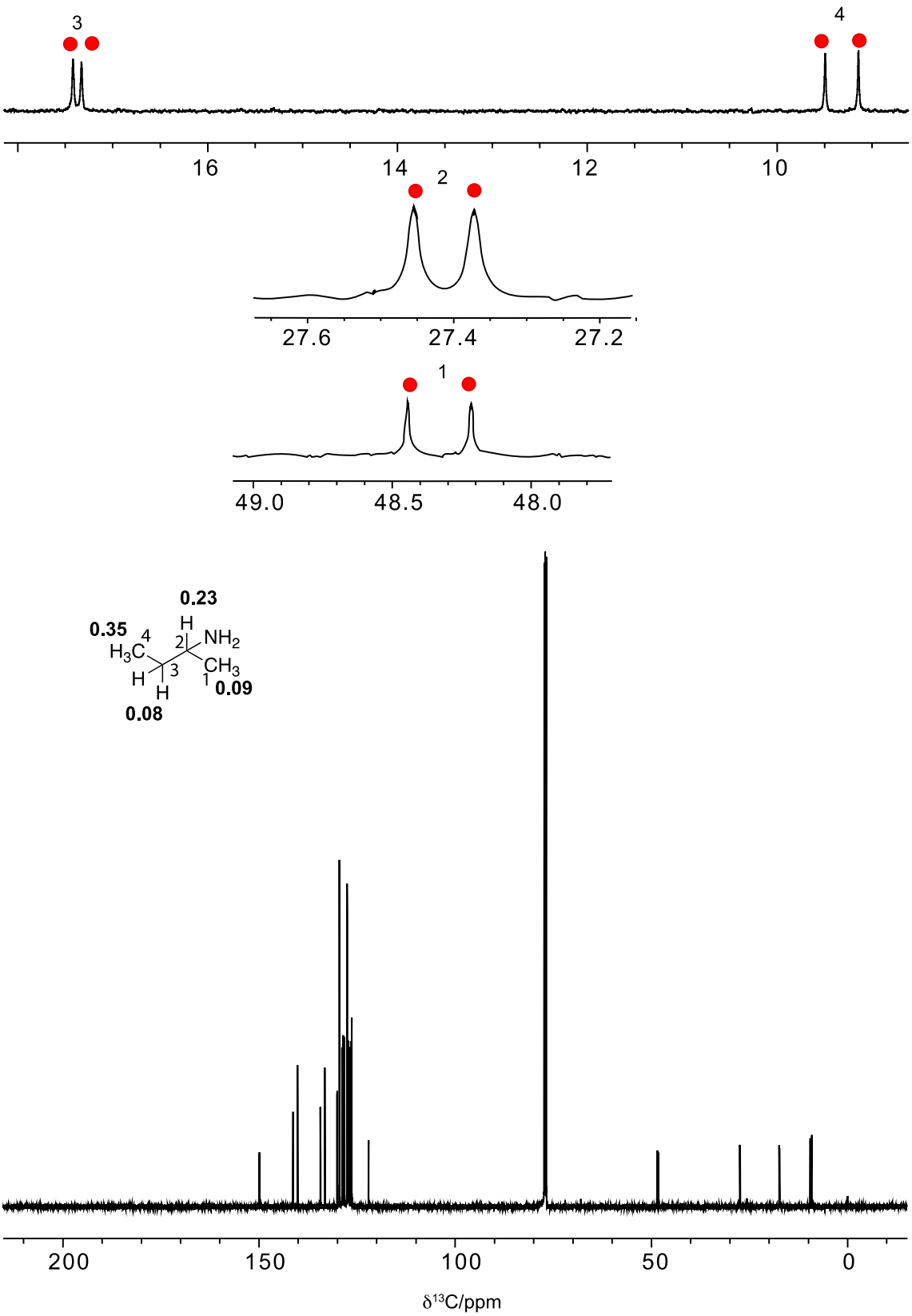
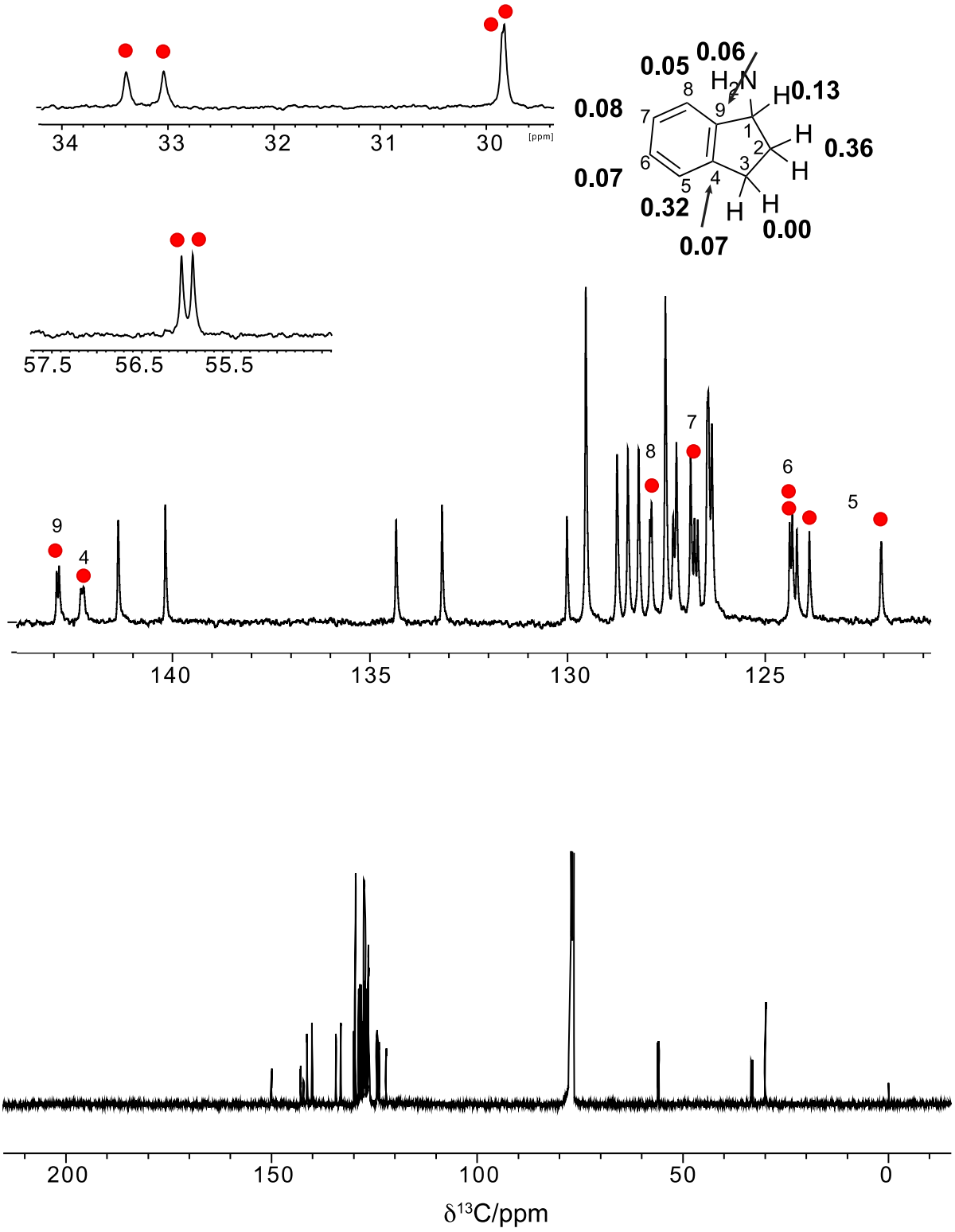

3
4
16
14
12
10
2
27.6
27.4
27.2
1
49.0
48.5
48.0
0.23
H
0.35
4
2
NH2
H3C
CH3
H
3
1
0.09
H
0.08
200
150
100
50
0
δ13C/ppm

Figure S6: ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of racemic 1-aminoindane (1 equivalent) in $CDCl_3$ with 1 equivalent of R-VAPOL PA added.



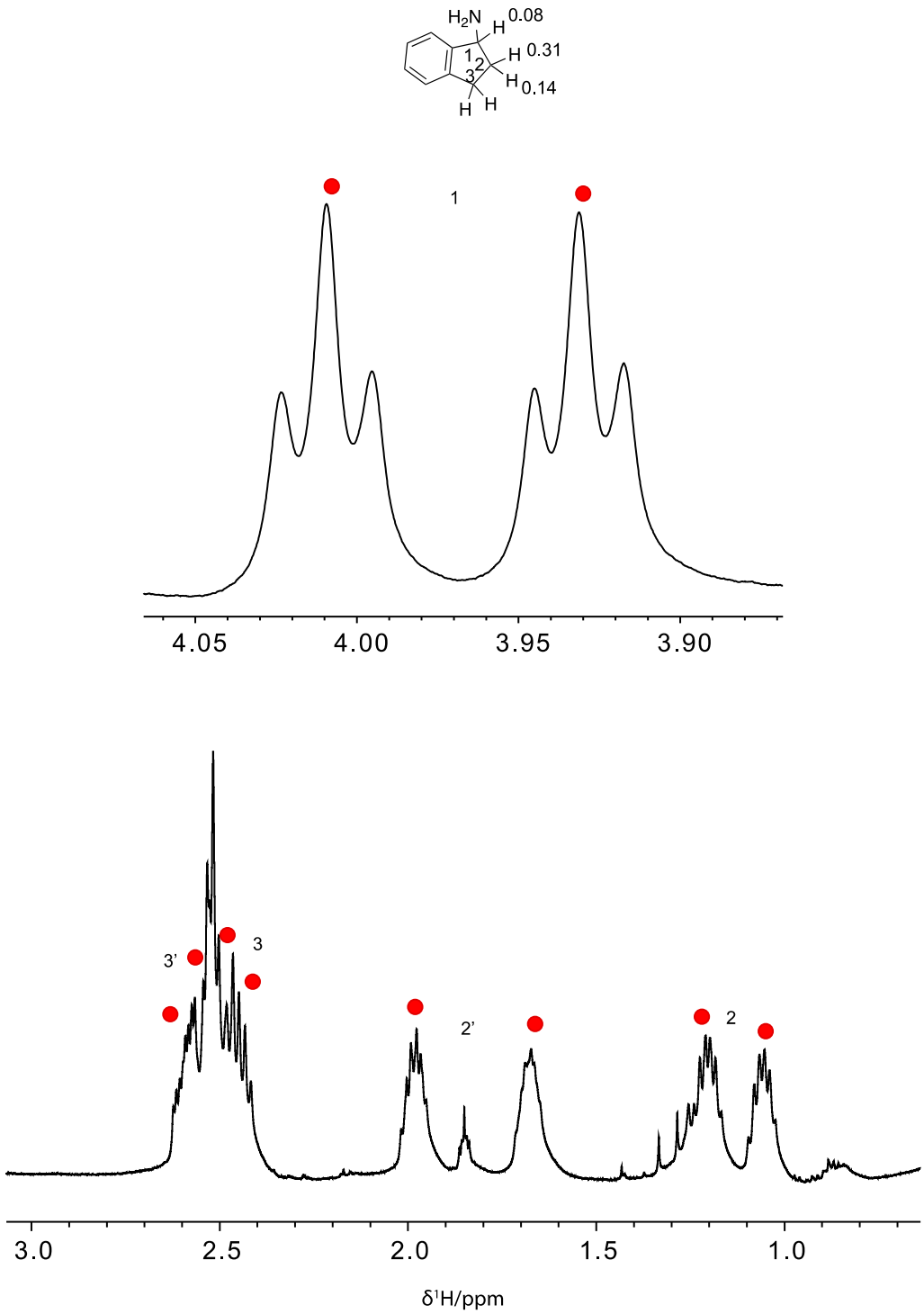

H2N
H
0.08
1
2
3
H
0.31
H
0.14
H
H
1
4.05
4.00
3.95
3.90
3'
3
2'
2
3.0
2.5
2.0
1.5
1.0
δ1H/ppm

Figure S7: ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of racemic 2-methylpiperidine (1 equivalent) in $CDCl_3$ with 1 equivalent of R-VAPOL PA added.

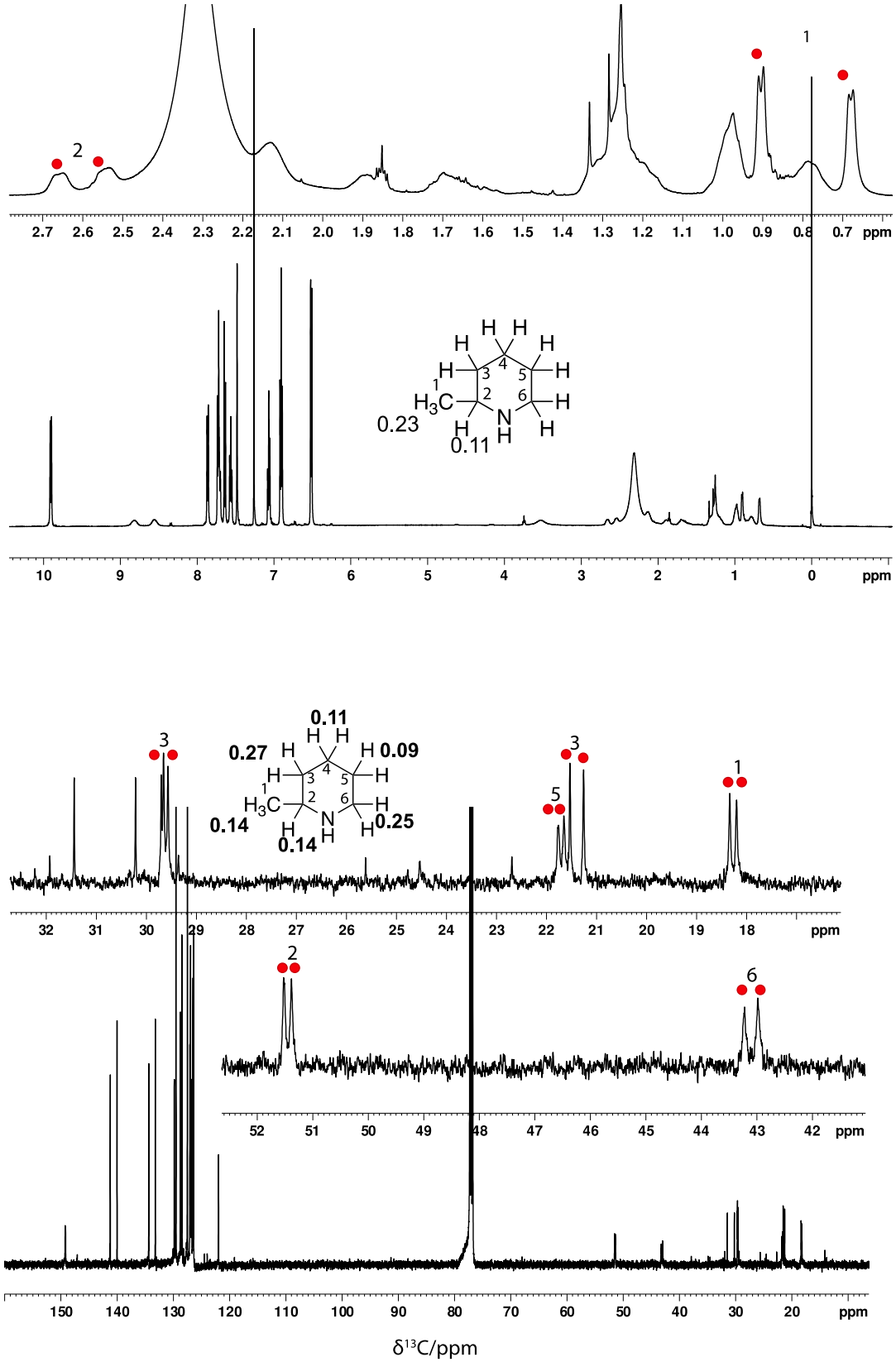
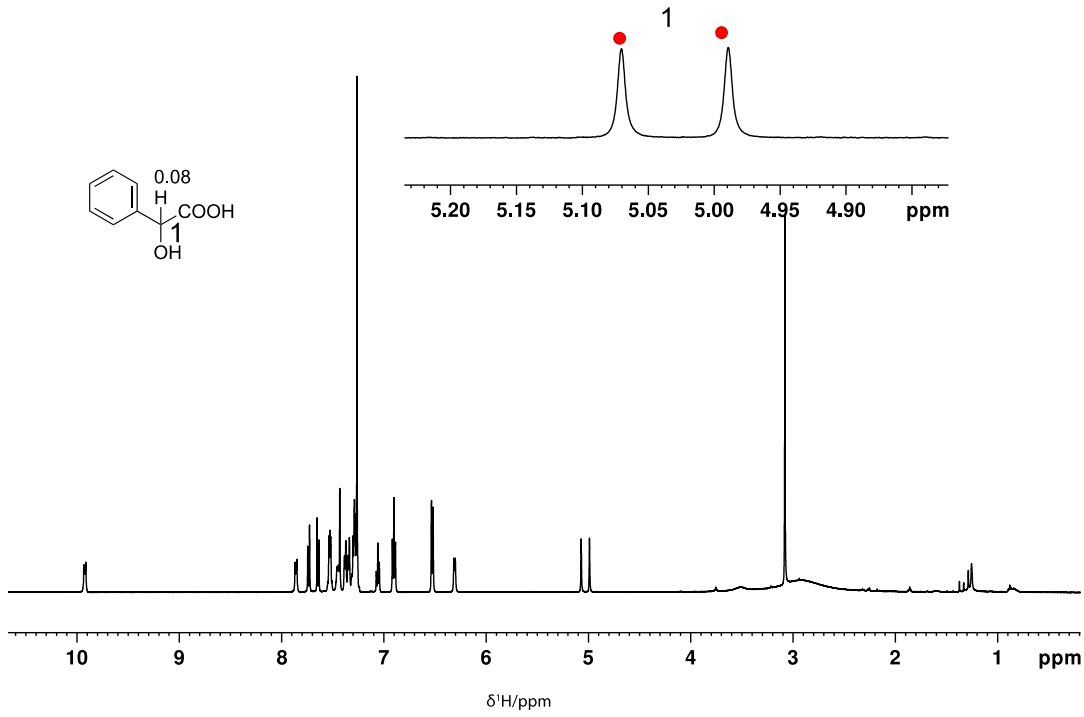


Figure S8: ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of racemic mandelic acid in $CDCl_3$ with 1 equivalent of *R*-VAPOL PA and DMAP added.



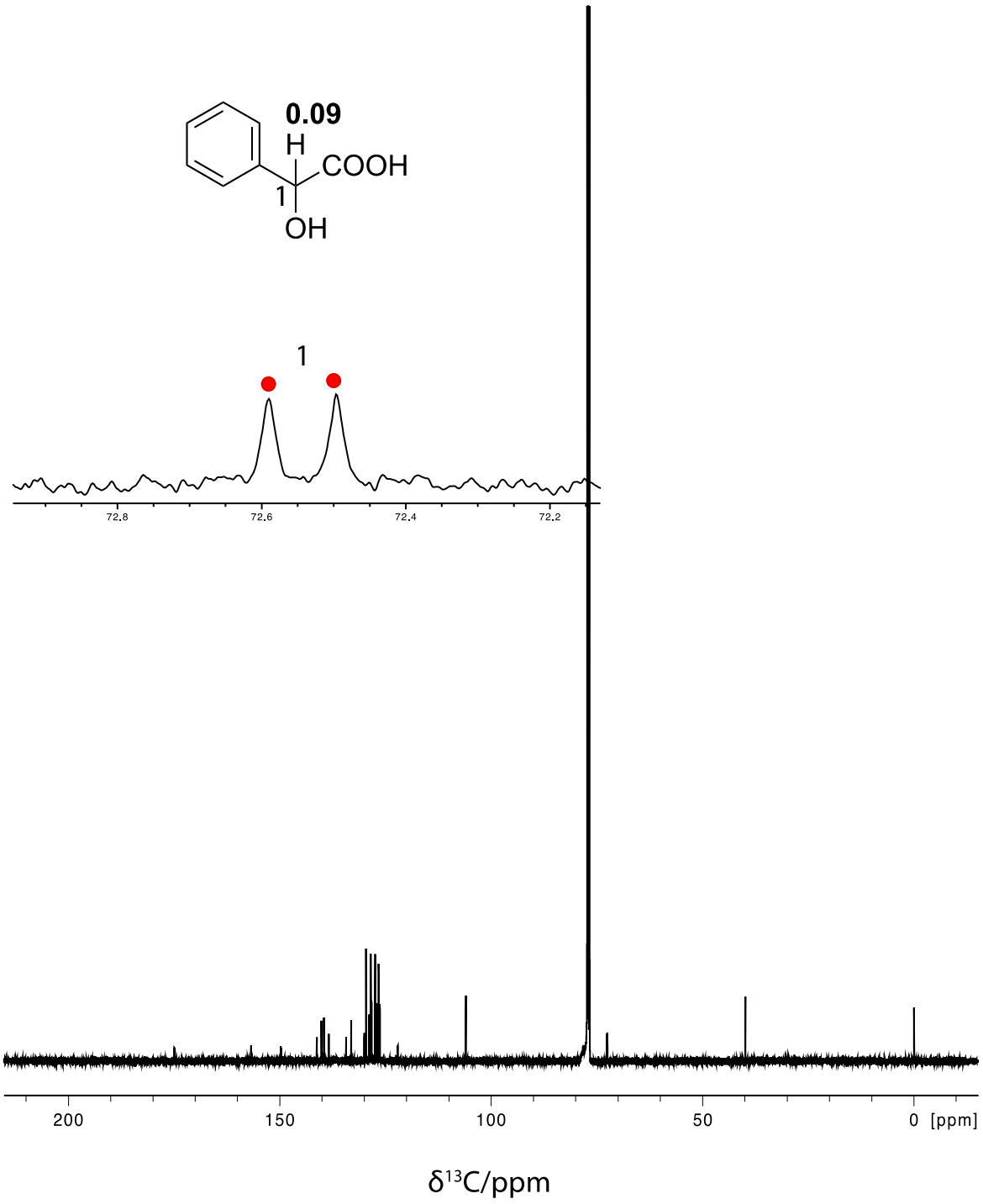
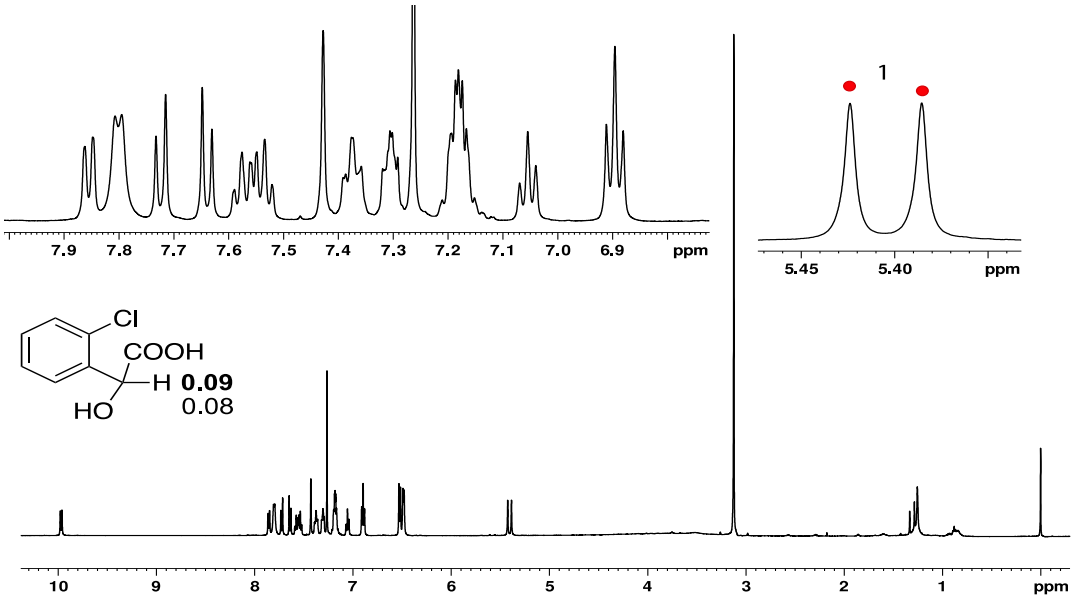

0.09
H
COOH
1
OH
1
72.8
72.6
72.4
72.2
200
150
100
50
0 [ppm]
δ13C/ppm

Figure S9: ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of racemic 2-chloro-mandelic acid (1 equivalent) in $CDCl_3$ with 1 equivalent of *R*-VAPOL PA and DMAP added.



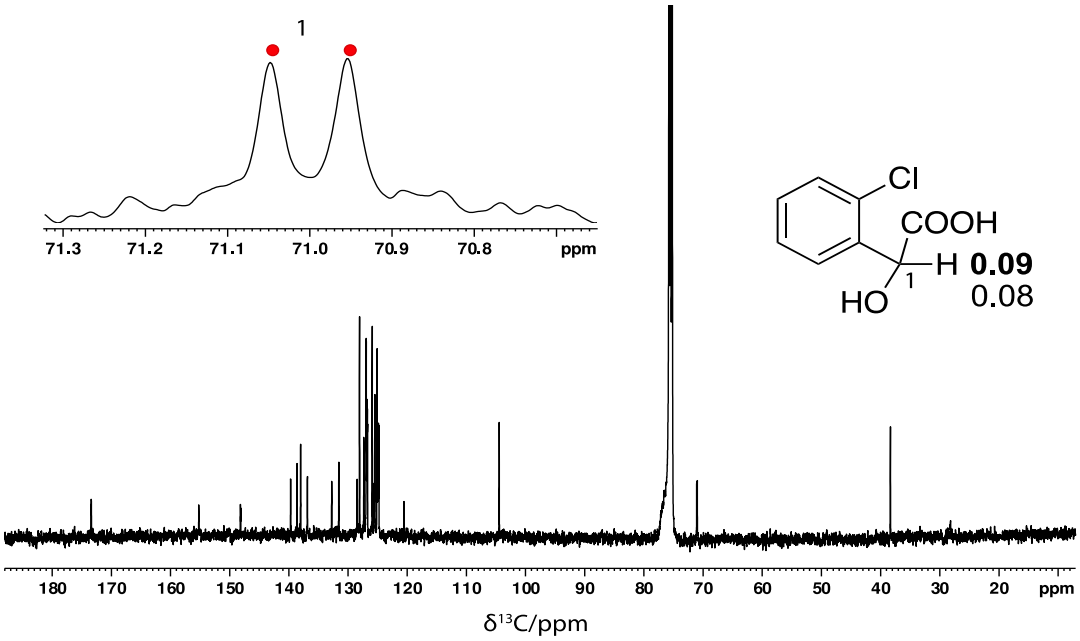


Figure S10: ^{1}H spectrum of racemic 2-chloropropanoic acidI(8)(1 equivalent) in $CDCl_3$ with 2 equivalent of *R*-VAPOL PA and DMAP added.

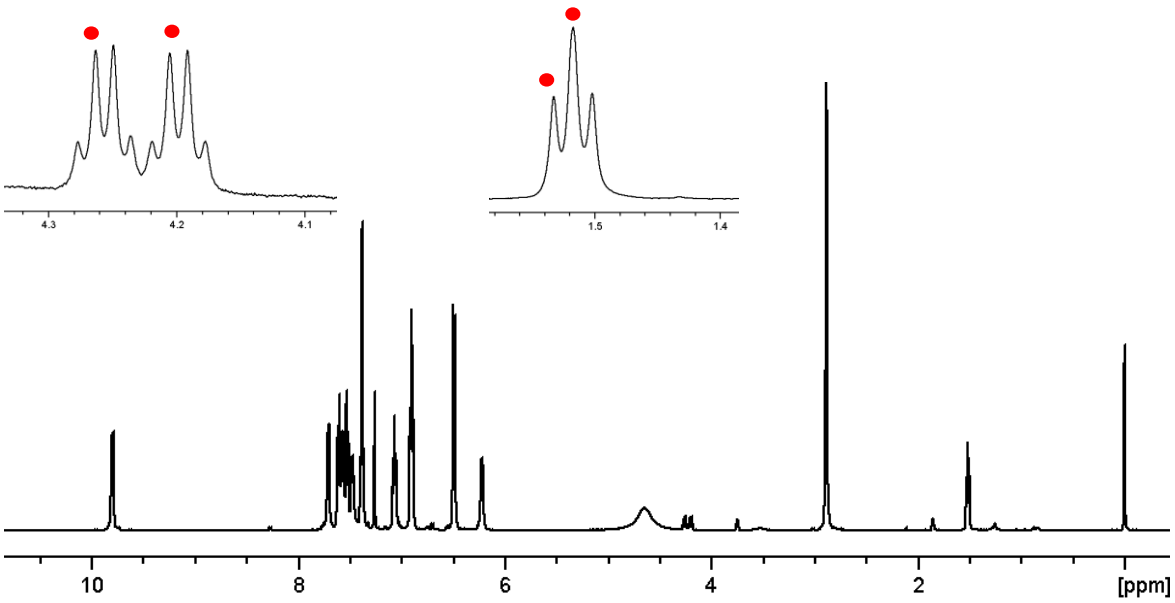


Figure S11: ^{1}H spectrum of racemic Ibuprofen (9) (1equivalent) in $CDCl_3$ with 2 equivalent of *R*-VAPOL PA and DMAP added.

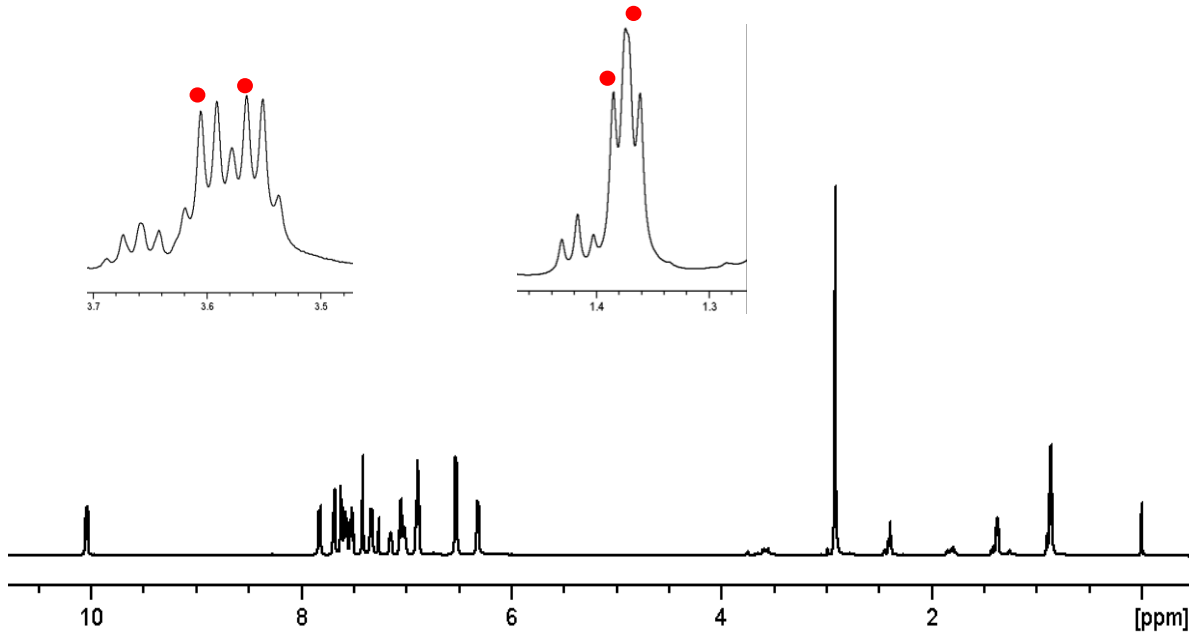


Figure S12: ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of racemic 1-aminoindane(4) (1 equivalent) in $CDCl_3$ with 1 equivalent of R-BINOL added.

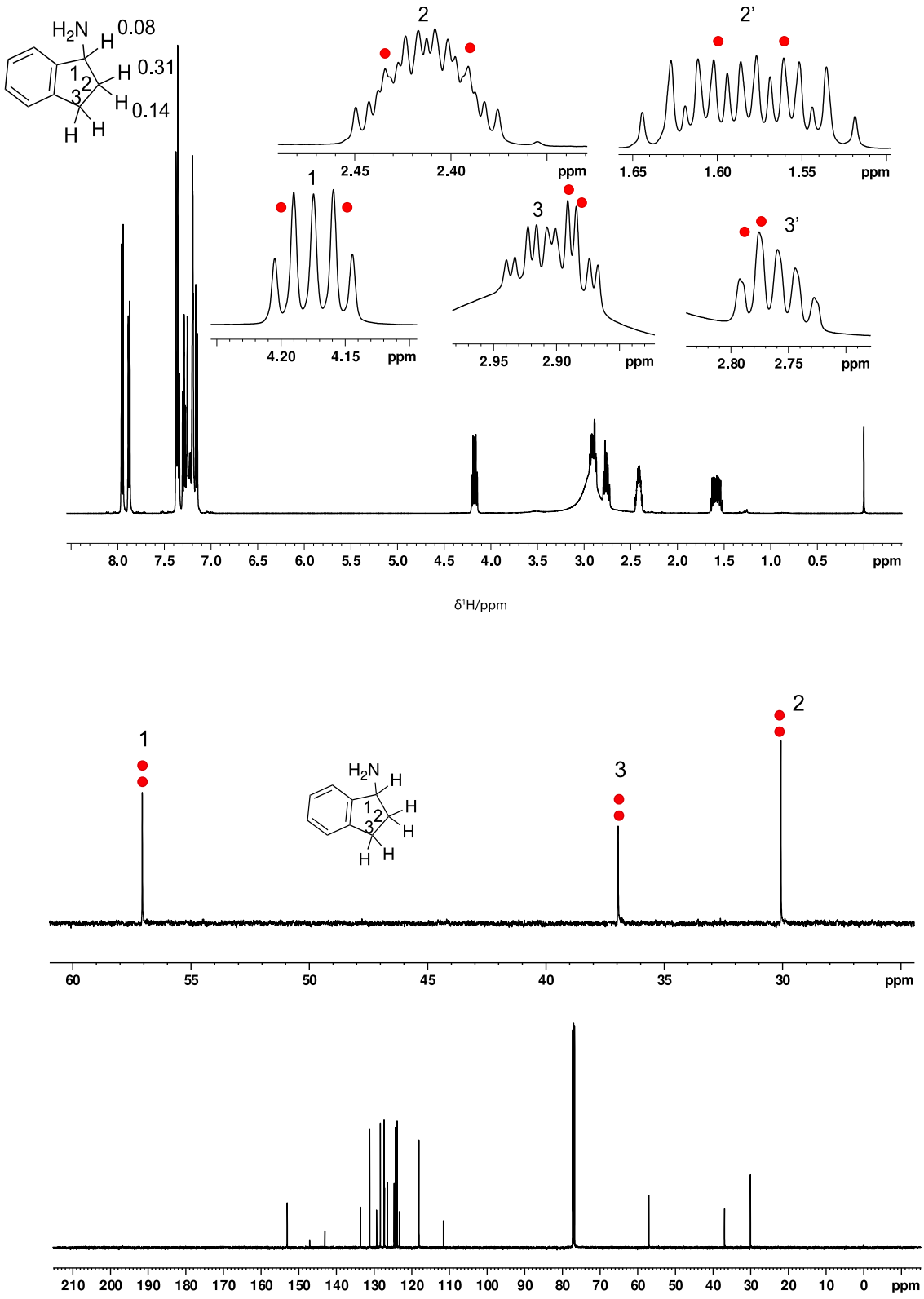


Figure S13: 2D ^{1}H J-resolved spectrum NMR spectra of racemic 9 (1 equivalent) in $CDCl_3$ with 2 equivalent of *R*-VAPOL PA and DMAP added.

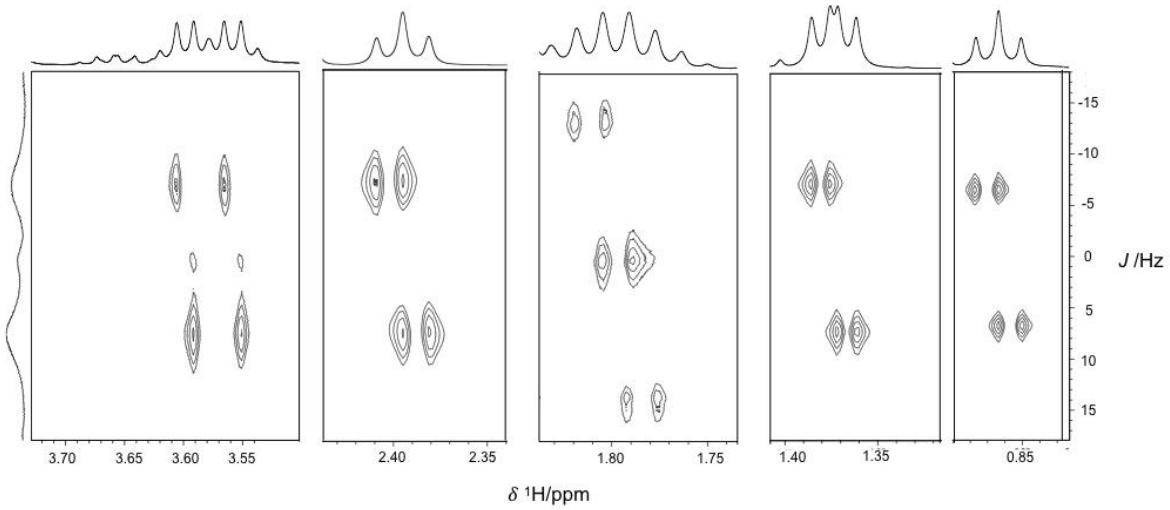


Figure S14: ^{1}H spectrum of racemic 2-Hydroxy 3-methyl butyric acid (10) (1 equivalent) in $CDCl_3$ with 2 equivalent of *R*-VAPOL PA and DMAP added.

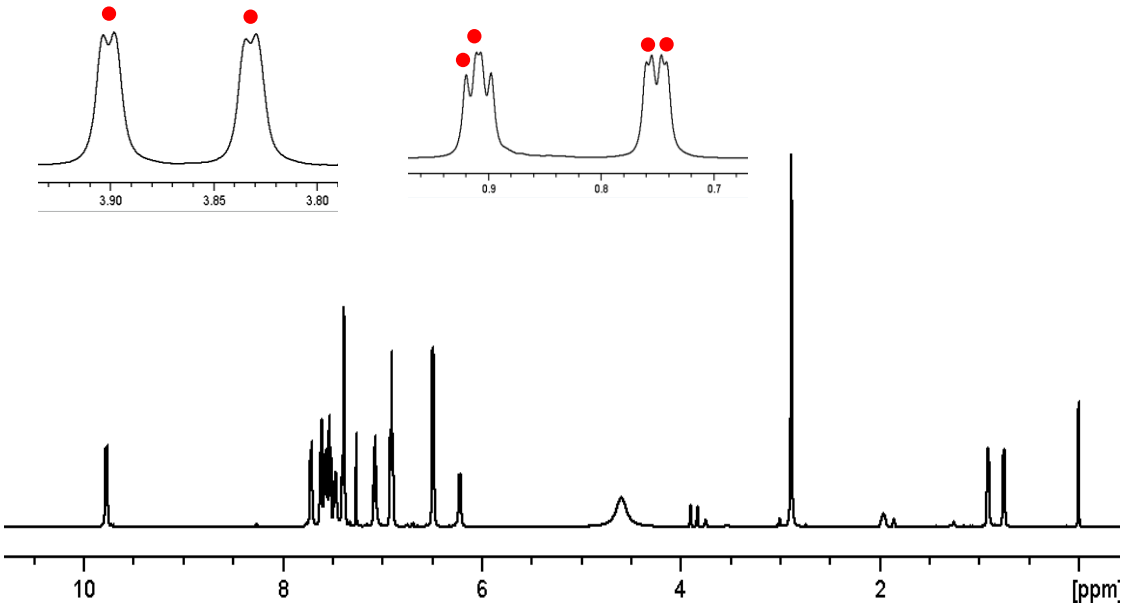


Figure S15: ^{1}H spectrum of racemic lactic acid (11) (1 equivalent) in $CDCl_3$ with 1 equivalent of *R*-VAPOL PA and DMAP added.

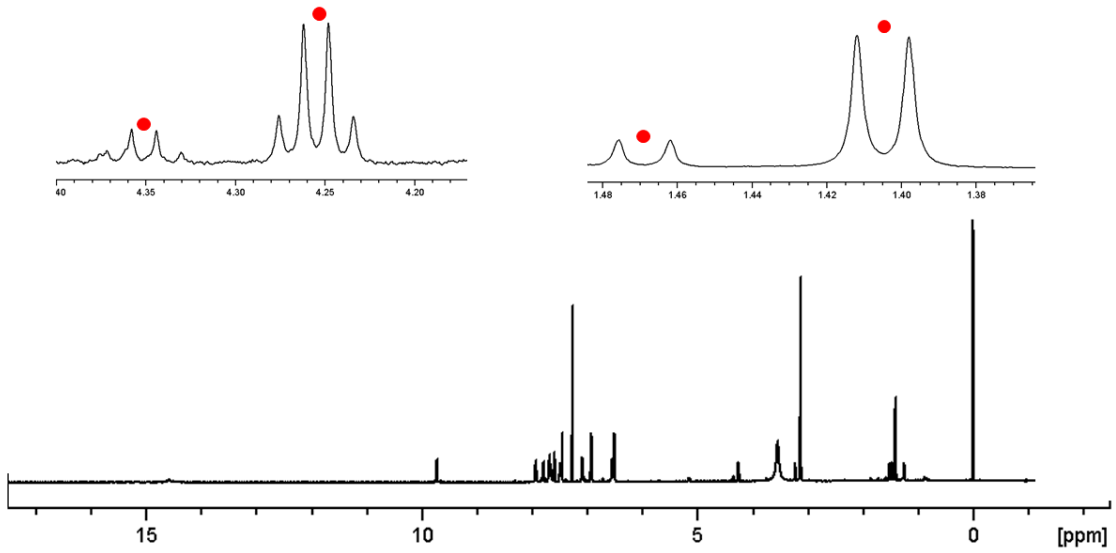


Figure S16: ^{1}H spectrum of racemic Phenylacetic acid (12) (1equivalent) in $CDCl_3$ with 2 equivalent of *R*-VAPOL PA and DMAP added.

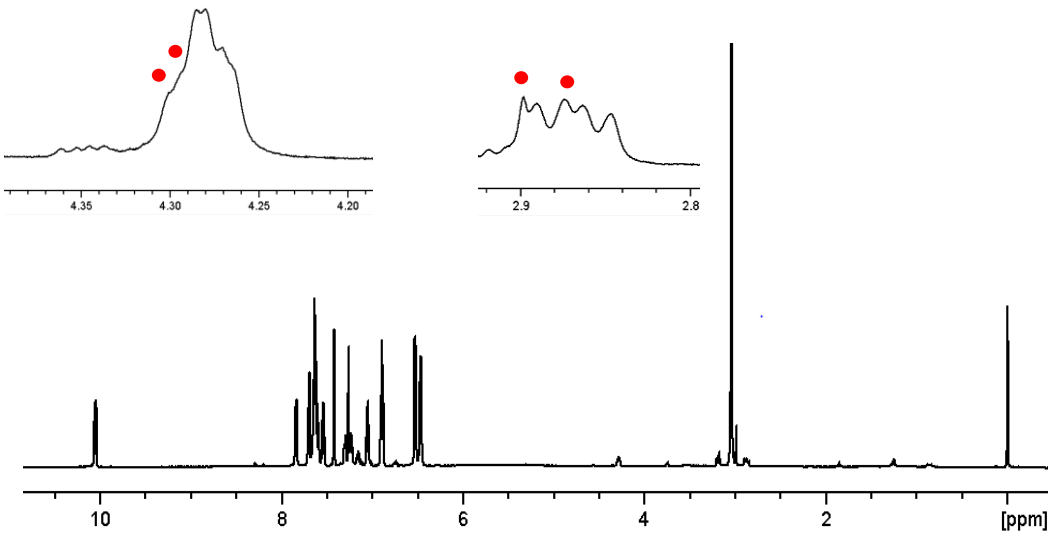


Figure S17: ^{1}H spectrum of racemic Bromosuccinic acid (13) (1equivalent) in $CDCl_3$ with 2 equivalent of *R*-VAPOL PA and DMAP added.

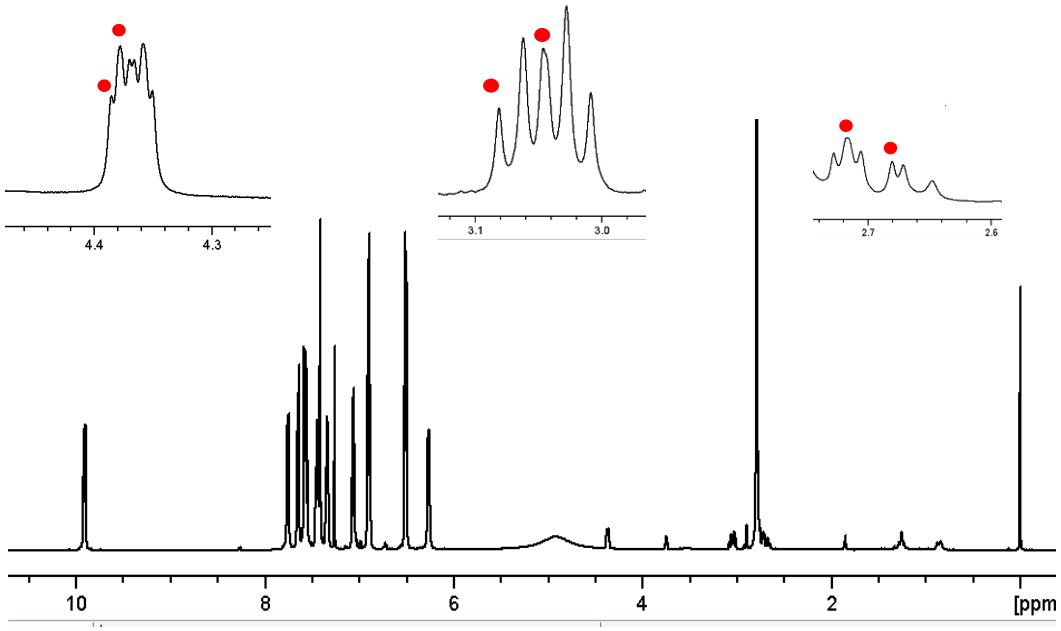


Table S3: The experimentally Determined and laboratory prepared scalemic ratio of (R)-(+)-α-Methylbenzylamine and (S)-(−)-α-Methylbenzylamine.The $C(H)NH_2$ peak was chosen to measure ee

***(R)* Enantiomer**			***(S)* Enantiomer**		
Gravimetric (ee)	**Experimental (NMR) (ee)**	**Intergral (abs)**	**Gravimetric**	**Experimental (NMR) (ee)**	**Intergral (abs)**
50.00	50.074	1339481586	50.00	49.93	1335540873
70.00	69.110	5834674654	30.00	30.89	2607902814
75.00	74.930	3757999390	25.00	25.07	1257315684
87.00	88.680	5621687032	13.00	11.32	717636699
95.00	94.827	8656606700	5.00	5.17	472201958

Figure S18: DFT optimized geometries of the molecule with I (right side) and 1 (left side). [see Figure 2 and 3 in the main paper for structural details]

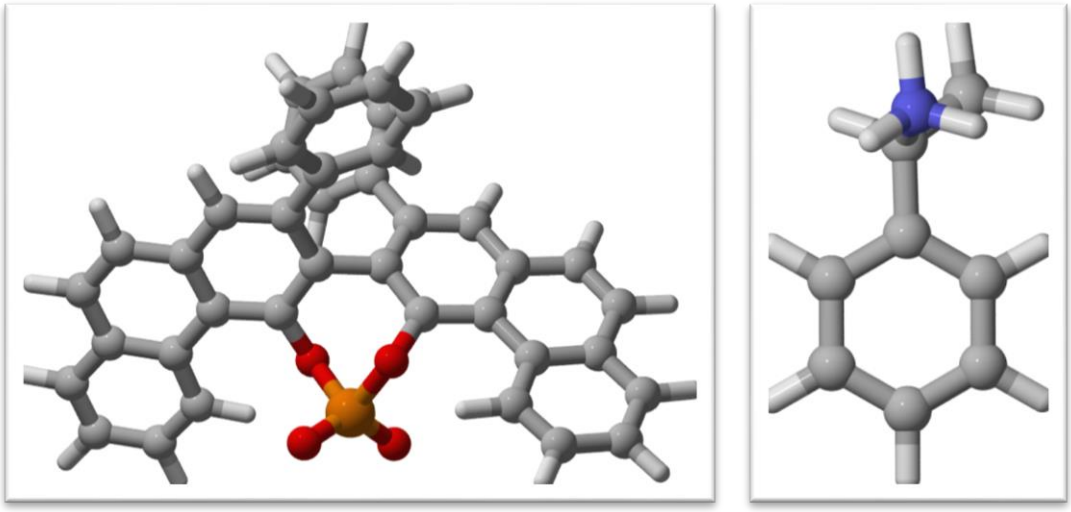


Figure S19: DFT optimized geometries of the R-1-I and S-1-I complexed structures.

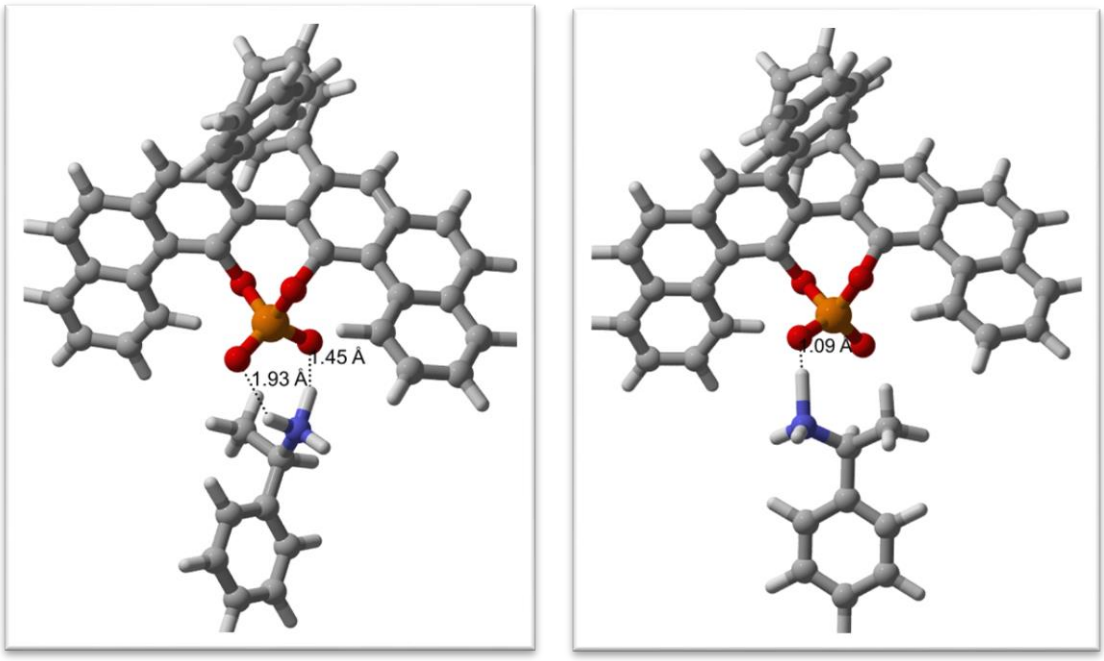


Figure S20: DFT optimized geometries of the molecule with I and 6. [see Figure 2 and 3 in the main paper for structural details]

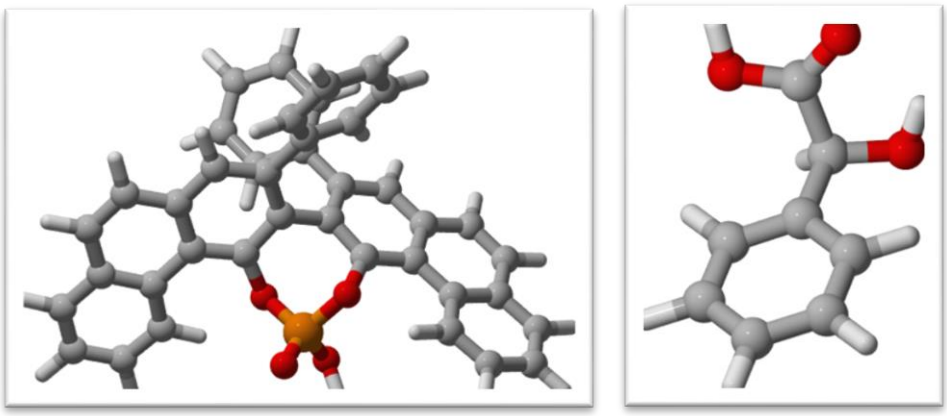


Figure S21: DFT optimized geometries of the R-6-I and S-6-I structures.

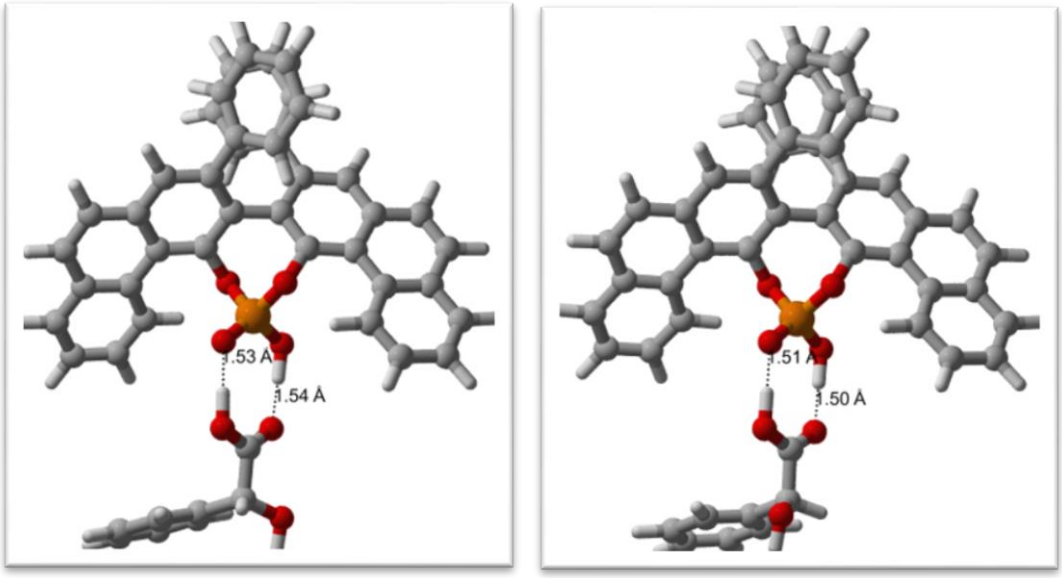


Figure S22: DFT optimized geometries of the molecule with I, 6 and DMAP. [see Figures 2 and 3 in the main paper for structural details]

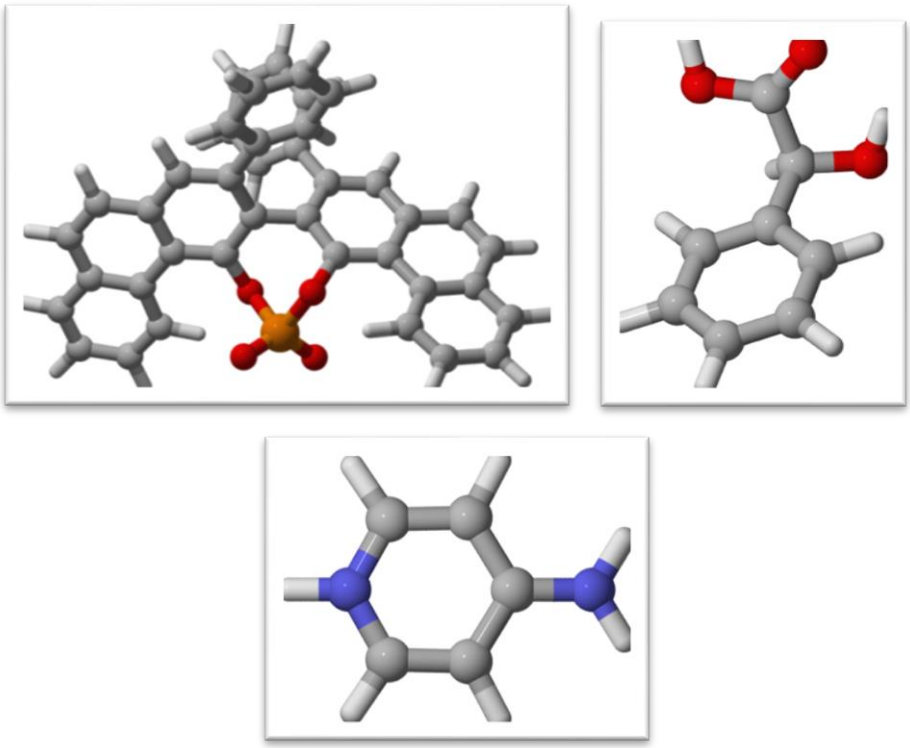


Figure S23: DFT optimized geometry of the complex R-1-I-DMAP.

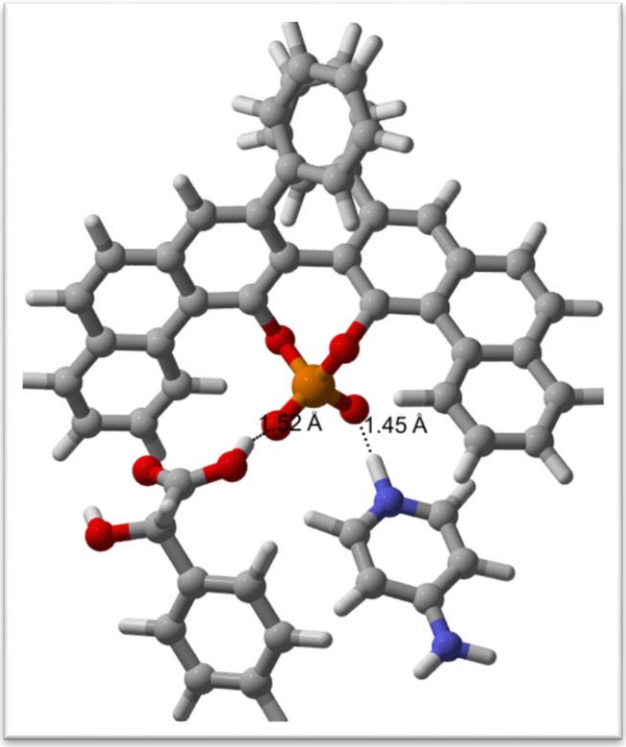
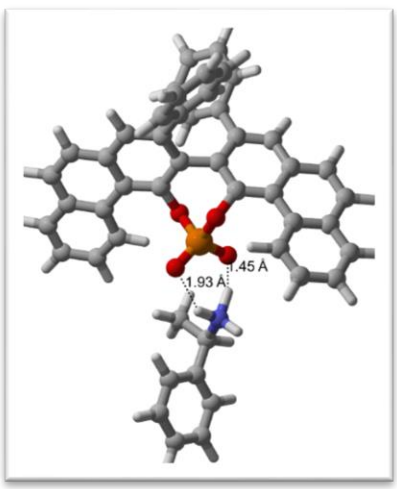
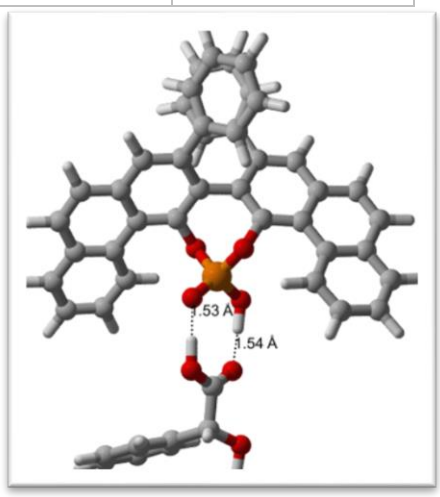
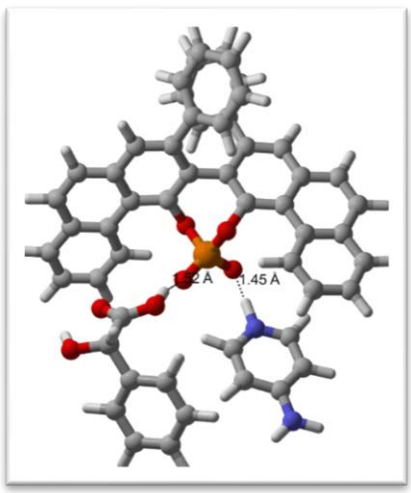


Table S4: Binding energies of different chiral assemblies.

System	Binding energy (kcal/mol)
VAPOL-PA:1 (S)	-104.38
VAPOL-PA:1 R)	-108.44
VAPOL-PA:10 (R)	-28.53
VAPOL-PA:10(S)	-28.46
VAPOL-PA:10: DMAP	-123.83







DFT optimized coordinates of PO4-NH3-R complex in xyz format

```
90

C       -2.488733938   2.209444180  -0.683384243
C       -2.033641157   3.513458628  -0.768592879
C       -0.864316932   3.956101360  -0.131315696
C       -0.071470007   3.054129099   0.633904747
C       -0.534499606   1.719988116   0.660629957
C       -1.733945784   1.298731286   0.101055517
C       -0.413590339   5.293696249  -0.337343464
C        1.144805184   3.535998101   1.262989601
C        1.568587136   4.870956018   0.988385967
C        0.767610350   5.722158753   0.171449559
C        2.763876791   5.359086254   1.552690722
H        3.069968599   6.373774468   1.313238595
C        3.521697025   4.585915644   2.402960623
C        3.082935142   3.294833171   2.723001592
C        1.927189912   2.783122551   2.167665698
H       -1.028767875   5.953726346  -0.942412221
H       -2.562109134   4.216330234  -1.405557524
H        1.117969460   6.732448658  -0.020466229
H        4.435044494   4.979955221   2.837780858
H        3.645893057   2.690162930   3.428496974
H        1.608320380   1.790443785   2.447906091
C       -3.674150122   1.807241665  -1.477161783
C       -3.692011106   0.627413446  -2.232468550
C       -4.803723596   2.635456202  -1.529435216
C       -4.802943811   0.282303715  -2.990903090
H       -2.823617418  -0.019720372  -2.241788653
C       -5.914753326   2.291758437  -2.289446678
H       -4.816998273   3.553376276  -0.948664687
C       -5.922355891   1.107859826  -3.019289287
H       -4.789711233  -0.637137938  -3.567859986
H       -6.779974865   2.947178922  -2.305288907
H       -6.791707816   0.832251898  -3.607802919
C       -3.254531267  -0.522432111   1.041023468
C       -3.644277699  -1.846275306   0.955043738
C       -2.955001702  -2.798579867   0.193069790
C       -1.730060253  -2.460749110  -0.454594098
C       -1.347153181  -1.103202289  -0.338107185
C       -2.133077008  -0.122952743   0.270012470
C       -3.460590273  -4.129144630   0.125527921
C       -1.009121881  -3.497645090  -1.177949984
C       -1.560169561  -4.816836916  -1.202794740
C       -2.790749020  -5.098468656  -0.541822571
C       -0.895030096  -5.848403105  -1.893195231
H       -1.342573380  -6.838770221  -1.891770224
C        0.286653773  -5.618789598  -2.559643914
C        0.827626802  -4.328069333  -2.554676711
C        0.197397292  -3.297735772  -1.886949607
H       -4.397996892  -4.345881547   0.629374091
H       -4.517190434  -2.173949615   1.511732403
H       -3.182319686  -6.110962486  -0.587196004
H        0.787450538  -6.425271285  -3.085474142
H        1.754923197  -4.126122541  -3.083240136
H        0.639063309  -2.316087587  -1.917574684
C       -3.905035117   0.320123177   2.077222087
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C	-4.438859941	1.596698128	1.879991172
C	-3.986556513	-0.228860806	3.367016591
C	-5.027380542	2.294676057	2.928936933
H	-4.426871928	2.042469715	0.896691335
C	-4.581045656	0.463647827	4.412522402
H	-3.553028539	-1.207510572	3.548084279
C	-5.103833284	1.734424115	4.198882158
H	-5.436316258	3.284003539	2.747206710
H	-4.626540343	0.011236031	5.398321721
H	-5.565790505	2.281372042	5.014722610
P	1.060978653	-0.159246023	0.071629712
O	0.255896123	0.714606925	1.200796272
O	1.882083529	0.752693111	-0.816192059
O	1.768564816	-1.261135341	0.785734654
O	-0.158044255	-0.667108099	-0.898426129
C	5.948972164	-2.560947194	0.341827117
C	7.058985778	-3.232180138	0.838975706
C	8.332068345	-2.930117765	0.363676142
C	8.490929361	-1.949341374	-0.608305525
C	7.379133159	-1.273872704	-1.100885132
C	6.099874245	-1.572052455	-0.633962814
H	4.960783609	-2.816384123	0.716225358
H	6.928969226	-3.996476032	1.598141855
H	9.196192923	-3.460471096	0.750283746
H	9.479936191	-1.705490696	-0.982813611
H	7.505263536	-0.506872536	-1.860737894
C	4.906018970	-0.835948141	-1.194091084
N	4.147265462	-0.146565644	-0.106648766
H	3.258121386	0.418128255	-0.498468563
H	3.626314298	-0.813739903	0.497968749
H	4.747628767	0.441759454	0.466141723
C	3.949829615	-1.725275298	-1.983905431
H	3.497361725	-2.491130171	-1.348116901
H	3.143947994	-1.132263444	-2.422314067
H	4.500659229	-2.222154089	-2.784848673
H	5.271375896	-0.037808059	-1.849051516

DFT optimized coordinates of PO4-NH3-S complex in xyz format

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90

C       -2.595382264   2.235089464  -0.890129529
C       -2.205237407   3.558055316  -0.966014806
C       -1.016927727   4.031962254  -0.392611440
C       -0.101902982   3.133368231   0.231651441
C       -0.506622807   1.775727329   0.242465417
C       -1.748703623   1.330142808  -0.198882297
C       -0.712282119   5.421931042  -0.479327286
C        1.131291737   3.666573527   0.788730154
C        1.386358309   5.067858800   0.667596316
C        0.439522797   5.919837265   0.029835827
C        2.574080105   5.618864732   1.186981696
H        2.740497120   6.686303483   1.071698998
C        3.505422296   4.834631495   1.827636695
C        3.252925908   3.466783296   1.976833212
C        2.098364481   2.901455014   1.476398340
H       -1.431586036   6.073204733  -0.967061023
H       -2.823520204   4.261812327  -1.515561514
H        0.661310749   6.981281149  -0.033120197
H        4.419014257   5.271409613   2.218134937
H        3.970885384   2.836539019   2.492449268
H        1.933212949   1.847369935   1.623344986
C       -3.845877221   1.814608041  -1.560693837
C       -3.882773059   0.699857238  -2.406189102
C       -5.020369468   2.558793316  -1.394762122
C       -5.059942721   0.329800111  -3.042654172
H       -2.977004646   0.131289552  -2.582594786
C       -6.200313995   2.183899246  -2.023420808
H       -5.012281891   3.430471000  -0.746063770
C       -6.226281923   1.062389516  -2.845274906
H       -5.063164501  -0.534247830  -3.699667562
H       -7.103032830   2.764933200  -1.862501565
H       -7.149154016   0.763007690  -3.331565525
C       -3.188718696  -0.505602761   0.872834474
C       -3.590455674  -1.828549557   0.790260938
C       -2.962453433  -2.777640214  -0.026868241
C       -1.794980946  -2.431051104  -0.768675273
C       -1.417568546  -1.071444900  -0.676207437
C       -2.137798186  -0.093447732   0.007142823
C       -3.450333192  -4.117530376  -0.040598342
C       -1.110816721  -3.466321036  -1.528921885
C       -1.619913297  -4.801094717  -1.466989690
C       -2.798359673  -5.090780915  -0.720345361
C       -0.967507854  -5.841125626  -2.157040699
H       -1.375054966  -6.845424808  -2.076409555
C        0.152783863  -5.602294587  -2.919634458
C        0.634932818  -4.292568519  -3.022206387
C        0.021013577  -3.254767326  -2.349067950
H       -4.348658401  -4.343085460   0.527054931
H       -4.423208436  -2.161756805   1.402372341
H       -3.164126604  -6.113862906  -0.713541271
H        0.646644572  -6.414666348  -3.443334231
H        1.498827887  -4.079182859  -3.644616598
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C       -3.747296919   0.312661906   1.979880258
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C	-4.158915168	1.645295491	1.881176195
C	-3.854313640	-0.302255402	3.239323387
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H	-4.112295657	2.154621783	0.932789129
C	-4.357922707	0.377706674	4.339816786
H	-3.507459131	-1.323500788	3.359472368
C	-4.762606656	1.702429141	4.218738157
H	-4.972155448	3.361565462	2.867793172
H	-4.422161881	-0.127259779	5.298901015
H	-5.147278903	2.242261250	5.078473167
P	1.005618577	-0.229239135	-0.367613371
O	0.343919996	0.788328959	0.723033094
O	2.079502594	0.334379311	-1.199547451
O	1.322222699	-1.450601893	0.531968488
O	-0.259355027	-0.628437614	-1.308556398
C	6.340647688	-3.096479229	-0.461605504
C	7.618607515	-3.603712583	-0.665266708
C	8.731186114	-2.793449909	-0.472836576
C	8.547746966	-1.474197159	-0.076683190
C	7.266918398	-0.973402463	0.130331904
C	6.136214126	-1.774398179	-0.054738982
H	5.499017094	-3.761371593	-0.634074583
H	7.741391976	-4.636163743	-0.976506770
H	9.729551886	-3.186869073	-0.631791170
H	9.405364293	-0.826875813	0.076122443
H	7.155140161	0.059176857	0.439939868
C	4.731197954	-1.212350567	0.138673154
C	4.664091830	-0.030174403	1.097658545
H	3.627337291	0.268125810	1.250745999
H	5.112531944	-0.273858178	2.066792820
H	5.178655465	0.840500148	0.689202911
N	3.752793910	-2.236575346	0.589975641
H	2.364826110	-1.762330176	0.552791761
H	3.769644797	-3.045955033	-0.024081568
H	4.003366396	-2.572986792	1.518244226
H	4.351293704	-0.866212068	-0.831274641

DFT optimized coordinates of PO4-COOH-R complex in xyz format

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C	-3.072948322	2.434370962	-1.095509617
C	-2.507038781	3.694707290	-1.070915591
C	-1.217716869	3.944380014	-0.574781594
C	-0.431088534	2.880205021	-0.045703971
C	-1.026690484	1.603400310	-0.123536395
C	-2.313072200	1.348802664	-0.587044558
C	-0.660912893	5.252874002	-0.680992236
C	0.902634364	3.163253527	0.459582251
C	1.434389360	4.472172264	0.253902802
C	0.623521034	5.493992952	-0.321164348
C	2.754929082	4.765316395	0.646116184
H	3.138956224	5.762666988	0.450677836
C	3.541913092	3.822461479	1.267343773
C	3.000493912	2.562802626	1.546908939
C	1.715611729	2.243109993	1.159006079
H	-1.281036947	6.044241181	-1.092740975
H	-3.057691068	4.525332652	-1.502120490
H	1.058339744	6.481075167	-0.450086617
H	4.562881069	4.056773623	1.551800781
H	3.595136154	1.821005459	2.071030097
H	1.334239269	1.266075084	1.411655234
C	-4.410026354	2.253675737	-1.697317720
C	-4.646181357	1.267218870	-2.662422654
C	-5.469658108	3.083868580	-1.317494517
C	-5.909949905	1.104102879	-3.213801962
H	-3.830490451	0.630896914	-2.989664473
C	-6.732173159	2.923466931	-1.872398586
H	-5.309518184	3.825540152	-0.541482721
C	-6.959237638	1.929378371	-2.818235808
H	-6.074307853	0.330870656	-3.958366901
H	-7.546838793	3.564638572	-1.549321550
H	-7.948526255	1.797832378	-3.245788827
C	-4.045934727	-0.353073207	0.164662517
C	-4.505017304	-1.653980513	0.104664119
C	-3.850217388	-2.665351462	-0.611436322
C	-2.643722824	-2.387990401	-1.318015351
C	-2.179650634	-1.059043342	-1.200763428
C	-2.849497223	-0.036907990	-0.530893990
C	-4.375964326	-3.989491892	-0.585554198
C	-2.000299925	-3.458424447	-2.065050314
C	-2.554948776	-4.772257638	-1.974661812
C	-3.741593400	-5.003847594	-1.220473843
C	-1.947788567	-5.843509946	-2.659100714
H	-2.387374981	-6.831535848	-2.559565442
C	-0.835563645	-5.652809340	-3.445790489
C	-0.311867421	-4.362838098	-3.577674479
C	-0.877967221	-3.297341966	-2.908858721
H	-5.289195352	-4.166346766	-0.025337702
H	-5.394110113	-1.921648706	0.666866395
H	-4.136489104	-6.014880889	-1.181493438
H	-0.379358524	-6.487066616	-3.969538542
H	0.549325913	-4.187857959	-4.214819639
H	-0.452607670	-2.319471942	-3.061064763
C	-4.802393582	0.627525916	0.970306708

C	-6.195546690	0.694287885	0.851537315
C	-4.169365014	1.485737315	1.876939193
C	-6.934246743	1.594381839	1.607009670
H	-6.692968802	0.066427314	0.119242965
C	-4.907843976	2.388334370	2.631194825
H	-3.092340974	1.440172514	1.997317313
C	-6.292709793	2.447921788	2.498885753
H	-8.011683439	1.643621397	1.481963912
H	-4.398719929	3.044476008	3.330795006
H	-6.867992689	3.158493480	3.084283388
P	0.312201409	-0.374383208	-0.953934693
O	-0.285915398	0.478487815	0.267917787
O	1.292742670	0.324400475	-1.819150043
O	0.802760667	-1.661195190	-0.238850921
O	-0.988372240	-0.700784415	-1.835888776
C	6.646515157	-1.408423017	0.219447128
C	7.496360585	-0.572268696	0.934458374
C	8.027777106	0.565635879	0.335265792
C	7.710683497	0.864103477	-0.986768883
C	6.867916549	0.024487065	-1.705103493
C	6.332216340	-1.116589038	-1.108227850
H	6.225484626	-2.296192484	0.680831897
H	7.748096956	-0.812259710	1.962643920
H	8.689755573	1.216849238	0.896783152
H	8.128726610	1.745986360	-1.462152973
H	6.616794744	0.255220725	-2.736261086
C	5.404886019	-2.031002969	-1.893202803
H	5.577871317	-1.863419799	-2.966209754
C	3.956640538	-1.616609327	-1.629468793
O	3.229456452	-2.227536517	-0.850317530
O	3.642170388	-0.541456023	-2.309213724
H	2.699755855	-0.200191108	-2.089060407
H	1.770808456	-1.904993058	-0.491235718
O	5.537984545	-3.398913183	-1.560113702
H	6.474395540	-3.618166255	-1.638894653

DFT optimized coordinates of PO4-COOH-S complex in xyz format

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C	-1.501793698	2.748836459	-0.169584406
C	-0.881234373	3.977111189	-0.055522193
C	0.319025439	4.169079476	0.641822867
C	0.981017808	3.070230474	1.262882077
C	0.349189586	1.820318865	1.076604312
C	-0.876151012	1.630989932	0.442653249
C	0.905804624	5.467343252	0.666815260
C	2.220966763	3.311935880	1.986179633
C	2.775268956	4.628915003	1.952808156
C	2.096158066	5.682211090	1.275463262
C	3.988630588	4.902987890	2.612382446
H	4.387974346	5.911887729	2.554051969
C	4.652839723	3.929019312	3.321310957
C	4.096856125	2.647263609	3.398221809
C	2.914141611	2.347725876	2.752386910
H	0.380391791	6.274944916	0.165904357
H	-1.315476962	4.833884290	-0.561761320
H	2.550414180	6.669258181	1.271156728
H	5.588123233	4.154578350	3.823591745
H	4.597886093	1.872978103	3.971057868
H	2.515884461	1.351439668	2.855146648
C	-2.746691808	2.656706563	-0.959785789
C	-2.957146364	1.640042279	-1.898733036
C	-3.739788496	3.630626281	-0.801819887
C	-4.127309733	1.595015424	-2.645314545
H	-2.194064970	0.885541012	-2.056184034
C	-4.906185259	3.589369798	-1.552528179
H	-3.609054145	4.401116816	-0.048554038
C	-5.106673940	2.569019838	-2.476307873
H	-4.269838411	0.798576004	-3.369250719
H	-5.668793780	4.347242863	-1.402653699
H	-6.018780522	2.533443301	-3.063868599
C	-2.793018406	0.067429360	0.992087373
C	-3.334225137	-1.198774555	0.902403985
C	-2.670383423	-2.269966174	0.288409080
C	-1.374328831	-2.092118190	-0.279117859
C	-0.828707805	-0.797348558	-0.121405647
C	-1.501052660	0.282058880	0.446755262
C	-3.289584122	-3.553152935	0.276356458
C	-0.739944639	-3.218558155	-0.948594316
C	-1.401192386	-4.485657101	-0.913133770
C	-2.670037611	-4.621411439	-0.278789419
C	-0.818498333	-5.605952811	-1.536295416
H	-1.344402493	-6.555096802	-1.482062841
C	0.375661151	-5.507791238	-2.212314724
C	1.011725699	-4.264304903	-2.287858989
C	0.470841236	-3.152839623	-1.674157794
H	-4.267797127	-3.652208503	0.737611187
H	-4.304080599	-1.390572909	1.351701994
H	-3.139213273	-5.601207261	-0.268701900
H	0.810574630	-6.378476103	-2.691996334
H	1.942192717	-4.163059124	-2.837935863
H	0.986835350	-2.212671897	-1.779042918
C	-3.568531522	1.128506917	1.666785651

C	-4.904371628	1.341147775	1.310925684
C	-3.010169960	1.921819739	2.675129223
C	-5.659805688	2.322524187	1.937971709
H	-5.333218704	0.762969287	0.497737874
C	-3.766360333	2.902616856	3.303168585
H	-1.980529558	1.761154204	2.975825115
C	-5.093263875	3.108651811	2.935748008
H	-6.688277336	2.486755767	1.630932121
H	-3.318306099	3.504911327	4.086798074
H	-5.681578019	3.877931368	3.426017081
P	1.654507252	-0.248982166	0.414138275
O	0.974241007	0.657842249	1.552955116
O	2.760513068	0.386578487	-0.343082472
O	1.998405951	-1.542191447	1.195862403
O	0.451617057	-0.530971376	-0.611597533
C	8.065821759	-0.561505271	1.265183033
C	8.758405571	-0.119117003	2.385908495
C	8.798169479	-0.899308531	3.537904999
C	8.146712549	-2.128704100	3.563233149
C	7.463669332	-2.578687920	2.439168079
C	7.422376604	-1.800133455	1.283653784
H	8.015388136	0.049370586	0.369582118
H	9.265011189	0.840579860	2.359129031
H	9.337382761	-0.551415827	4.413011841
H	8.177266052	-2.743319229	4.457143598
H	6.953833272	-3.536928159	2.458388635
C	6.659687845	-2.284331392	0.063072865
H	6.527362659	-3.371931451	0.137385304
C	5.251984075	-1.694968466	0.116057398
O	4.373670629	-2.311919040	0.730950455
O	5.122185329	-0.542675180	-0.470533204
H	4.163304019	-0.172793852	-0.397655471
H	2.964941078	-1.864001119	1.002379962
O	7.264152031	-1.921198585	-1.166103561
H	8.188101430	-2.193698894	-1.121612242

DFT optimized coordinates of PO4-COOH-NH complex in xyz format

102

C	-1.887845577	2.890722120	-0.710015479
C	-1.289262505	4.133043740	-0.626358764
C	-0.016744546	4.325691113	-0.070391656
C	0.732895751	3.217009867	0.418659915
C	0.119988561	1.952533289	0.261835939
C	-1.173451776	1.767679566	-0.223325052
C	0.550904274	5.633147801	-0.052111743
C	2.041561094	3.456693896	1.005630943
C	2.576436191	4.781439809	0.960114495
C	1.803706276	5.849015043	0.417664230
C	3.857800534	5.042932036	1.485495248
H	4.241454895	6.058151629	1.426756366
C	4.602094303	4.051476689	2.085564391
C	4.059740905	2.765375436	2.191777297
C	2.816908537	2.475530601	1.665589663
H	-0.042729472	6.454060325	-0.443651456
H	-1.804096488	4.994871156	-1.040152488
H	2.234549370	6.846188054	0.410880127
H	5.585099341	4.270408048	2.492189979
H	4.618783293	1.977827528	2.689493685
H	2.428427314	1.474659206	1.774401031
C	-3.218868025	2.776116273	-1.338362966
C	-3.478261203	1.820945024	-2.327601106
C	-4.246595646	3.648541044	-0.965337609
C	-4.731432089	1.739171741	-2.919601531
H	-2.690290236	1.145295029	-2.642481921
C	-5.500435127	3.565395321	-1.556233912
H	-4.069816419	4.362497691	-0.167052073
C	-5.748408689	2.608431060	-2.535176653
H	-4.913304946	0.995476077	-3.689626111
H	-6.290816173	4.239063246	-1.238798792
H	-6.727617991	2.538422862	-2.999437780
C	-2.944375605	0.147617601	0.582690456
C	-3.440876256	-1.140765053	0.583870327
C	-2.826944476	-2.194188269	-0.109181562
C	-1.642868512	-1.971021856	-0.872194848
C	-1.147040621	-0.645875763	-0.834179659
C	-1.767696044	0.406607797	-0.163685933
C	-3.367225659	-3.507519030	0.008353204
C	-1.039940348	-3.093710324	-1.577006141
C	-1.602789347	-4.393717031	-1.388826517
C	-2.766254371	-4.566253756	-0.585709754
C	-1.023852883	-5.513341829	-2.015523285
H	-1.468449313	-6.488667253	-1.837782993
C	0.071847686	-5.384861162	-2.836603298
C	0.602280792	-4.111609339	-3.065476885
C	0.060403390	-2.998286024	-2.457024568
H	-4.262511495	-3.639239784	0.608702058
H	-4.314968412	-1.368294108	1.186923272
H	-3.168444005	-5.568889099	-0.469496751
H	0.513203267	-6.257924940	-3.306997715
H	1.454921668	-3.990041787	-3.726866824
H	0.494322206	-2.035923776	-2.671563082
C	-3.627427076	1.177852876	1.392988693

C	-5.014889149	1.329795200	1.299298106
C	-2.928006865	1.997774546	2.286602019
C	-5.682604198	2.274998398	2.066655152
H	-5.565103507	0.728266214	0.582483470
C	-3.594440873	2.946268639	3.051197137
H	-1.854529666	1.884898317	2.390421870
C	-4.974827776	3.091103461	2.943142544
H	-6.758062661	2.386511708	1.966325352
H	-3.033203537	3.570952469	3.739882571
H	-5.495046761	3.834500201	3.539481553
P	1.366851696	-0.092914170	-0.644599949
O	0.809446261	0.803253547	0.611997958
O	2.277555089	0.719906106	-1.524703967
O	1.898764283	-1.349848364	-0.048756176
O	0.018074058	-0.318867153	-1.518385538
H	3.647534583	0.626126240	-1.071596645
C	5.033434872	-0.614755185	-0.062244251
C	6.244569897	-0.741018543	0.568152039
C	7.119105946	0.364139578	0.618605819
C	6.699462382	1.561928628	0.004818059
C	5.470811338	1.613460701	-0.601930475
N	4.666535775	0.542173489	-0.642217901
H	4.298393527	-1.411740709	-0.108081077
H	6.501421030	-1.684460562	1.038524769
H	7.319527923	2.450557881	0.028561050
H	5.081774241	2.517579448	-1.055280292
N	8.313930448	0.279077876	1.245666188
H	8.596219853	-0.570872835	1.701774263
H	8.925038487	1.073744033	1.314151027
C	5.075451532	-3.694896758	3.192362231
C	6.447236835	-3.476994839	3.130296850
C	7.272155052	-4.379294263	2.461723203
C	6.712025968	-5.501550589	1.860011283
C	5.340188171	-5.722406239	1.927174665
C	4.509563647	-4.821405981	2.591134450
H	4.436885779	-2.987106495	3.711823317
H	6.874667683	-2.610383043	3.628564028
H	8.346806891	-4.223819948	2.431442476
H	7.347168529	-6.218073604	1.347782877
H	4.897604217	-6.607402649	1.483301512
C	3.008580215	-5.066496182	2.651702020
H	2.649013566	-4.772102549	3.649154134
O	1.703135520	-4.694204275	0.680004978
O	2.364422576	-2.895045443	1.889026183
C	2.278874407	-4.181548200	1.622569401
O	2.670191829	-6.407086320	2.398031152
H	2.136026215	-6.362491236	1.580054656
H	2.022576361	-2.321990957	1.116151492

DFT optimized coordinates of PO4-OH-R complex in xyz format

89

C	-1.685599466	2.162204915	-0.926215423
C	-1.004347856	3.359374644	-0.832650908
C	0.219621753	3.486283669	-0.157761077
C	0.825260771	2.358177219	0.468600409
C	0.116730436	1.145665636	0.325252140
C	-1.121172878	1.024873989	-0.294014059
C	0.898775117	4.738709471	-0.176300639
C	2.104454617	2.522676565	1.142251761
C	2.768821042	3.782719578	1.027785858
C	2.134420558	4.872479176	0.363153810
C	4.045632258	3.961114768	1.594657853
H	4.532620808	4.924522526	1.471796545
C	4.663449811	2.952569789	2.298635738
C	3.988611943	1.741841611	2.481168121
C	2.742701633	1.533251336	1.924585749
H	0.406901295	5.575734032	-0.662694027
H	-1.396266924	4.231956662	-1.347362294
H	2.661041154	5.821349816	0.311024339
H	5.653676127	3.097955452	2.719051162
H	4.451172251	0.948278890	3.059233686
H	2.254721984	0.587618366	2.103196367
C	-2.926705750	2.089452677	-1.726294652
C	-3.092586599	1.111721611	-2.714084018
C	-3.955651016	3.014981131	-1.525420312
C	-4.258724078	1.051541425	-3.465333989
H	-2.295030810	0.400370511	-2.900564879
C	-5.124628414	2.951454446	-2.272950091
H	-3.854638638	3.757365700	-0.739912639
C	-5.283516185	1.967112293	-3.242603153
H	-4.367781774	0.286416902	-4.227709150
H	-5.923751025	3.660978418	-2.081209951
H	-6.200838591	1.910590396	-3.820444146
C	-3.125925114	-0.366350060	0.340664054
C	-3.794696979	-1.568907603	0.240675708
C	-3.254838231	-2.685469141	-0.414665291
C	-1.944175364	-2.642964253	-0.978265779
C	-1.266279327	-1.411648945	-0.811903328
C	-1.838573213	-0.273742073	-0.247005035
C	-4.023123244	-3.883613131	-0.475217105
C	-1.435364764	-3.824175045	-1.663333643
C	-2.253488360	-4.996742286	-1.691895273
C	-3.539915103	-4.995033823	-1.079274854
C	-1.799426612	-6.160537648	-2.342818723
H	-2.442814025	-7.035972478	-2.339032587
C	-0.580537629	-6.196526480	-2.979974022
C	0.216363611	-5.047286072	-2.981361957
C	-0.197104517	-3.897104858	-2.340575544
H	-5.007386749	-3.880466450	-0.016144276
H	-4.768997914	-1.675383436	0.708834046
H	-4.130689454	-5.905962147	-1.116310744
H	-0.243870991	-7.099982509	-3.478499908
H	1.176453676	-5.052289783	-3.488224066
H	0.449187985	-3.036434897	-2.374202860
C	-3.745858125	0.750974358	1.086334403

C	-5.076015298	1.108402531	0.839752770
C	-3.041037917	1.456157717	2.070132726
C	-5.680525995	2.141490087	1.544296673
H	-5.623305870	0.600468383	0.051558340
C	-3.646288589	2.487709686	2.776306725
H	-2.013848269	1.188051338	2.294176747
C	-4.968108301	2.838001948	2.515082916
H	-6.707179144	2.414209371	1.319158197
H	-3.081628315	3.019809335	3.535585335
H	-5.435982928	3.649247046	3.065060607
P	1.256431949	-1.073332166	-0.264406888
O	0.661489906	-0.034292015	0.827892535
O	2.232518688	-0.281615285	-1.207465410
O	1.792101316	-2.256729987	0.419889345
O	0.032360969	-1.269737605	-1.297713233
C	7.583023823	-1.576696099	0.801825115
C	8.614403687	-1.362832013	1.710791830
C	9.054233331	-0.070917126	1.978826585
C	8.452668567	1.007919937	1.337774068
C	7.421783492	0.790726075	0.433002869
C	6.975837538	-0.502242012	0.150610860
H	7.258216156	-2.592964075	0.600877512
H	9.077808874	-2.209326321	2.207467888
H	9.863668168	0.095466045	2.682498870
H	8.790103096	2.019697942	1.540739317
H	6.947296325	1.633953865	-0.061590804
C	5.815928391	-0.678179577	-0.803703628
O	4.566429265	-0.533303310	-0.072193852
H	3.172261249	-0.336277358	-0.841598557
C	5.812283905	-1.954142925	-1.626780157
H	5.718073675	-2.845070155	-0.997668679
H	4.969426113	-1.946268060	-2.321810116
H	6.737327186	-2.045303705	-2.201778318
H	5.805171213	0.185154334	-1.476859403
H	4.439760623	-1.306960702	0.496589872

DFT optimized coordinates of PO4-OH-S complex in xyz format

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89

C       -1.411848048   2.442810376  -0.547006479
C       -0.740896825   3.628810439  -0.329467635
C        0.255165302   3.761741058   0.649537322
C        0.636364716   2.648151395   1.454702792
C        0.000291915   1.428721155   1.134298811
C       -1.050881574   1.316447698   0.231776713
C        0.930837011   5.008455831   0.796858847
C        1.614014352   2.846600768   2.510794336
C        2.280640754   4.107367217   2.591221965
C        1.927910707   5.163506573   1.701188633
C        3.253981262   4.325200378   3.585227195
H        3.761242667   5.285841478   3.608081933
C        3.543109116   3.361692723   4.524867483
C        2.840465885   2.152078061   4.499039523
C        1.905656966   1.898239476   3.515354809
H        0.634999633   5.827935823   0.148167676
H       -0.964172675   4.486829808  -0.956878236
H        2.453124941   6.110521883   1.788036757
H        4.290803224   3.545717827   5.289491394
H        3.028168385   1.399131570   5.258334614
H        1.377597385   0.957172592   3.534613353
C       -2.425483896   2.355915238  -1.619438627
C       -2.314390112   1.394140518  -2.629905487
C       -3.496547095   3.252882187  -1.660663004
C       -3.252790385   1.329057470  -3.650762903
H       -1.476850508   0.704108924  -2.621478462
C       -4.437640377   3.185219543  -2.681108982
H       -3.610843364   3.978455701  -0.861044784
C       -4.320470583   2.221960479  -3.677586666
H       -3.146336364   0.580549889  -4.429652609
H       -5.272485324   3.879185871  -2.690040256
H       -5.057900559   2.165475307  -4.472214184
C       -3.186872437  -0.027710310   0.427665323
C       -3.823732563  -1.237736074   0.235869538
C       -3.163143163  -2.381012214  -0.236872020
C       -1.766492986  -2.348567621  -0.526330229
C       -1.137732607  -1.110931512  -0.268605583
C       -1.801778825   0.041628127   0.131327029
C       -3.888336596  -3.601445536  -0.361186628
C       -1.119699994  -3.551073530  -1.025752419
C       -1.889753663  -4.752311761  -1.096438638
C       -3.271657319  -4.743771499  -0.748138419
C       -1.292219318  -5.947659927  -1.540522906
H       -1.900921038  -6.847139432  -1.568145211
C        0.022967158  -5.982820850  -1.943506197
C        0.770541239  -4.800290789  -1.928488987
C        0.215286667  -3.618099765  -1.483669305
H       -4.946893780  -3.593728514  -0.117474315
H       -4.871247691  -1.329495651   0.507390753
H       -3.825928032  -5.675504629  -0.817212864
H        0.469749559  -6.912046022  -2.282372072
H        1.801178764  -4.805073431  -2.269266061
H        0.822921881  -2.727971049  -1.504945651
C       -3.946149603   1.101781726   1.004812663
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C	-5.225992484	1.409834038	0.528504156
C	-3.437088419	1.852696361	2.071439654
C	-5.970774891	2.434499802	1.097414169
H	-5.622572048	0.860393876	-0.319505685
C	-4.179432651	2.880497552	2.637149798
H	-2.457216094	1.619473578	2.472915299
C	-5.449873228	3.177057969	2.152399798
H	-6.958357307	2.662208691	0.708124165
H	-3.765201461	3.445316972	3.467006131
H	-6.029895692	3.980120060	2.595951383
P	1.132075607	-0.893983134	0.906044763
O	0.397368256	0.251687565	1.773652424
O	2.465815180	-0.300505232	0.335643477
O	1.257997143	-2.127780029	1.705794559
O	0.244617600	-0.979654364	-0.436970038
C	6.543747646	0.017701197	2.471740842
C	7.695562922	0.610003988	1.959866826
C	8.412379733	-0.014097263	0.947039086
C	7.976388703	-1.240215006	0.451178017
C	6.832790298	-1.832427711	0.967913274
C	6.099381227	-1.209206175	1.982180421
H	5.991855932	0.527259098	3.254501503
H	8.026898306	1.565751553	2.353814693
H	9.305782570	0.451447437	0.543030904
H	8.529604787	-1.735761382	-0.340503822
H	6.489554927	-2.784068933	0.573961194
C	4.851793012	-1.894502055	2.494007919
O	4.014922846	-2.141868738	1.331965059
H	3.235540385	-0.882845708	0.655382813
C	4.077316341	-1.144584729	3.561393989
H	3.797420917	-0.146610929	3.217017995
H	3.159562547	-1.684767794	3.808182458
H	4.664145377	-1.042204259	4.478720391
H	5.143019289	-2.880190208	2.888060505
H	3.165940536	-2.524621082	1.639498226

DFT optimized coordinates of PO4-OH-NH3-R complex in xyz format

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102

C       -1.490359657   2.190067377  -1.407427245
C       -0.820396272   3.399048649  -1.374619144
C        0.364672084   3.581668747  -0.647286247
C        0.964470879   2.489052222   0.044291509
C        0.340636997   1.231979940  -0.143594537
C       -0.908657466   1.083661659  -0.740200471
C        0.990669090   4.862785967  -0.622289427
C        2.108439341   2.742168557   0.903034783
C        2.674618730   4.053951115   0.916471267
C        2.111758571   5.084303938   0.108117243
C        3.766952673   4.338494820   1.758207825
H        4.180463865   5.343512568   1.741239120
C        4.290809368   3.381817827   2.599298315
C        3.730462340   2.100334721   2.606696041
C        2.672103613   1.785990046   1.777548025
H        0.539507302   5.663544699  -1.201533218
H       -1.221984780   4.240994007  -1.931298330
H        2.579799543   6.065186880   0.120081588
H        5.123391589   3.621810643   3.253728126
H        4.133023415   1.331582397   3.258653299
H        2.275370265   0.782554513   1.802497119
C       -2.750091500   2.084734940  -2.172008457
C       -2.967803144   1.038420358  -3.076462686
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C       -4.143298314   0.970087432  -3.812447458
H       -2.203011575   0.281926687  -3.214925823
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H       -3.607175001   3.851464544  -1.297321441
C       -5.125947413   1.943780641  -3.656521220
H       -4.290239032   0.152353525  -4.511989482
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H       -6.046054944   1.885527192  -4.229817861
C       -2.856725617  -0.232934610   0.145594458
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C       -3.067506174  -2.601544497  -0.400886926
C       -1.826168675  -2.609279267  -1.105237464
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C        0.069310127  -5.132024434  -3.218622124
C       -0.263464599  -3.944281484  -2.599053200
H       -4.748434532  -3.767858718   0.292131977
H       -4.449543704  -1.487034542   0.803086977
H       -3.987637072  -5.869620568  -0.748726512
H       -0.445728800  -7.207597652  -3.538485276
H        0.954635175  -5.171705805  -3.845830028
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C       -3.372111110   0.949814762   0.870646030
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C	-3.057484292	2.732986852	2.484579778
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C	-4.366584765	3.162704402	2.282451329
H	-6.202960291	2.805454013	1.220208674
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H	-4.749838447	4.020841743	2.826349060
P	1.472275344	-1.005185127	-0.803074628
O	0.937232918	0.084349068	0.325656687
O	2.382128228	-0.327979432	-1.791252884
O	1.926228494	-2.186491581	-0.028444604
O	0.122777047	-1.284284658	-1.690570078
C	7.472084383	-1.048883832	-0.961104839
C	8.681447433	-0.379447704	-0.811047296
C	9.052150975	0.122483991	0.433621922
C	8.206474473	-0.059104143	1.524048626
C	6.997242443	-0.731264889	1.371411875
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H	7.179636891	-1.420790831	-1.940143571
H	9.335083794	-0.243574250	-1.667322131
H	9.996052585	0.645873982	0.553563164
H	8.492019952	0.320847673	2.500859796
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H	3.232047087	0.804082006	-1.606618353
C	5.417774651	-3.455250795	0.025844648
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DFT optimized coordinates of PO4-OH-NH3-S complex in xyz format

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102

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C       -4.333053665   3.382765179  -1.177396156
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H       -2.531123045   0.895587932  -2.611581401
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H	8.711938454	-0.531179003	0.794799641
H	8.725371872	1.075483341	1.297410034

--- End of the supporting information: S. R. Chaudhari and S. Mogurampelly 2018 ---