# Two Modifications of Nitrilotris(methylenephenylphosphinic) Acid: A Polymeric Network with Intermolecular $(O{=}P{-}O{-}H)_3$ vs. Monomeric Molecules with Intramolecular $(O{=}P{-}O{-}H)_3$ Hydrogen Bond Cyclotrimers

*Steven Knerr [1,2], Erica Brendler [2], Robert Gericke [3], Edwin Kroke [1,4] and Jörg Wagler [1,]**

[1] Institut für Anorganische Chemie, TU Bergakademie Freiberg, D-09596 Freiberg, Germany

[2] Institut für Analytische Chemie, TU Bergakademie Freiberg, D-09596 Freiberg, Germany

[3] Institute of Resource Ecology, Helmholtz-Zentrum Dresden-Rossendorf eV, D-01328 Dresden, Germany

[4] Zentrum für Effiziente Hochtemperaturstoffwandlung (ZeHS), TU Bergakademie Freiberg, D-09596 Freiberg, Germany

## Supporting Information:

Content:

- $^{1}H$, $^{13}C\{^{1}H\}$ and $^{31}P\{^{1}H\}$ NMR spectra of a $(CD_3)_2SO$ solution of **NTPAH$_3$** 2
- $^{1}H$, $^{13}C\{^{1}H\}$, $^{29}Si\{^{1}H\}$ and $^{31}P\{^{1}H\}$ NMR spectra of a $CDCl_3$ solution of **NTPA(SiMe$_3$)$_3$** 5
- $^{1}H$, $^{13}C$ and $^{31}P$ MAS NMR spectra of **NTPAH$_3^P$** and **NTPAH$_3^M$** 10
- Selected Hirshfeld $d_{norm}$ isosurface views of the asymmetric units of **NTPAH$_3^P$** and **NTPAH$_3^M$** 16
- Selected Hirshfeld surface analysis fingerprint traces ($d_e$ vs. $d_i$) for H-O-contacts of the asymmetric units of **NTPAH$_3^P$** and **NTPAH$_3^M$** 18
- Comparison of percentages of atom contact contributions in Hirshfeld surface analyses of **NTPAH$_3^P$** and **NTPAH$_3^M$** for free refinement of OH groups and for OH refinement in idealized H-positions 19
- Graphics and tables with Cartesian coordinates of optimized molecular structures of **NTPAH$_3^P$** and **NTPAH$_3^M$** (as single molecules and in their crystal environment) 20

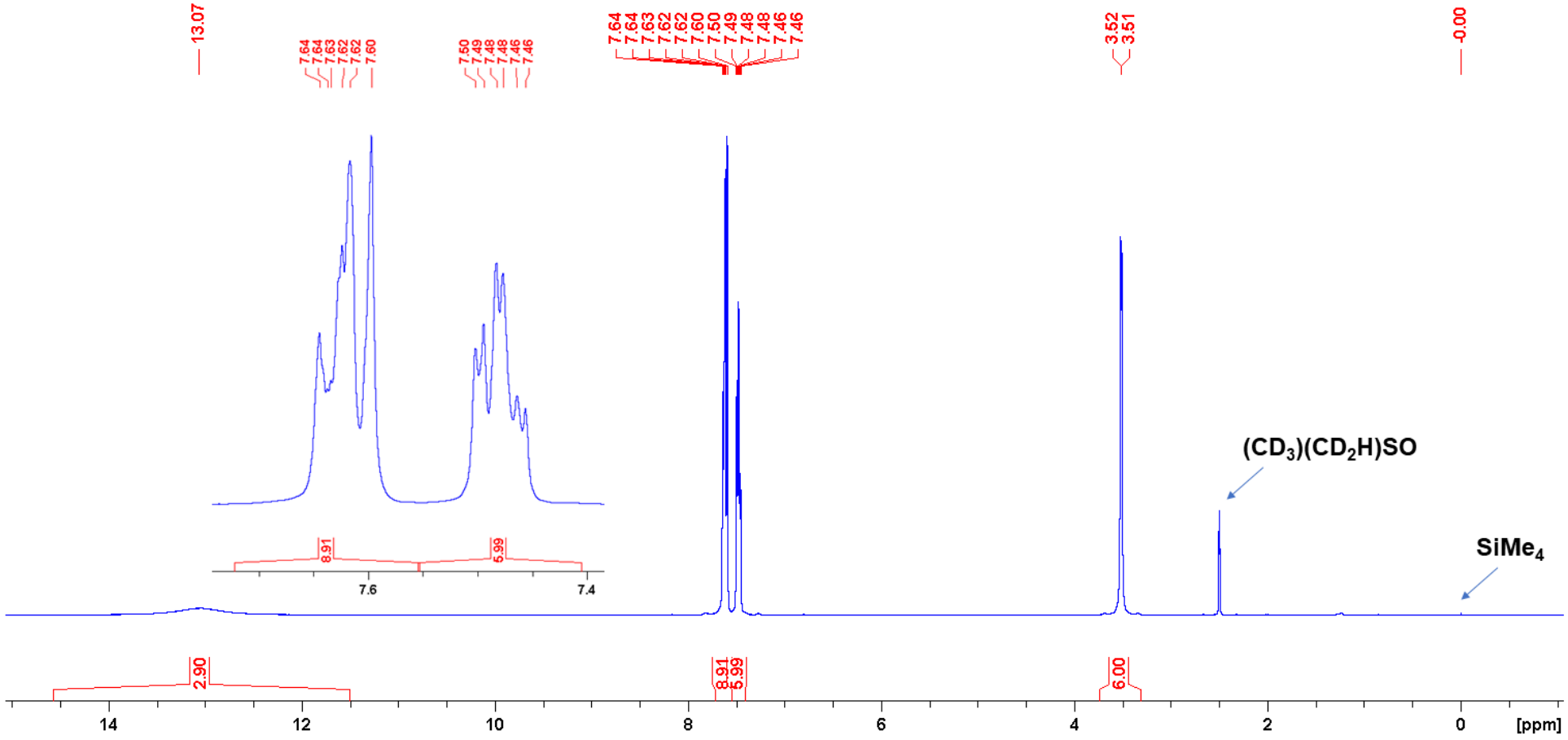



**Figure S1.** $^{1}$H NMR spectrum of a solution of **NTPAH$_3$** in $(CD_3)_2SO$ (full spectrum and magnified inset of the aryl section of $^{1}$H signals).

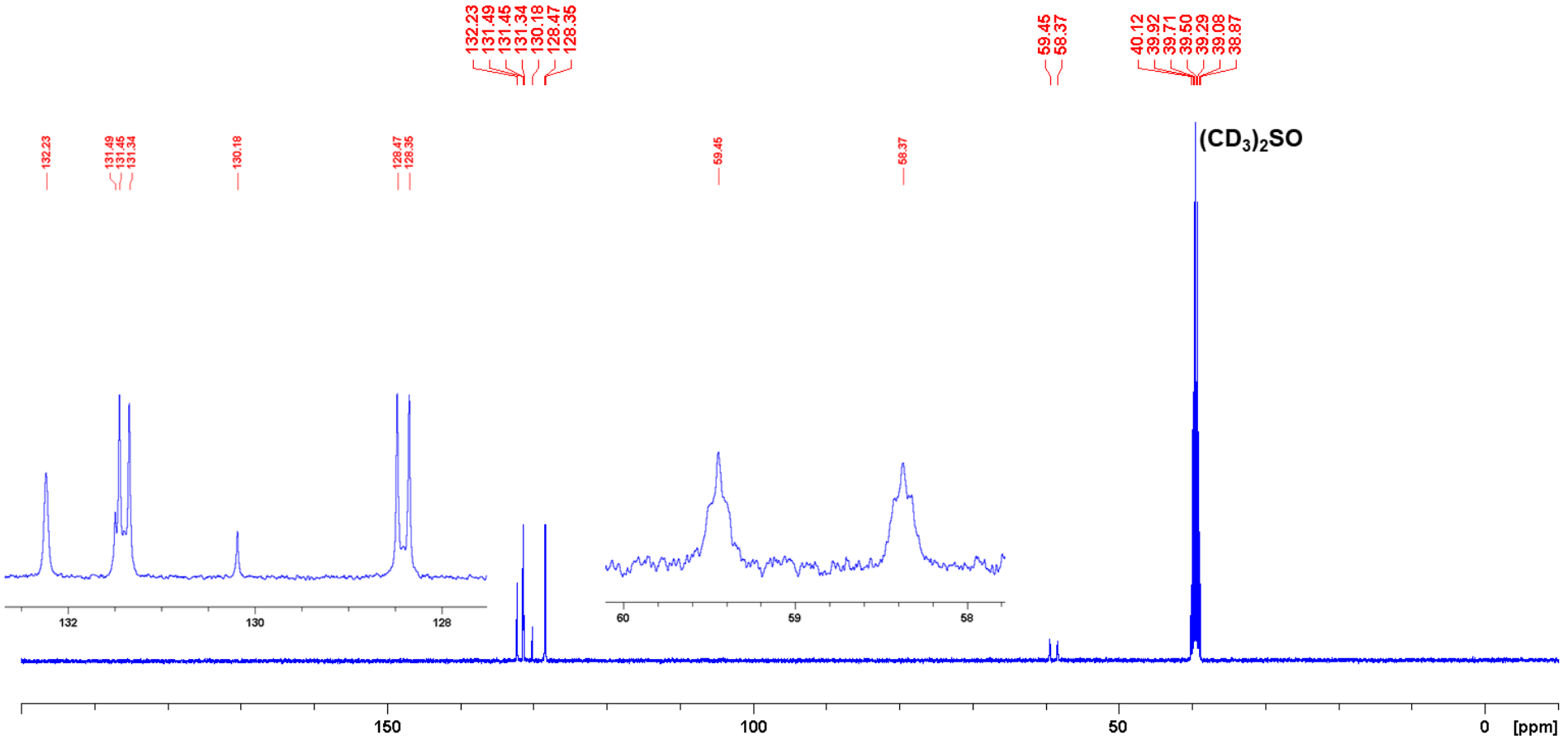



**Figure S2.** $^{13}C\{^{1}H\}$ NMR spectrum of a solution of **NTPAH3** in $(CD_3)_2SO$ (full spectrum and magnified insets of the aryl section and the $CH_2$ section of $^{13}C$ signals). As the internal reference signal ($SiMe_4$ at 0 ppm) is not visible, the spectrum is referenced to the solvent signal, $(CD_3)_2SO$ at 39.5 ppm.

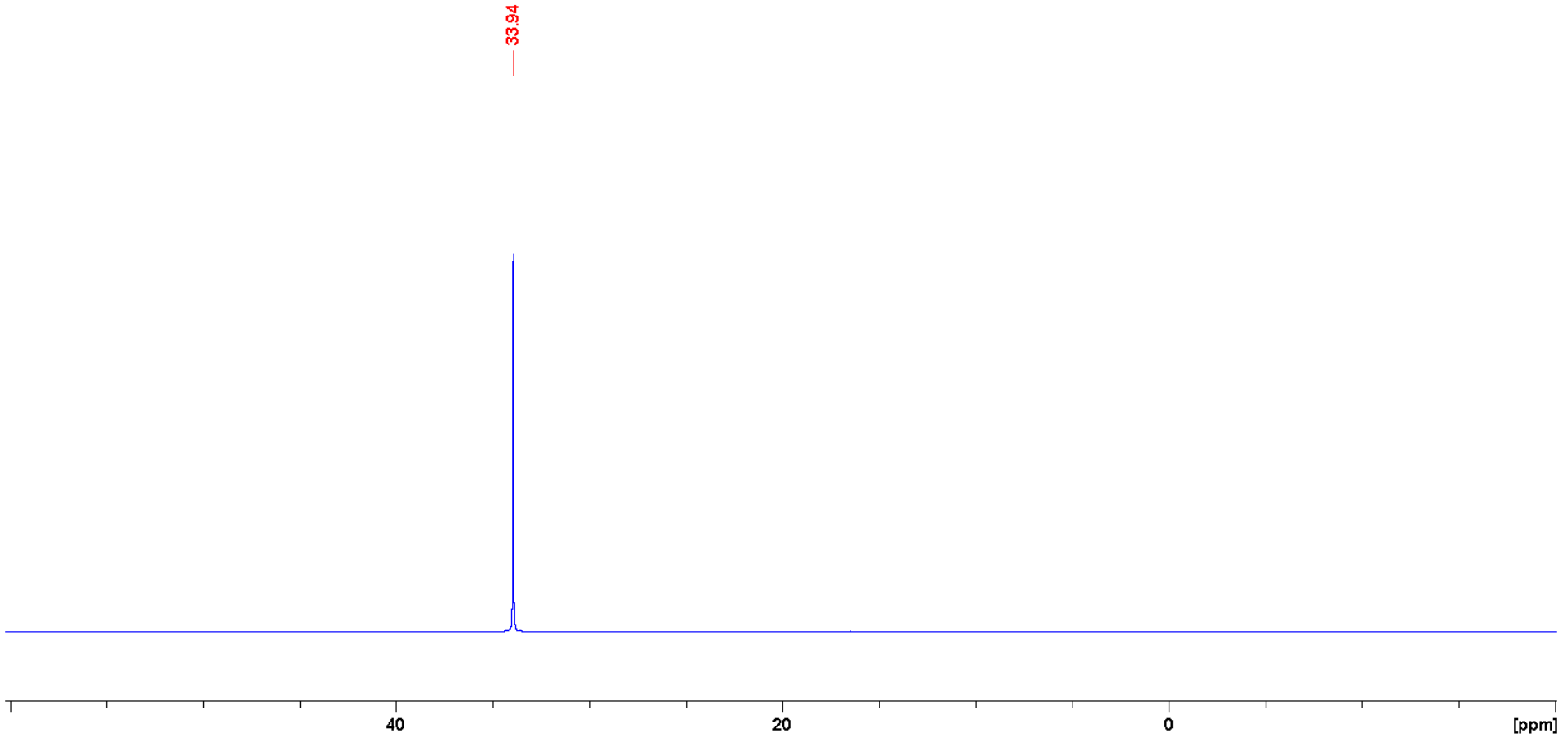



**Figure S3.** $^{31}P\{^{1}H\}$ NMR spectrum of a solution of **NTPAH$_3$** in $(CD_3)_2SO$.

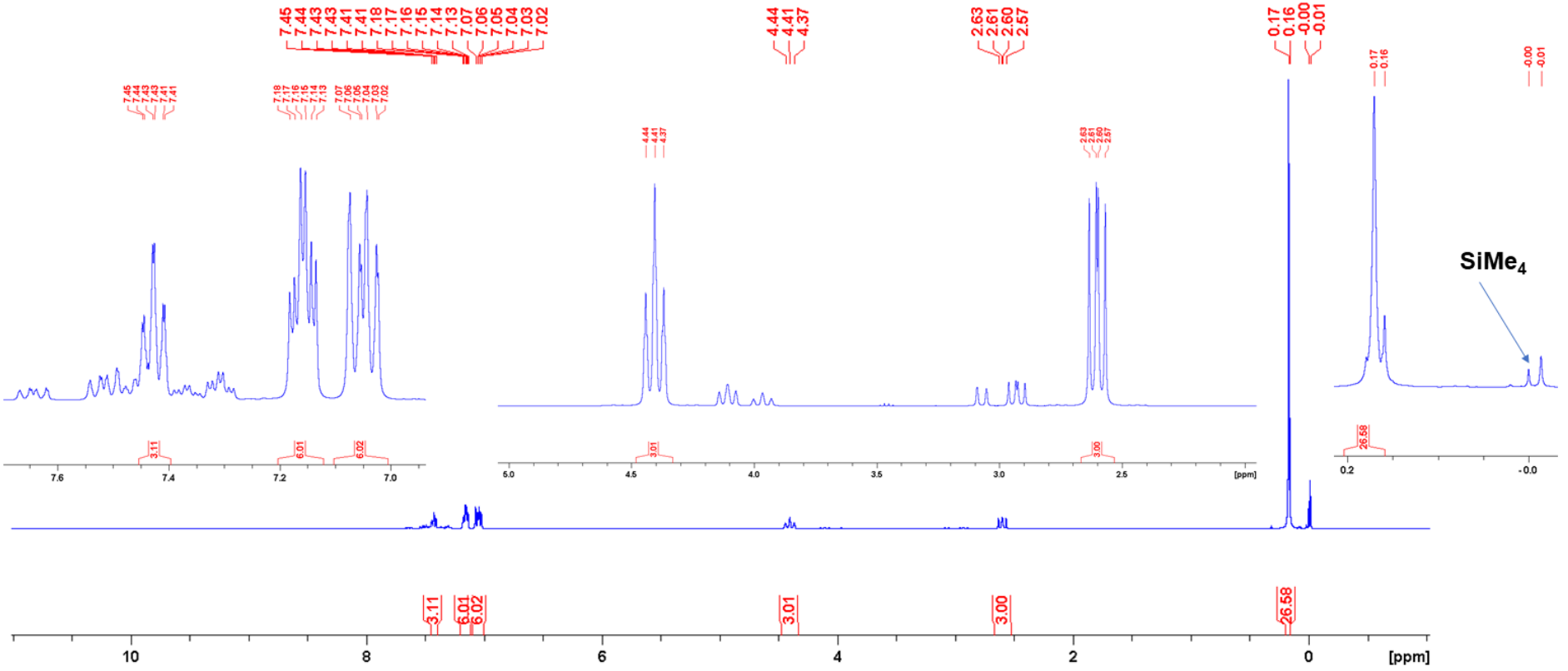



**Figure S4.** $^{1}$H NMR spectrum of a solution of **NTPA(SiMe$_3$)$_3$** in $CDCl_3$ (full spectrum and magnified insets of the aryl section, $CH_2$ section and $SiMe_3$ section of $^{1}$H signals). In the former two sections, only the shifts of the signals of the predominant isomer (RRR/SSS pair of enantiomers) are shown, and the integrals are also set for this isomer. The corresponding set of pairs of smaller signals (in relative 2:1 ratio) is assigned to the diastereomeric RRS/SSR pair of enantiomers.

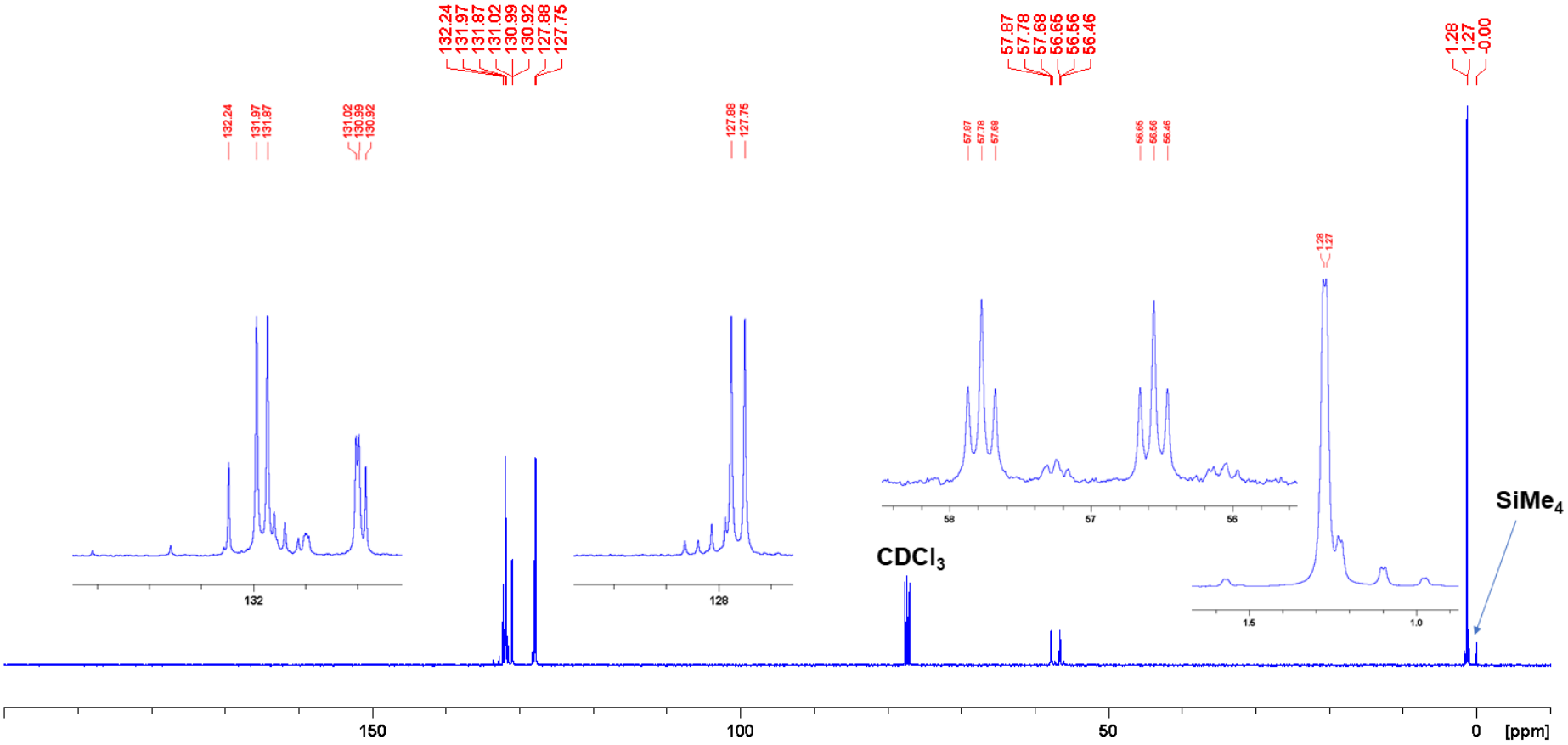



**Figure S5.** $^{13}C\{^{1}H\}$ NMR spectrum of a solution of **NTPA(SiMe$_3$)$_3$** in $CDCl_3$ (full spectrum and magnified insets of the aryl section, $CH_2$ section and $SiMe_3$ section of $^{1}H$ signals). Only the shifts of the signals of the predominant isomer (RRR/SSS pair of enantiomers) are shown. The corresponding set of smaller signals (only in part resolved, in relative 2:1 ratio) is assigned to the diastereomeric RRS/SSR pair of enantiomers.

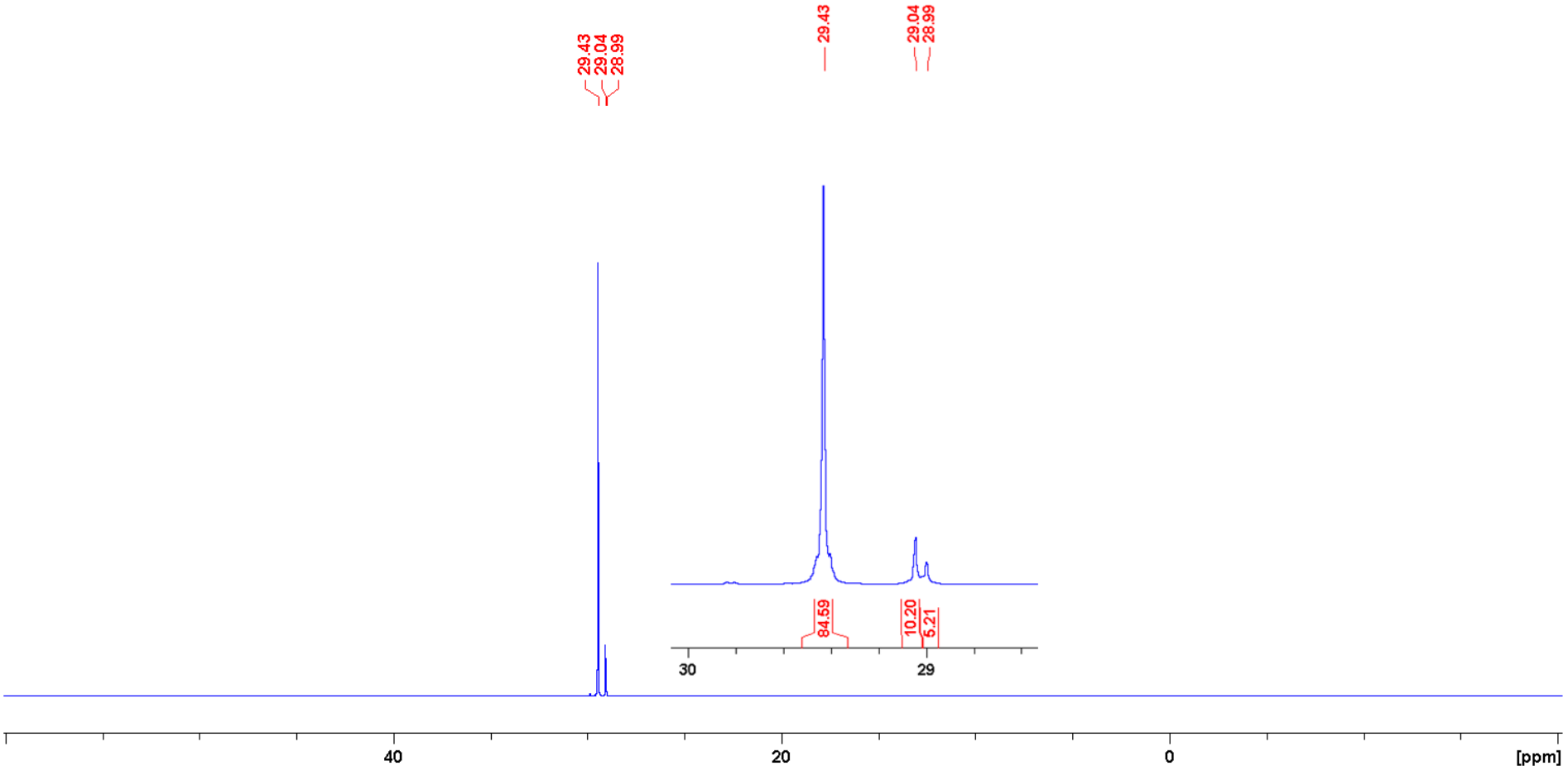



**Figure S6.** $^{31}P\{^{1}H\}$ NMR spectrum of a solution of **NTPA(SiMe$_3$)$_3$** in $CDCl_3$ (full spectrum and magnified inset). The latter is complemented by integrals, which indicate the relative 2:1 intensity ratio of the pair of smaller signals (assigned to the RRS/SSR pair of enantiomers) and the ca. 85% : 15% ratio of the diastereomeric RRR/SSS and RRS/SSR pairs of enantiomers.

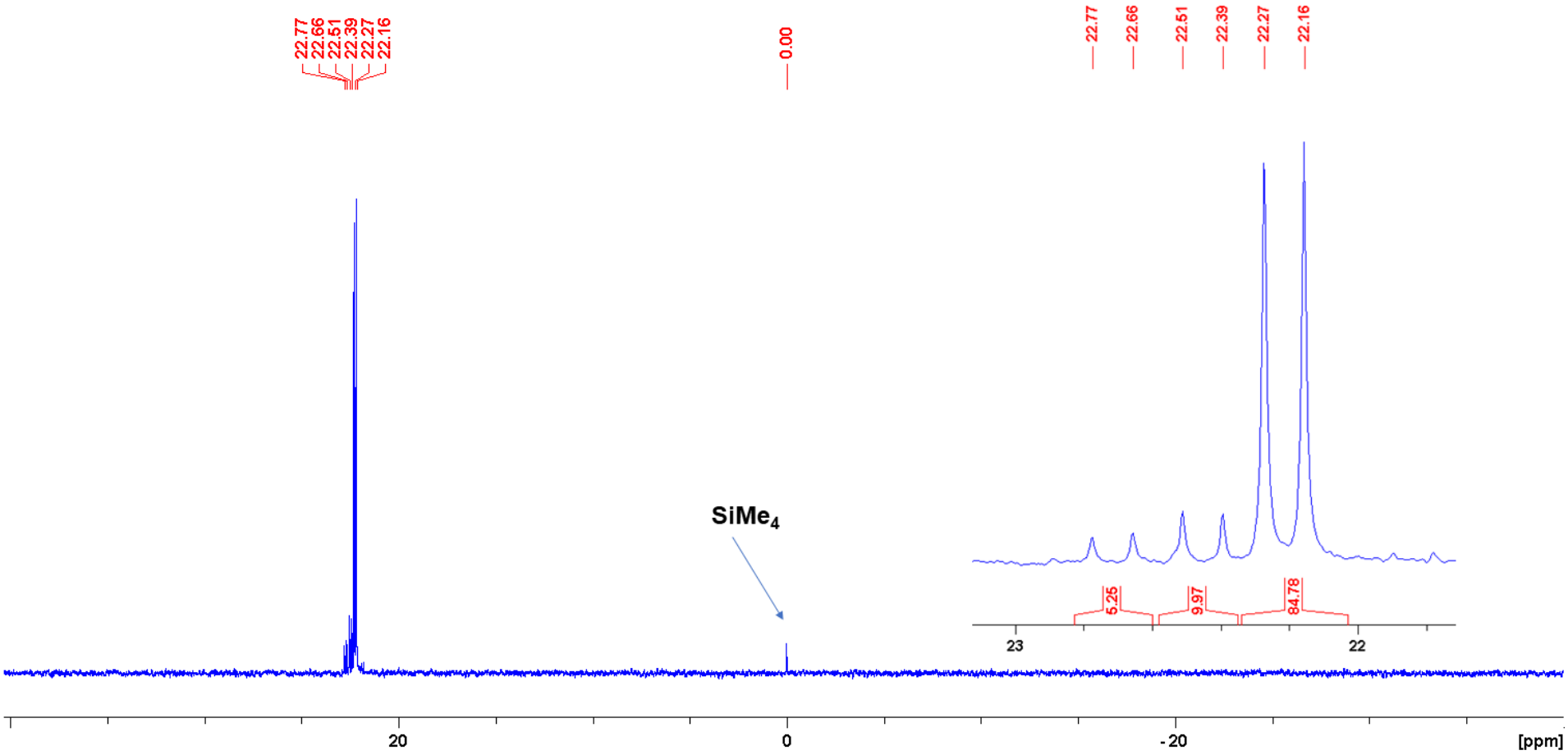



**Figure S7.** $^{29}Si\{^{1}H\}$ NMR spectrum of a solution of **NTPA(SiMe$_3$)$_3$** in $CDCl_3$ (full spectrum and magnified inset). The latter is complemented by integrals, which indicate the relative 2:1 intensity ratio of the pair of smaller signals (assigned to the RRS/SSR pair of enantiomers) and the ca. 85% : 15% ratio of the diastereomeric RRR/SSS and RRS/SSR pairs of enantiomers.

**Table S1.** $^{1}H$, $^{13}C$, $^{31}P$ and $^{29}Si$ NMR data of the main isomers (pairs of RRR and SSS pair of enantiomers) in column 1 and corresponding signals of the minor isomers (RRS and SSR pair of enantiomers) of **NTPA(SiMe$_3$)$_3$** in $CDCl_3$. The pair of minor isomers produces two sets of signals in 2:1 relative intensity ratio because of the chemically non-equivalent moieties within one molecule. Columns 2 and 3 contain the data of the bigger and the smaller signal, respectively, of each set.

| $^{1}H$ | | |
|---|---|---|
| 7.43 (tq, 7.5 Hz, 1.3 Hz) | contained in the in part superimposed multiplets in the range 7.4 – 7.7 ppm | contained in the in part superimposed multiplets in the range 7.4 – 7.7 ppm |
| 7.16 (td, 7.8 Hz, 3.6 Hz) | 7.31 (td, 7.5 Hz, 3.4 Hz) | 7.37 (td, 7.6 Hz, 3.4 Hz) |
| 7.05 (ddd, 12.2 Hz, 8.1 Hz, 1.4 Hz) | 7.52 (ddd, 12.1 Hz, 8.2 Hz, 1.4 Hz) | contained in the in part superimposed multiplets in the range 7.4 – 7.7 ppm |
| 4.41 (tt, 14.7 Hz, 2.6 Hz) | 4.11 (tt, 14.7 Hz, 2.0 Hz) | 3.97 (tt, 14.6 Hz, 2.2 Hz) |
| 2.60 (dd, 14.8 Hz, 11.4 Hz) | 2.93 (dd, 15.0 Hz, 11.5 Hz) | 3.07 (dd, 15.1 Hz, 1.6 Hz) |
| 0.17 (s) | 0.16 (s) | –0.01 (s) |
| $^{13}C$ | | |
| 131.9 (d, 10.5 Hz) | 131.8 (d, 10.4 Hz) | 131.5 (d, 10.2 Hz) |
| 131.6 (d, 132.3 Hz) | 132.1 (d, 130 Hz) | 132.9 (d, 127 Hz) |
| 131.0 (d, 2.8 Hz) | 131.5 (d, 2.6 Hz) | 131.5 (d, 2.6 Hz) |
| 127.8 (d, 13.1 Hz) | 128.0 (d, 12.9 Hz) | 128.3 (d, 12.5 Hz) |
| 57.2 (dt, 122.6 Hz, 9.8 Hz) | 56.6 (dt, not resolved) | 56.6 (dt, not resolved) |
| 1.27 (d, 1.2 Hz) | 1.23 (d, 1.2 Hz) | 1.10 (d, 1.2 Hz) |
| $^{31}P$ | | |
| 29.43 | 29.04 | 28.99 |
| $^{29}Si$ | | |
| 22.2 (d, 9.3 Hz) | 22.5 (d, 9.3 Hz) | 22.7 (d, 9.3 Hz) |

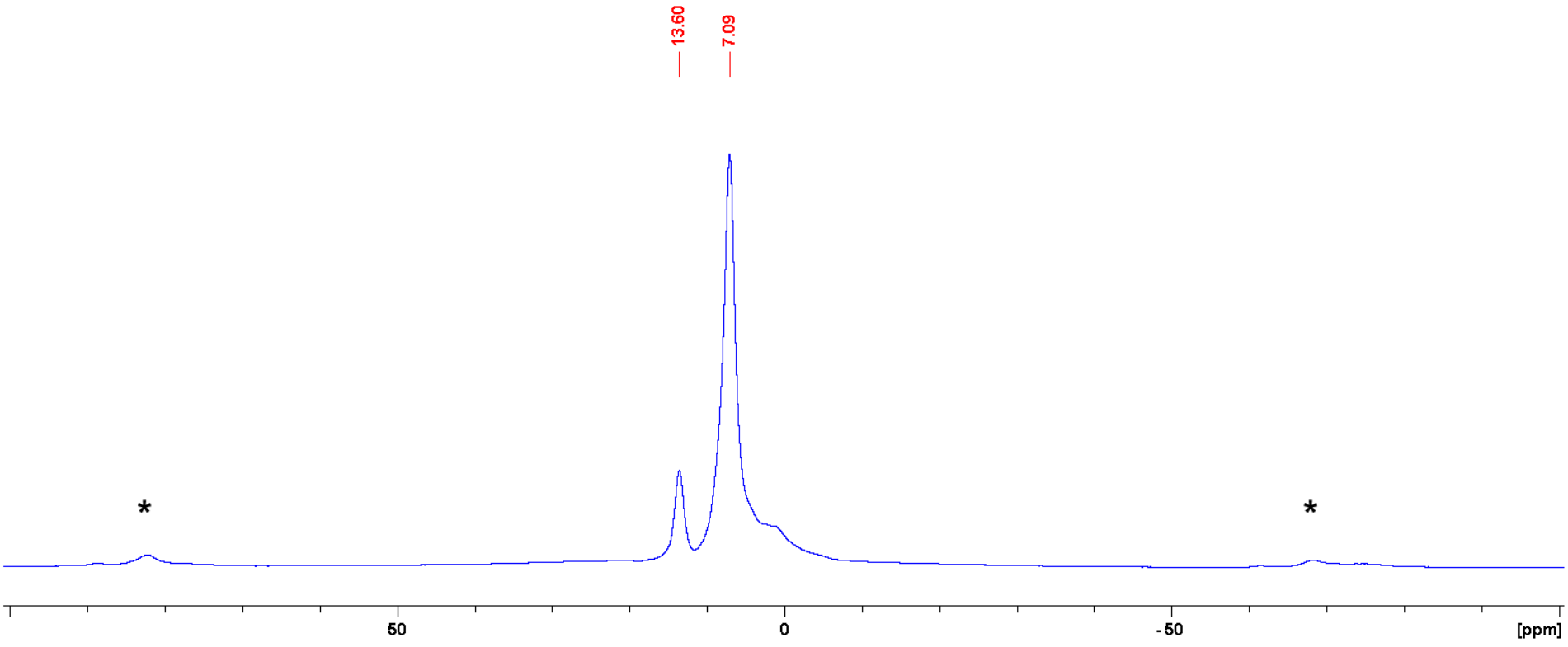



**Figure S8.** $^{1}$H MAS NMR spectrum of **NTPAH$_3^P$** recorded at an MAS frequency of 30 kHz. The spectrum is not corrected for the probe background (broad underlying signal).

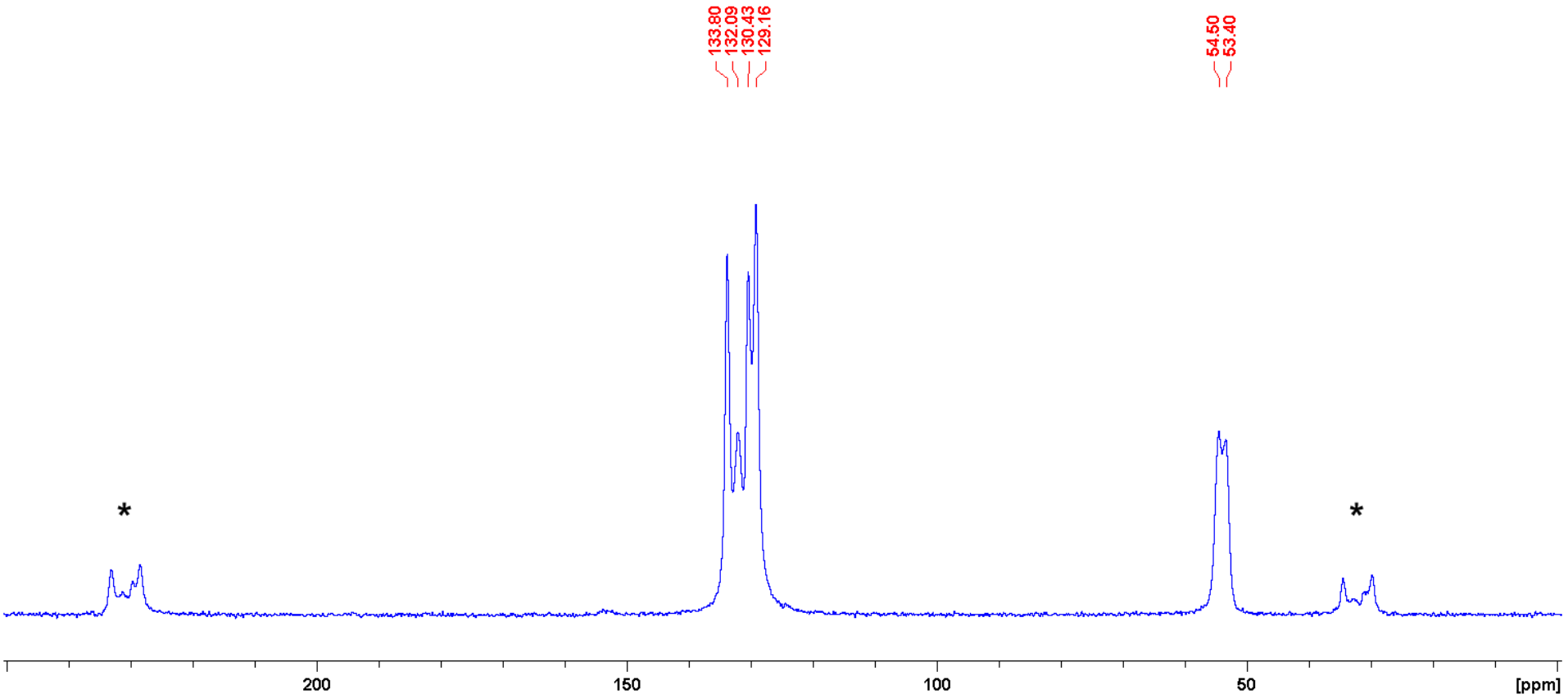



**Figure S9.** $^{13}$C CP/MAS NMR spectrum of **NTPAH$_3^P$**. (The spectrum was recorded at an MAS frequency of 10 kHz and with a CP contact time of $\tau$ = 2 ms.) The asterisks (*) indicate spinning sidebands.

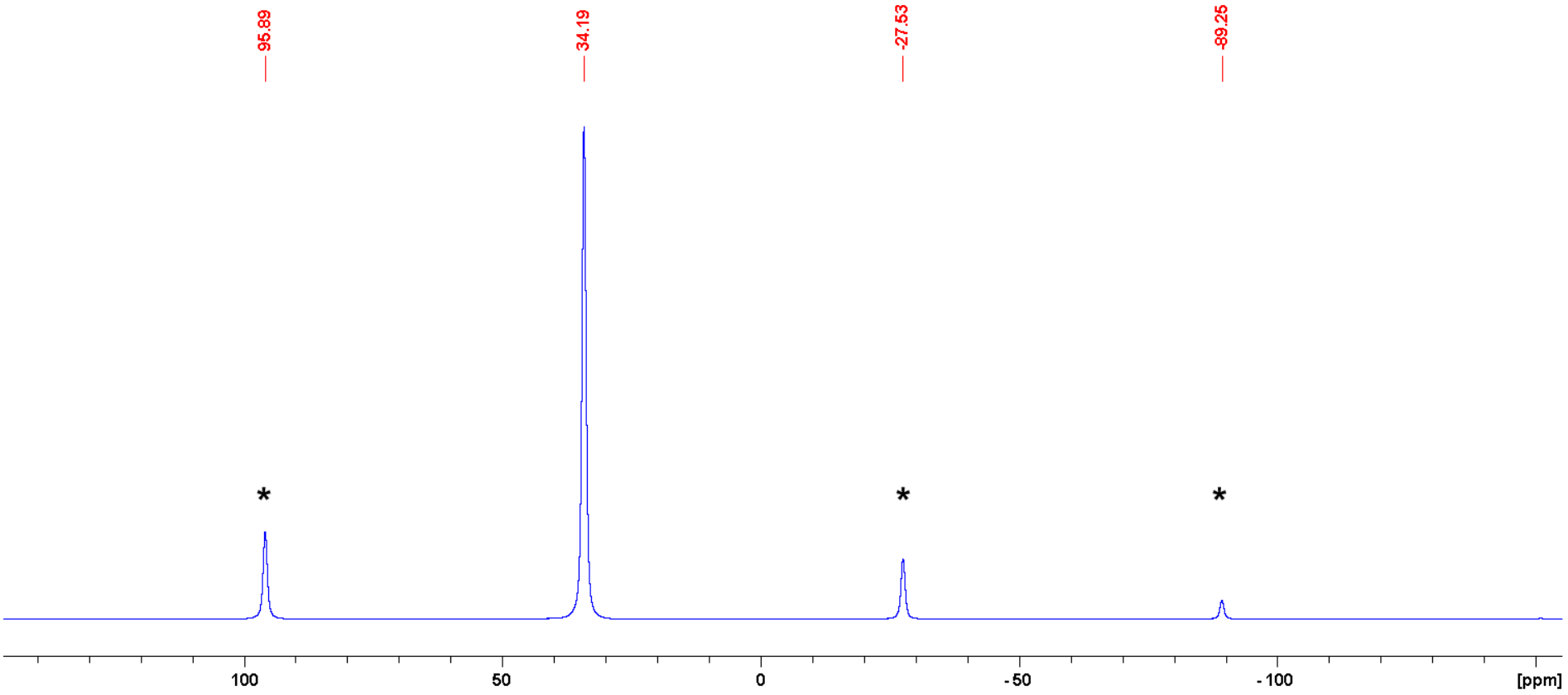



**Figure S10.** $^{31}$P CP/MAS NMR spectrum of **NTPAH$_3^P$**. (The spectrum was recorded at an MAS frequency of 10 kHz and with a CP contact time of $\tau$ = 1 ms.) The asterisks (*) indicate spinning sidebands.

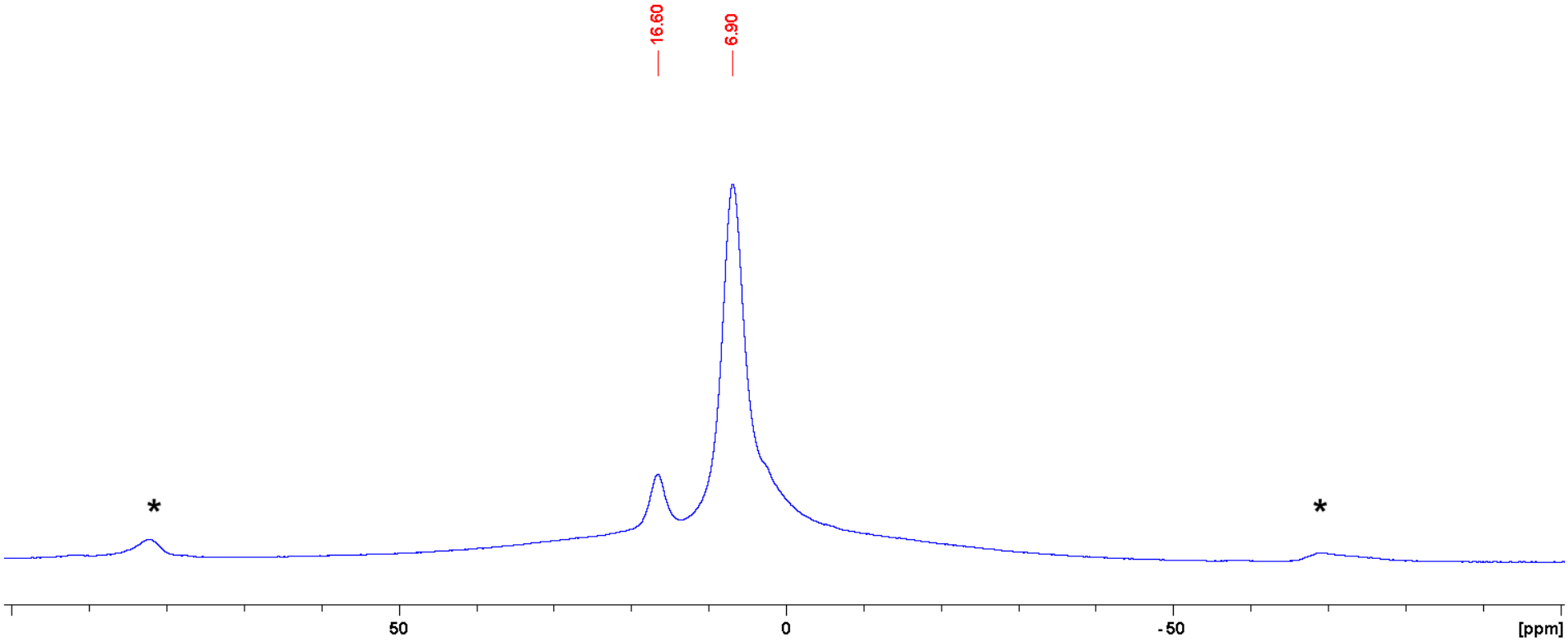



**Figure S11.** $^{1}$H MAS NMR spectrum of **NTPAH$_3^{M}$** recorded at an MAS frequency of 30 kHz. The spectrum is not corrected for the probe background (broad underlying signal).

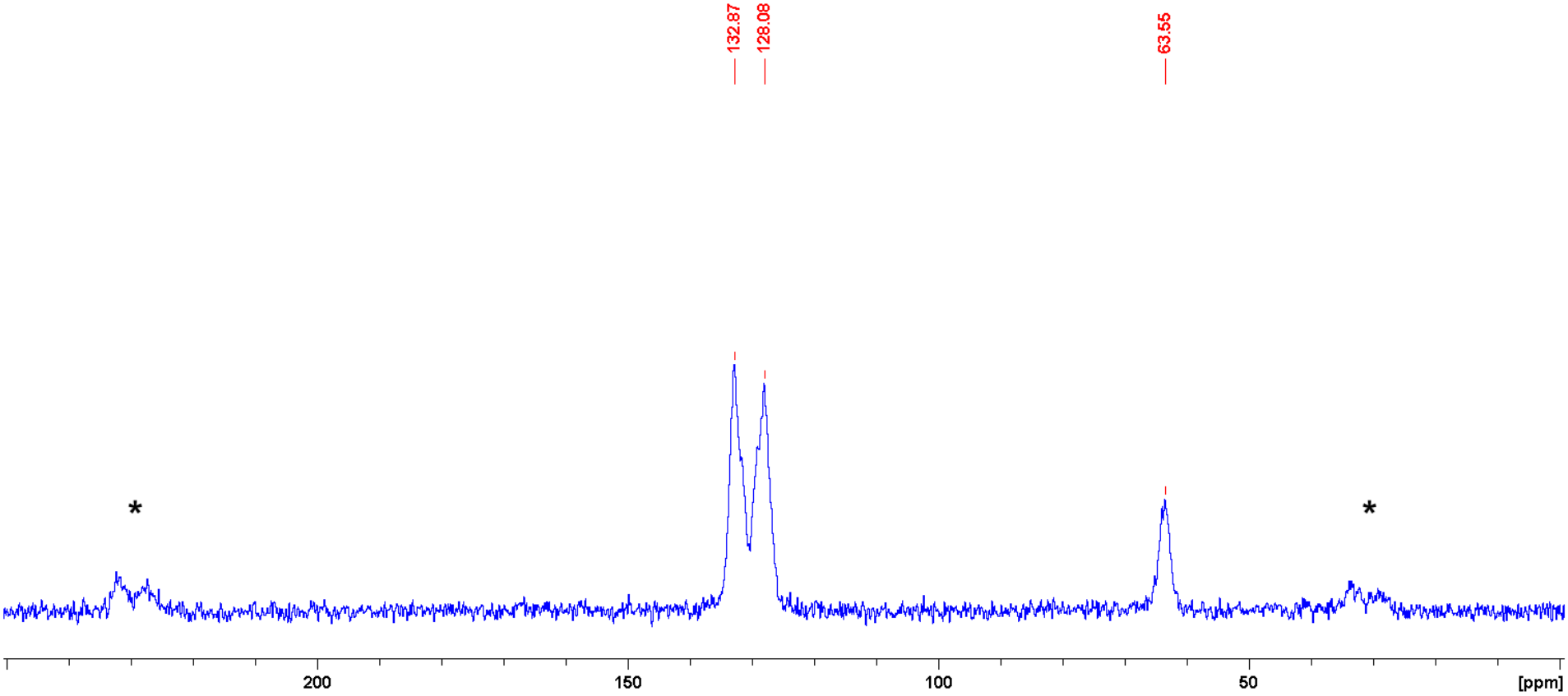



**Figure S12.** $^{13}$C CP/MAS NMR spectrum of **NTPAH$_3^M$**. (The spectrum was recorded at an MAS frequency of 10 kHz and with a CP contact time of $\tau$ = 2 ms.) The asterisks (*) indicate spinning sidebands.

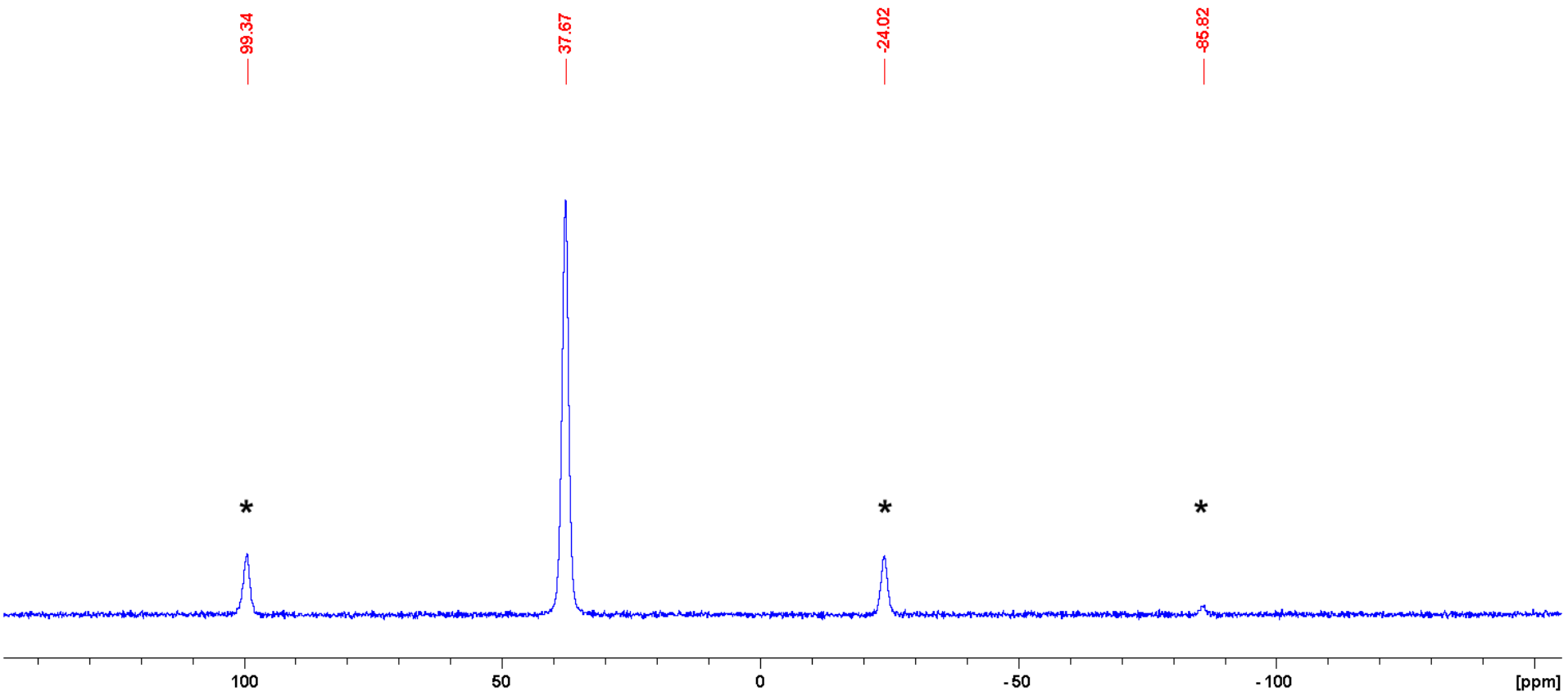



**Figure S13.** $^{31}$P CP/MAS NMR spectrum of **NTPAH$_3^M$**. (The spectrum was recorded at an MAS frequency of 10 kHz and with a CP contact time of $\tau$ = 1 ms.) The asterisks (*) indicate spinning sidebands.

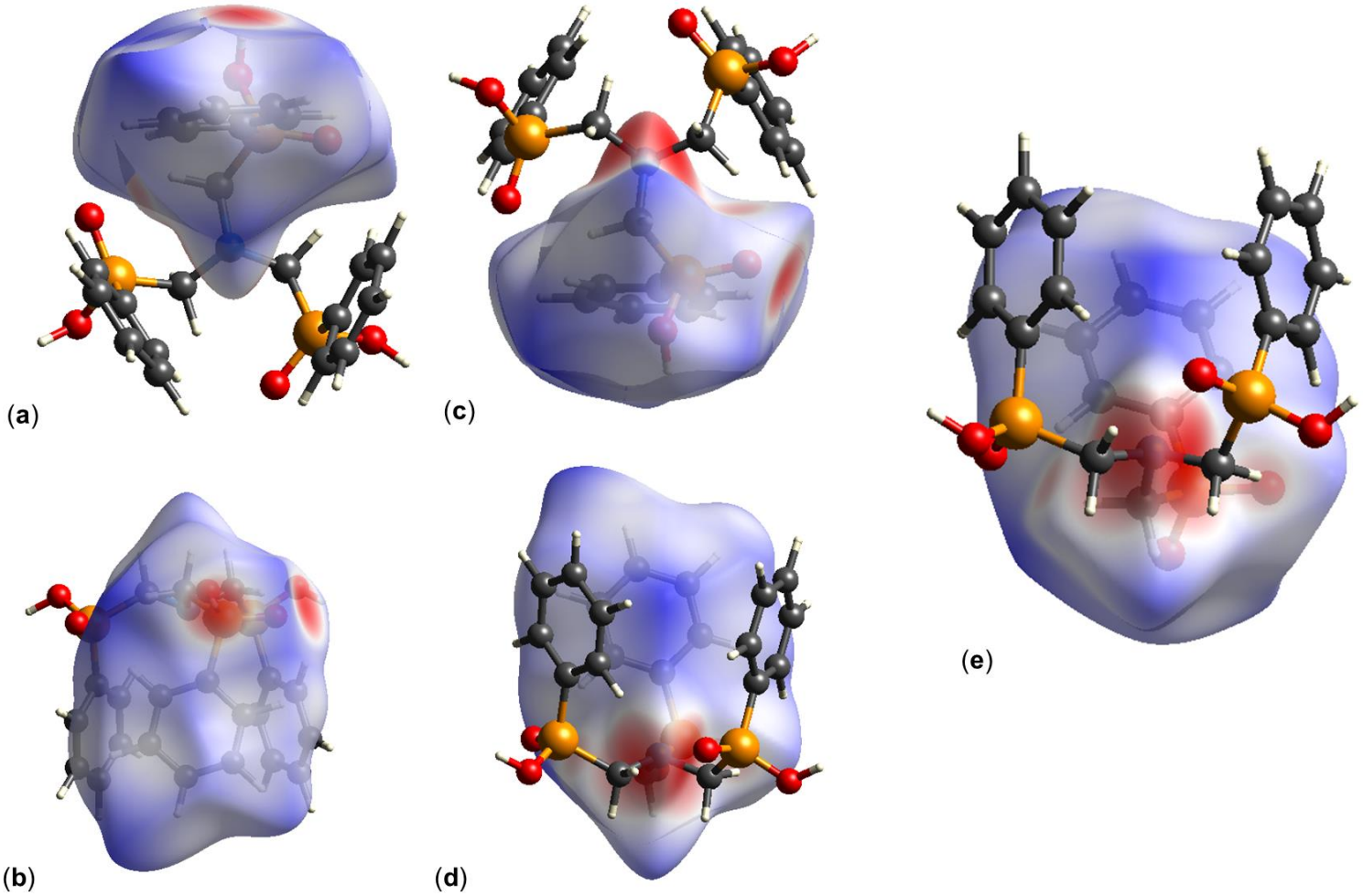



**Figure S14.** Selected views of the Hirshfeld surface analysis of the asymmetric unit of **NTPAH$_3^P$** ($d_{norm}$ isosurface). Views (**a**), (**b**), (**c**), (**d**) correspond to step-wise 90° rotation about a horizontal axis. View (**e**) shows the area of the C–N bonds to the other two symmetry equivalent parts of the molecule.

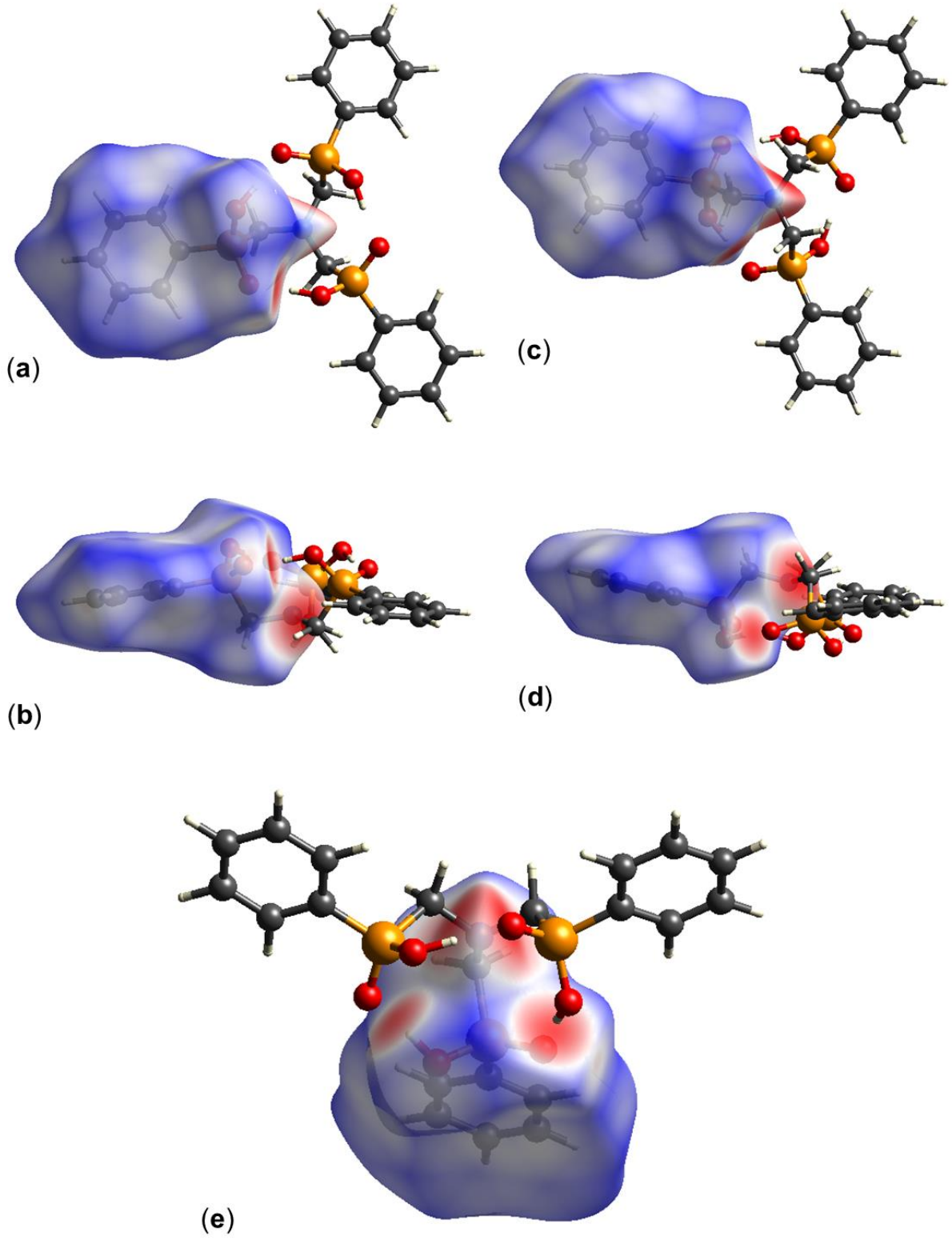



**Figure S15.** Selected views of the Hirshfeld surface analysis of the asymmetric unit of **NTPAH$_3^M$** ($d_{norm}$ isosurface). Views (**a**), (**b**), (**c**), (**d**) correspond to step-wise 90° rotation about a horizontal axis. View (**e**) shows the area of the C–N bonds to the other two symmetry equivalent parts of the molecule.

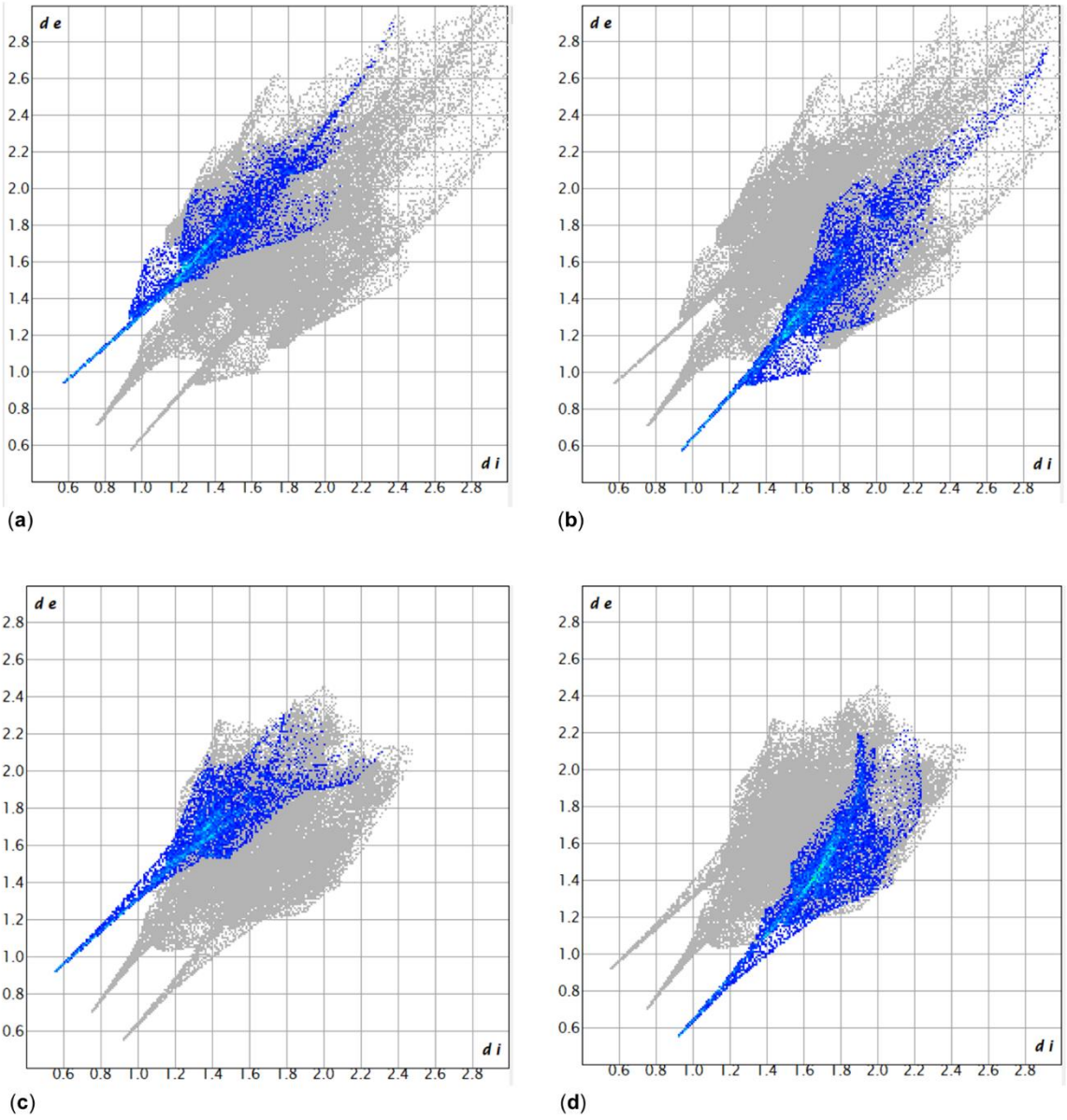



**Figure S16.** Selected Hirshfeld surface analysis fingerprint traces ($d_e$ vs. $d_i$) for H-O-contacts of the asymmetric units of **NTPAH$_3^P$** in (**a**) and (**b**), and **NTPAH$_3^M$** in (**c**) and (**d**). In (**a**) and (**c**) the H(inside)-O(outside) contacts are highlighted, O(inside)-H(outside) in (**b**) and (**d**).

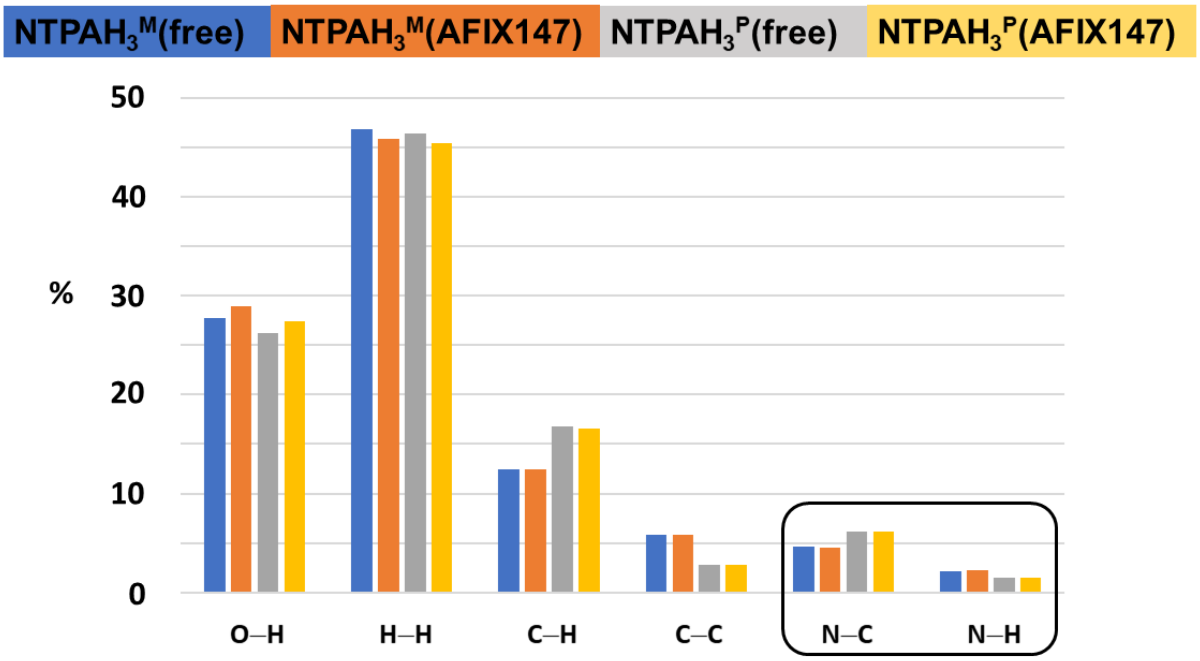



**Figure S17.** Percentages of atom contacts on the Hirshfeld surface of **NTPAH$_3^P$** and **NTPAH$_3^M$** depending on the refinement of OH groups (**free** = refinement of OH hydrogen atoms without restraints, **AFIX147** = refinement in idealized position, riding model, with ShelX code AFIX 147).

**Atomic coordinates and total energies:**

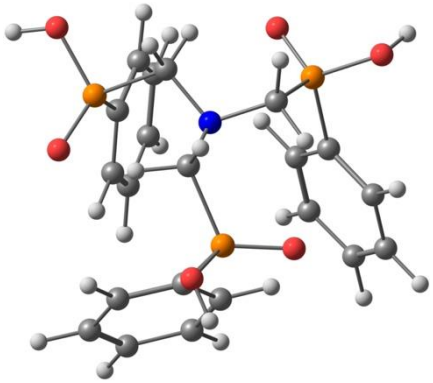


**Figure S18.** Optimized molecular structure of **NTPAH$_3^P$** (**NTPAH$_3^P$$_{OPT-1}$**).

PBE0:

final single point energy: -2348.869022402735 a.u.
final Gibbs free energy: -2348.49503933 a.u.

**Table S2.** Atomic coordinates for optimized structure of **NTPAH$_3^P$$_{OPT-1}$**.

| | | | |
|---|---|---|---|
| C | 3.76121794846030 | 1.90747597652116 | 11.68515192802194 |
| C | 3.01011413549261 | 0.74269921593217 | 11.54042611008714 |
| H | 2.75066041822339 | 0.15004625645209 | 12.40845317226296 |
| C | 2.58391711255943 | 0.34883476034499 | 10.28318617837626 |
| H | 2.00001357107682 | -0.55634819508446 | 10.17161098578147 |
| C | 2.89776234134742 | 1.11936331940007 | 9.17074324550923 |
| H | 2.56405498758526 | 0.80695843552388 | 8.18802753071916 |
| C | 3.62831366171806 | 2.28921827712551 | 9.31569897239551 |
| H | 3.86188487988831 | 2.89900940959178 | 8.45164198652148 |
| C | 4.06217694170913 | 2.68395414188158 | 10.57123172107125 |
| H | 4.64017775163166 | 3.58957930641568 | 10.69988211400675 |
| P | 4.38320655918548 | 2.42524871869237 | 13.28774933573494 |
| O | 5.41993227146868 | 3.47039005342716 | 13.18044318245078 |
| O | 4.84269280980758 | 1.07235060190016 | 14.02542133688974 |
| H | 5.68716561929447 | 0.75304106994126 | 13.69576666685333 |
| C | 2.97019598518887 | 2.82099565037409 | 14.34520038861737 |
| H | 3.31295724390479 | 2.83414462432819 | 15.39221932929502 |
| H | 2.25187759063108 | 2.00572735175152 | 14.23275170727540 |
| N | 2.34505310021956 | 4.06378532496751 | 13.93642126751137 |
| C | 0.95661346122032 | 4.14494767147377 | 14.34584928579682 |
| H | 0.79741832695325 | 3.84501721747469 | 15.39397511561714 |
| H | 0.60919116378094 | 5.17410252213565 | 14.23005993885015 |
| C | 3.10947423156408 | 5.22786349698306 | 14.33981131922823 |
| H | 2.92985013539447 | 5.52086681740475 | 15.38659284338203 |
| H | 4.17447947756879 | 5.01380805863898 | 14.22455320287413 |
| P | -0.09258979882508 | 3.11516609784340 | 13.29208719441564 |
| C | -0.23345762677129 | 3.90923941582650 | 11.68808156894788 |
| C | -0.86194211518994 | 5.14436313998784 | 11.54258553774898 |
| H | -1.23942972499341 | 5.66965318796185 | 12.41064582443218 |
| C | -0.99243271193828 | 5.70756713666456 | 10.28437309574760 |
| H | -1.48043338260526 | 6.66778631325232 | 10.17221608672217 |
| C | -0.48930819989708 | 5.04539513621167 | 9.17163149761459 |
| H | -0.59481774236474 | 5.48857123428752 | 8.18819794557598 |
| C | 0.15347809925262 | 3.82518034492588 | 9.31721071020373 |
| H | 0.55898831097789 | 3.31390535323487 | 8.45282504244157 |
| C | 0.28095942970993 | 3.25492117268569 | 10.57378199223291 |
| H | 0.77285201084696 | 2.29982455726019 | 10.70327871531074 |
| O | 0.29557679042393 | 1.69501842819368 | 13.18598083787001 |
| O | -1.49297157574816 | 3.39339314140178 | 14.03206750258044 |
| H | -2.19145647431104 | 2.81977258888956 | 13.70519868036946 |
| P | 2.74085838659887 | 6.64616025490394 | 13.27916407007065 |
| C | 3.50078502396642 | 6.36543341348651 | 11.67695744394579 |
| C | 4.88497798513249 | 6.29709829970763 | 11.53189615787576 |
| H | 5.52828078706719 | 6.36826821387360 | 12.39972006471699 |
| C | 5.43880271757242 | 6.12545301871687 | 10.27442195024824 |
| H | 6.51463611068810 | 6.07223253599791 | 10.16248989317153 |
| C | 4.61427055584994 | 6.01262090068034 | 9.16209773404325 |
| H | 5.05144441239735 | 5.88016587962601 | 8.17923343502491 |
| C | 3.23588287366688 | 6.06053306117070 | 9.30743358110554 |
| H | 2.59074317197851 | 5.95828431644289 | 8.44349750908096 |
| C | 2.67750591726006 | 6.23850561306697 | 10.56317814007713 |
| H | 1.60423767967724 | 6.28624179411203 | 10.69246183852779 |
| O | 1.31640828741993 | 7.01740281814203 | 13.17008913868394 |
| O | 3.67877265035352 | 7.72549850941291 | 14.01473016083245 |
| H | 3.52768242592906 | 8.61549303843447 | 13.68480178525067 |

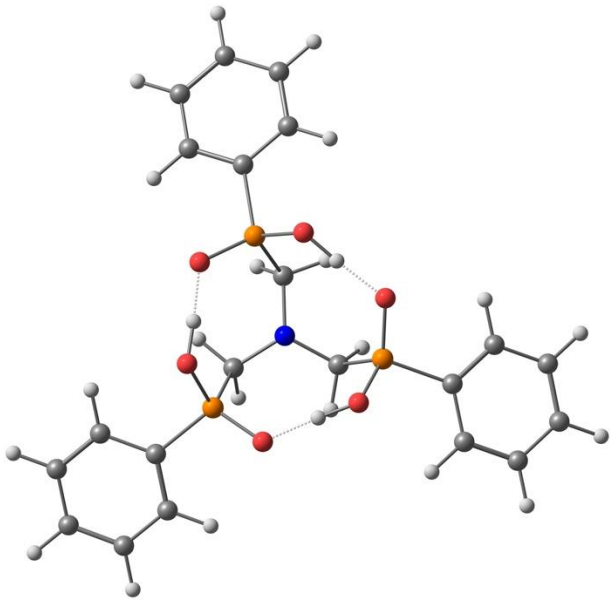


**Figure S19.** Optimized molecular structure of **NTPAH$_3^M$** (**NTPAH$_3^M$$_{OPT-1}$**).

PBE0:

final single point energy: -2348.900548358977 a.u.
final Gibbs free energy: -2348.52785692 a.u.

**Table S3.** Atomic coordinates for optimized structure of **NTPAH$_3^{M}$$_{OPT-1}$**.

| | | | |
|---|---|---|---|
| H | 0.98831318344109 | -4.60615290538773 | 0.26587278334104 |
| C | 2.01195743722759 | -4.45973091200257 | -0.05713036603967 |
| C | 2.76978478232884 | -5.53212752957144 | -0.49854041221812 |
| H | 2.33404145339421 | -6.52304204591401 | -0.53492351186580 |
| C | 4.08906213262498 | -5.33762567083341 | -0.88283425652546 |
| H | 4.68124006836767 | -6.17828026961394 | -1.22403822448184 |
| C | 4.65528819143750 | -4.07222221438131 | -0.82185197353873 |
| H | 5.68871540092302 | -3.92542600786301 | -1.11107658429634 |
| C | 3.90071007772713 | -2.99663713672845 | -0.38216659745271 |
| H | 4.33404075612577 | -2.00650479744592 | -0.31098367630782 |
| C | 2.57517321908463 | -3.18718603073305 | -0.00035890851860 |
| P | 1.59093039865609 | -1.77840148976859 | 0.49438857724339 |
| O | 2.47520466014086 | -0.65967037315976 | 0.94625732788739 |
| O | 0.55733546381517 | -2.31792668921029 | 1.51972897418322 |
| H | -0.42486456312344 | -2.05388899802423 | 1.36266445207726 |
| C | 0.63347068612570 | -1.25337394409861 | -0.97269739174954 |
| H | 1.30598916370579 | -1.20862230611849 | -1.84038109013986 |
| H | -0.11547980879534 | -2.02126306907218 | -1.17519387449106 |
| N | -0.01502143590573 | 0.01009753835281 | -0.71114900506883 |
| C | 0.75561708442017 | 1.20394502130843 | -0.96894611076611 |
| H | 0.37873913589607 | 1.76970202099843 | -1.83201185019495 |
| H | 1.79413190645077 | 0.93876370951417 | -1.17585413564515 |
| C | -1.43504914455803 | 0.07923737876759 | -0.96559813445082 |
| H | -1.73831079503089 | -0.54340865653663 | -1.81814549570968 |
| H | -1.72476226645921 | 1.10778023431325 | -1.18910084762741 |
| P | 0.73709925194713 | 2.28782297974544 | 0.50370475820191 |
| O | -0.67341690635493 | 2.51925934030192 | 0.94421452179132 |
| O | 1.69584002554829 | 1.63711830955664 | 1.53734947461326 |
| H | 1.99250789032994 | 0.67048114101197 | 1.34686149556287 |
| C | 1.49704614996934 | 3.83432117825708 | 0.02490037657169 |
| C | 0.69283583375316 | 4.90437954335895 | -0.35881051529871 |
| H | -0.38403669915229 | 4.80359931157605 | -0.30065298217309 |
| C | 1.27346733516060 | 6.08851978676253 | -0.78339810225326 |
| C | 2.88372769289873 | 3.95817880886035 | -0.01474883165072 |
| H | 3.50389899520866 | 3.13124899637714 | 0.30975824521770 |
| H | 0.64790508439546 | 6.92366617570956 | -1.07385619308133 |
| P | -2.36116415325225 | -0.45592064211833 | 0.51894638861765 |
| O | -1.82018003639701 | -1.76150477659782 | 1.00755055355148 |
| O | -2.32635317862948 | 0.73848618267311 | 1.51027677205406 |
| H | -1.61663710193196 | 1.46229443010543 | 1.33251934807677 |
| C | -4.07262056537229 | -0.63871579248432 | 0.03263405957760 |
| C | -4.55592725939549 | -1.89858919197798 | -0.31124806601840 |
| H | -3.90397284078400 | -2.75838867572752 | -0.21688202668404 |
| C | -5.86461505941366 | -2.04348697277594 | -0.74236552501860 |
| C | -4.90756902590747 | 0.47267523518824 | -0.05319094452430 |
| H | -4.53381169382620 | 1.44600928557242 | 0.24093433387372 |
| H | -6.24291274079613 | -3.02474698420770 | -1.00161580386857 |
| C | 2.65542115864725 | 6.20632141541557 | -0.82734487064983 |
| H | 3.10803649238999 | 7.13400243034260 | -1.15648867036256 |
| C | -6.69178217054668 | -0.93298576288875 | -0.83272970403394 |
| H | -7.71584425529621 | -1.04826927556457 | -1.16710503572439 |
| C | 3.46004010779306 | 5.14358341080228 | -0.44110899375571 |
| H | 4.53837266256534 | 5.24249778247587 | -0.46397507007347 |
| C | -6.21506404896920 | 0.32343274138650 | -0.48618865099479 |
| H | -6.86654813260214 | 1.18667473407223 | -0.54521450418808 |

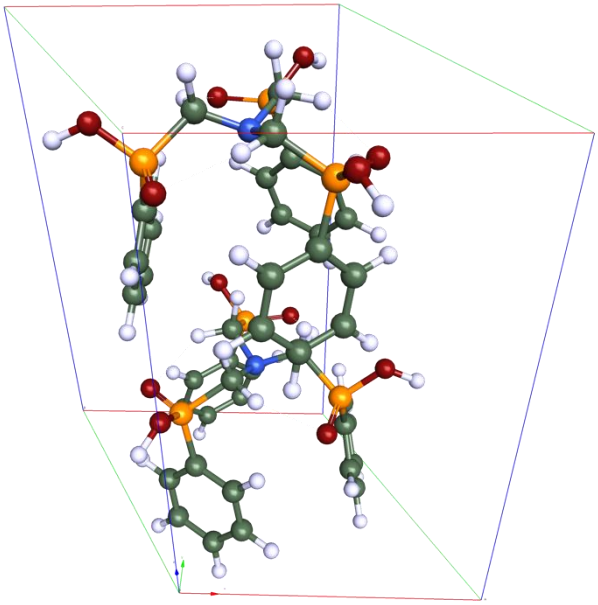


**Figure S20.** Optimized crystal structure of **NTPAH$_3^P$** (**NTPAH$_3^P$$_{OPT\text{-}CRYST}$**, perspective view of the optimized unit cell with the two molecules of **NTPAH$_3^P$** contained therein).

PBE:

final single point energy: -4686.9847106362 a.u.

PBE0:

final single point energy: -4687.2802116227 a.u.

cell parameters: a = 17.72411936 Å, b = 17.72411936 Å, c = 29.58347365 Å,
$\alpha$ = 90°, $\beta$ = 90°, $\gamma$ = 120°,

**Table S4.** Atomic coordinates for optimized structure of **NTPAH$_3^P$$_{OPT\text{-}CRYST}$**.

| | | | |
|---|---|---|---|
| C | 4.098292000 | 1.819955000 | 11.702242000 |
| C | 2.933794000 | 1.111634000 | 11.381782000 |
| H | 2.202300000 | 0.854348000 | 12.150590000 |
| C | 2.699909000 | 0.737469000 | 10.061236000 |
| H | 1.792254000 | 0.183242000 | 9.814250000 |
| C | 3.638039000 | 1.035771000 | 9.071364000 |
| H | 3.475625000 | 0.703416000 | 8.044672000 |
| C | 4.798240000 | 1.743067000 | 9.390337000 |
| H | 5.531487000 | 1.983475000 | 8.617323000 |
| C | 5.021637000 | 2.153657000 | 10.701286000 |
| H | 5.926294000 | 2.708104000 | 10.956885000 |
| P | 4.475537000 | 2.307591000 | 13.405021000 |
| O | 5.554515000 | 3.431963000 | 13.362106000 |
| O | 4.854890000 | 1.025694000 | 14.297403000 |
| H | 5.374108000 | 0.205843000 | 13.867271000 |
| C | 2.968223000 | 2.826138000 | 14.305909000 |
| H | 3.248970000 | 2.890678000 | 15.378504000 |
| H | 2.249030000 | 2.003400000 | 14.203317000 |
| N | 2.346118000 | 4.063071000 | 13.805316000 |

| | | | |
|---|---|---|---|
| C | 0.961149000 | 4.148027000 | 14.298354000 |
| H | 0.870550000 | 3.891460000 | 15.375082000 |
| H | 0.607745000 | 5.179963000 | 14.174826000 |
| C | 3.110284000 | 5.221361000 | 14.297063000 |
| H | 2.931320000 | 5.428821000 | 15.373294000 |
| H | 4.181033000 | 5.012507000 | 14.175566000 |
| P | -0.238273000 | 3.092070000 | 13.405400000 |
| C | -0.473761000 | 3.656837000 | 11.700612000 |
| C | -0.502510000 | 5.017888000 | 11.373099000 |
| H | -0.359711000 | 5.784878000 | 12.137038000 |
| C | -0.707508000 | 5.400613000 | 10.050226000 |
| H | -0.732051000 | 6.462483000 | 9.797332000 |
| C | -0.919508000 | 4.433832000 | 9.065653000 |
| H | -1.124101000 | 4.735777000 | 8.037171000 |
| C | -0.891077000 | 3.077097000 | 9.391949000 |
| H | -1.054023000 | 2.318773000 | 8.623096000 |
| C | -0.647773000 | 2.685321000 | 10.704983000 |
| H | -0.622189000 | 1.626404000 | 10.967289000 |
| O | 0.200485000 | 1.596751000 | 13.366864000 |
| O | -1.539241000 | 3.403832000 | 14.296576000 |
| H | -2.509178000 | 3.362611000 | 13.866318000 |
| P | 2.797340000 | 6.787360000 | 13.404140000 |
| C | 3.403304000 | 6.708546000 | 11.699428000 |
| C | 4.599174000 | 6.057110000 | 11.373170000 |
| H | 5.194541000 | 5.554233000 | 12.138083000 |
| C | 5.032645000 | 6.042469000 | 10.050173000 |
| H | 5.966980000 | 5.537251000 | 9.797479000 |
| C | 4.298221000 | 6.704245000 | 9.064364000 |
| H | 4.661339000 | 6.729846000 | 8.035756000 |
| C | 3.105708000 | 7.352484000 | 9.389332000 |
| H | 2.526829000 | 7.867782000 | 8.619740000 |
| C | 2.645258000 | 7.338704000 | 10.702453000 |
| H | 1.712284000 | 7.841173000 | 10.963863000 |
| O | 1.283290000 | 7.154588000 | 13.366908000 |
| O | 3.719228000 | 7.755172000 | 14.296802000 |
| H | 4.171641000 | 8.615444000 | 13.868908000 |
| C | 1.721393000 | 2.826136000 | 6.478424000 |
| H | 1.440649000 | 2.890714000 | 7.551005000 |
| H | 2.440578000 | 2.003408000 | 6.375833000 |
| N | 2.343481000 | 4.063069000 | 5.977826000 |
| C | 3.728439000 | 4.148042000 | 6.470868000 |
| H | 3.819007000 | 3.891458000 | 7.547584000 |
| H | 4.081842000 | 5.179965000 | 6.347342000 |
| C | 1.579307000 | 5.221345000 | 6.469577000 |
| H | 1.758304000 | 5.428784000 | 7.545795000 |
| H | 0.508574000 | 5.012493000 | 6.348086000 |
| P | 4.927863000 | 3.092102000 | 5.577944000 |
| O | 4.489155000 | 1.596789000 | 5.539408000 |
| O | 6.228835000 | 3.403879000 | 6.469096000 |

| | | | |
|---|---|---|---|
| H | 7.198740000 | 3.362639000 | 6.038892000 |
| C | 5.163386000 | 3.656817000 | 3.873184000 |
| C | 5.192099000 | 5.017882000 | 3.545640000 |
| H | 5.049287000 | 5.784886000 | 4.309539000 |
| C | 5.397085000 | 5.400625000 | 2.222786000 |
| H | 5.421657000 | 6.462490000 | 1.969841000 |
| C | 5.609113000 | 4.433871000 | 1.238174000 |
| H | 5.813723000 | 4.735786000 | 0.209701000 |
| C | 5.580672000 | 3.077086000 | 1.564497000 |
| H | 5.743652000 | 2.318790000 | 0.795603000 |
| C | 5.337383000 | 2.685355000 | 2.877525000 |
| H | 5.311799000 | 1.626398000 | 3.139786000 |
| P | 0.214102000 | 2.307566000 | 5.577565000 |
| C | 0.591306000 | 1.819932000 | 3.874823000 |
| C | 1.755787000 | 1.111661000 | 3.554328000 |
| H | 2.487325000 | 0.854361000 | 4.323087000 |
| C | 1.989749000 | 0.737468000 | 2.233805000 |
| H | 2.897339000 | 0.183238000 | 1.986757000 |
| C | 1.051557000 | 1.035765000 | 1.243873000 |
| H | 1.213976000 | 0.703390000 | 0.217198000 |
| C | -0.108614000 | 1.743065000 | 1.562896000 |
| H | -0.841896000 | 1.983446000 | 0.789817000 |
| C | -0.332024000 | 2.153635000 | 2.873813000 |
| H | -1.236700000 | 2.708099000 | 3.129384000 |
| O | -0.864910000 | 3.431909000 | 5.534647000 |
| O | -0.165246000 | 1.025674000 | 6.469917000 |
| H | -0.684461000 | 0.205864000 | 6.039850000 |
| P | 1.892224000 | 6.787340000 | 5.576686000 |
| C | 1.286300000 | 6.708576000 | 3.871996000 |
| C | 0.090447000 | 6.057102000 | 3.545727000 |
| H | -0.504940000 | 5.554203000 | 4.310579000 |
| C | -0.343041000 | 6.042448000 | 2.222705000 |
| H | -1.277396000 | 5.537248000 | 1.969984000 |
| C | 0.391344000 | 6.704223000 | 1.236909000 |
| H | 0.028242000 | 6.729860000 | 0.208275000 |
| C | 1.583897000 | 7.352487000 | 1.561842000 |
| H | 2.162740000 | 7.867794000 | 0.792253000 |
| C | 2.044320000 | 7.338692000 | 2.875026000 |
| H | 2.977309000 | 7.841178000 | 3.136355000 |
| O | 3.406256000 | 7.154603000 | 5.539447000 |
| O | 0.970332000 | 7.755146000 | 6.469312000 |
| H | 0.517950000 | 8.615393000 | 6.041484000 |

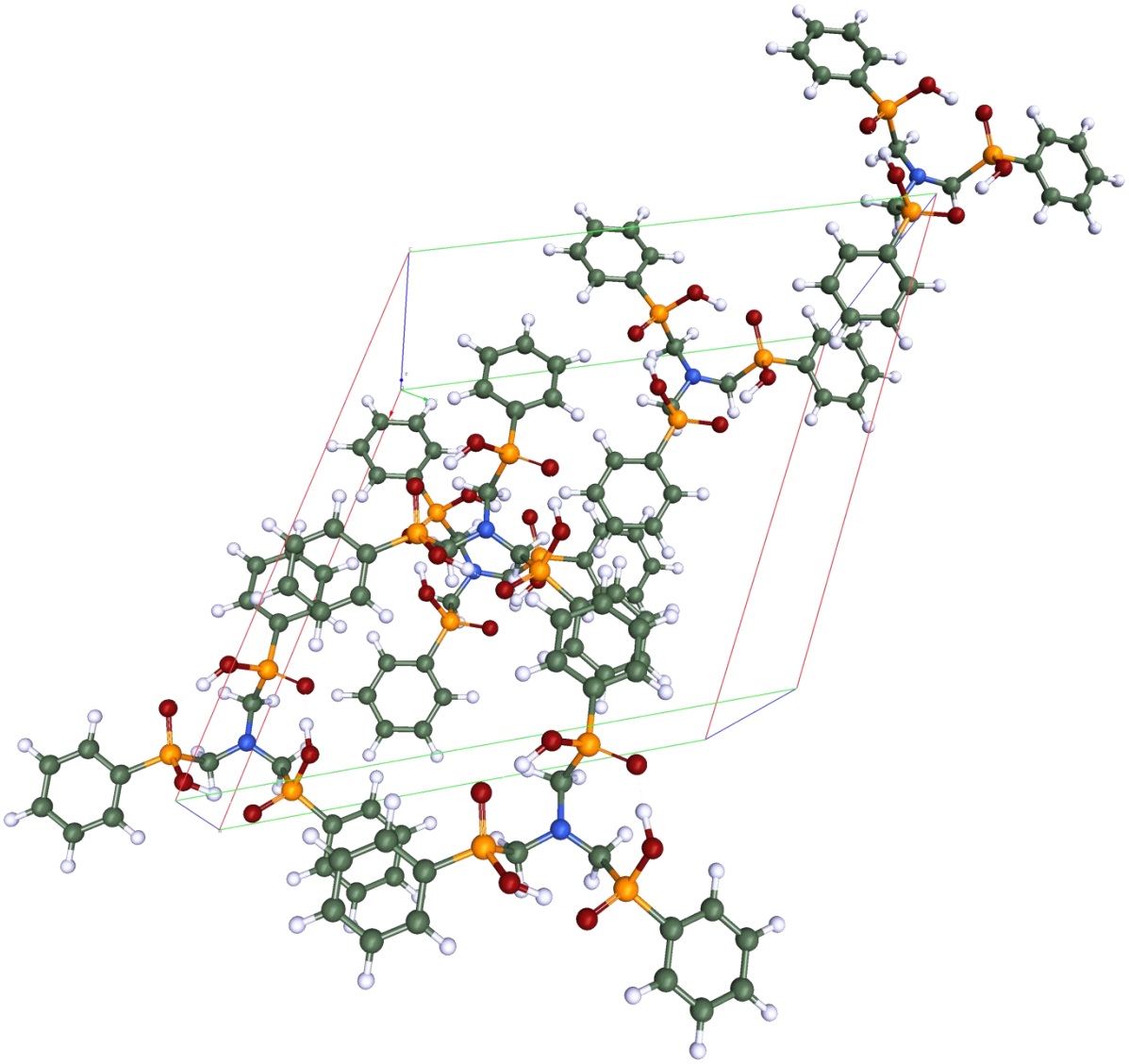


**Figure S21.** Optimized crystal structure of **NTPAH$_3^M$** (**NTPAH$_3^M$$_{OPT\text{-}CRYST}$**, perspective view of the optimized unit cell with the six molecules of **NTPAH$_3^M$** contained therein).

PBE:

final single point energy: -14060.9508473912 a.u.

PBE0:

final single point energy: -14061.8247619937 a.u.

cell parameters: a = 34.49770647 Å, b = 34.49770647 Å, c = 21.57632608 Å,
$\alpha = 90°$, $\beta = 90°$, $\gamma = 120°$,

**Table S5.** Atomic coordinates for optimized structure of **NTPAH$_3^M$$_{OPT\text{-}CRYST}$**.

| | | | |
|---|---|---|---|
| H | 0.867323000 | 7.929940000 | 4.798729000 |
| C | 1.585120000 | 8.753794000 | 4.771426000 |
| C | 2.930672000 | 8.490810000 | 4.543311000 |
| H | 3.255327000 | 7.467334000 | 4.356679000 |
| C | 3.853255000 | 9.536230000 | 4.512565000 |
| H | 4.906833000 | 9.327127000 | 4.315128000 |
| C | 3.437526000 | 10.850000000 | 4.723668000 |
| H | 4.166823000 | 11.661373000 | 4.702512000 |

| | | | |
|---|---|---|---|
| C | 2.094038000 | 11.123593000 | 4.958784000 |
| H | 1.755373000 | 12.145279000 | 5.133497000 |
| C | 1.167400000 | 10.074767000 | 4.982169000 |
| P | -0.568283000 | 10.406867000 | 5.344407000 |
| O | -0.726249000 | 11.871648000 | 5.851827000 |
| O | -1.006589000 | 9.270588000 | 6.397489000 |
| H | -1.887927000 | 8.715595000 | 6.145770000 |
| C | -1.638014000 | 10.144746000 | 3.848063000 |
| H | -1.204663000 | 10.691864000 | 2.995656000 |
| H | -1.603559000 | 9.076130000 | 3.595971000 |
| N | -3.014192000 | 10.545308000 | 4.120692000 |
| C | -3.352853000 | 11.941304000 | 3.867811000 |
| H | -4.041262000 | 12.059219000 | 3.015910000 |
| H | -2.442397000 | 12.505836000 | 3.624511000 |
| C | -4.052204000 | 9.556089000 | 3.852089000 |
| H | -3.806710000 | 8.914608000 | 2.990842000 |
| H | -4.998421000 | 10.061855000 | 3.615557000 |
| P | -4.107638000 | 12.726240000 | 5.373720000 |
| O | -5.283750000 | 11.845336000 | 5.892256000 |
| O | -2.896907000 | 12.926629000 | 6.415262000 |
| H | -1.983139000 | 12.424866000 | 6.164919000 |
| C | -4.699288000 | 14.389850000 | 5.005104000 |
| C | -6.072578000 | 14.656205000 | 4.961966000 |
| H | -6.782952000 | 13.847935000 | 5.138751000 |
| C | -6.514879000 | 15.949130000 | 4.701996000 |
| C | -3.769731000 | 15.415839000 | 4.787866000 |
| H | -2.696234000 | 15.214099000 | 4.829554000 |
| H | -7.583540000 | 16.166260000 | 4.664076000 |
| P | -4.342681000 | 8.487701000 | 5.344273000 |
| O | -2.989139000 | 7.891414000 | 5.834337000 |
| O | -5.099392000 | 9.426425000 | 6.411490000 |
| H | -5.126022000 | 10.471080000 | 6.176728000 |
| C | -5.500560000 | 7.153047000 | 4.980360000 |
| C | -5.056752000 | 5.825988000 | 4.953234000 |
| H | -4.003531000 | 5.606877000 | 5.132245000 |
| C | -5.965419000 | 4.801594000 | 4.707901000 |
| C | -6.852348000 | 7.454510000 | 4.765348000 |
| H | -7.205930000 | 8.488181000 | 4.796802000 |
| H | -5.628562000 | 3.764015000 | 4.681458000 |
| C | -5.590755000 | 16.970160000 | 4.485580000 |
| H | -5.941605000 | 17.981703000 | 4.269646000 |
| C | -7.309598000 | 5.100958000 | 4.491940000 |
| H | -8.016553000 | 4.294336000 | 4.285497000 |
| C | -4.222339000 | 16.705722000 | 4.534579000 |
| H | -3.503411000 | 17.501993000 | 4.341233000 |
| C | -7.753028000 | 6.422668000 | 4.527562000 |
| H | -8.800636000 | 6.654305000 | 4.335940000 |
| C | -6.197090000 | 13.760635000 | 8.349320000 |
| H | -5.872364000 | 12.737062000 | 8.162647000 |
| C | -5.274534000 | 14.806035000 | 8.318368000 |
| H | -4.220846000 | 14.596935000 | 8.120991000 |
| C | -7.542543000 | 14.023676000 | 8.577322000 |
| H | -8.260399000 | 13.199771000 | 8.604721000 |
| C | -7.960366000 | 15.344641000 | 8.788024000 |
| P | -9.696036000 | 15.676730000 | 9.150261000 |
| O | -10.134229000 | 14.540330000 | 10.203487000 |

| | | | |
|---|---|---|---|
| H | -11.015668000 | 13.985430000 | 9.951554000 |
| C | -10.765806000 | 15.414592000 | 7.653844000 |
| H | -10.731257000 | 14.345880000 | 7.401857000 |
| H | -10.332309000 | 15.961827000 | 6.801465000 |
| C | -5.690177000 | 16.119842000 | 8.529479000 |
| H | -4.960820000 | 16.931299000 | 8.508238000 |
| C | -7.033639000 | 16.393441000 | 8.764630000 |
| H | -7.372363000 | 17.415146000 | 8.939265000 |
| N | -12.141919000 | 15.815276000 | 7.926821000 |
| C | -12.480574000 | 17.211248000 | 7.673639000 |
| H | -13.169069000 | 17.329110000 | 6.821724000 |
| H | -11.570038000 | 17.775721000 | 7.430422000 |
| C | -13.179870000 | 14.826057000 | 7.657843000 |
| H | -12.934435000 | 14.184391000 | 6.796590000 |
| H | -14.126224000 | 15.331779000 | 7.421482000 |
| O | -9.853920000 | 17.141552000 | 9.657773000 |
| P | -13.470418000 | 13.757605000 | 9.150126000 |
| O | -12.116749000 | 13.161154000 | 9.640200000 |
| O | -14.227184000 | 14.696263000 | 10.217517000 |
| H | -14.253653000 | 15.740939000 | 9.982582000 |
| C | -14.628265000 | 12.422844000 | 8.786158000 |
| C | -14.184525000 | 11.095704000 | 8.759146000 |
| H | -13.131332000 | 10.876755000 | 8.938090000 |
| C | -15.093197000 | 10.071422000 | 8.513794000 |
| H | -14.756359000 | 9.033979000 | 8.487363000 |
| C | -16.437283000 | 10.370753000 | 8.297826000 |
| H | -17.144249000 | 9.564331000 | 8.091489000 |
| C | -16.880828000 | 11.692528000 | 8.333532000 |
| H | -17.928398000 | 11.924221000 | 8.141887000 |
| C | -15.980004000 | 12.724333000 | 8.571257000 |
| H | -16.333670000 | 13.758124000 | 8.602700000 |
| P | -13.235237000 | 17.996063000 | 9.179632000 |
| O | -14.411532000 | 17.115211000 | 9.698243000 |
| O | -12.024504000 | 18.196616000 | 10.221222000 |
| H | -11.110880000 | 17.694748000 | 9.970804000 |
| C | -13.826964000 | 19.659698000 | 8.810955000 |
| C | -15.200309000 | 19.926169000 | 8.767894000 |
| H | -15.910689000 | 19.117741000 | 8.944638000 |
| C | -15.642527000 | 21.219121000 | 8.507841000 |
| H | -16.711233000 | 21.436115000 | 8.469915000 |
| C | -14.718395000 | 22.240042000 | 8.291394000 |
| H | -15.069266000 | 23.251462000 | 8.075553000 |
| C | -13.350012000 | 21.975622000 | 8.340557000 |
| H | -12.631183000 | 22.771802000 | 8.147182000 |
| C | -12.897483000 | 20.685727000 | 8.593791000 |
| H | -11.823966000 | 20.484009000 | 8.635489000 |
| C | 3.055140000 | 9.386367000 | 1.156046000 |
| H | 2.344719000 | 8.578088000 | 1.332805000 |
| C | 2.612856000 | 10.679321000 | 0.896047000 |
| H | 1.544237000 | 10.896436000 | 0.858074000 |
| C | 3.537029000 | 11.700278000 | 0.679534000 |
| H | 3.186117000 | 12.711849000 | 0.463710000 |
| C | 4.905353000 | 11.435789000 | 0.728755000 |
| H | 5.624215000 | 12.232090000 | 0.535368000 |
| C | 5.357898000 | 10.145975000 | 0.981960000 |
| H | 6.431443000 | 9.944285000 | 1.023689000 |

| | | | |
|---|---|---|---|
| C | 4.428417000 | 9.120044000 | 1.199244000 |
| P | 5.020086000 | 7.456392000 | 1.567728000 |
| O | 3.844009000 | 6.575649000 | 2.086395000 |
| O | 6.230855000 | 7.656744000 | 2.609322000 |
| H | 7.144490000 | 7.155029000 | 2.359005000 |
| C | 5.774848000 | 6.671485000 | 0.061825000 |
| H | 6.685269000 | 7.235968000 | -0.181372000 |
| N | 6.113470000 | 5.275528000 | 0.315029000 |
| C | 5.075581000 | 4.286339000 | 0.046033000 |
| H | 4.129237000 | 4.791938000 | -0.190316000 |
| C | 7.489553000 | 4.874880000 | 0.042004000 |
| H | 7.524208000 | 3.806118000 | -0.209923000 |
| H | 5.320938000 | 3.644605000 | -0.815132000 |
| H | 7.923139000 | 5.422003000 | -0.810259000 |
| H | 5.086403000 | 6.789392000 | -0.789963000 |
| P | 4.784980000 | 3.217968000 | 1.538308000 |
| O | 6.138557000 | 2.621415000 | 2.028504000 |
| O | 4.028243000 | 4.156622000 | 2.605692000 |
| H | 4.001718000 | 5.201167000 | 2.370758000 |
| C | 3.627174000 | 1.883085000 | 1.174477000 |
| C | 4.070896000 | 0.555996000 | 1.147315000 |
| H | 5.124185000 | 0.336958000 | 1.326371000 |
| C | 2.275377000 | 2.184606000 | 0.959447000 |
| H | 1.921707000 | 3.218367000 | 0.990896000 |
| C | 1.374601000 | 1.152775000 | 0.721674000 |
| H | 0.326954000 | 1.384404000 | 0.530023000 |
| P | 8.559448000 | 5.137055000 | 1.538423000 |
| O | 8.401559000 | 6.601764000 | 2.045964000 |
| O | 8.121190000 | 4.000709000 | 2.591732000 |
| H | 7.239699000 | 3.445706000 | 2.339768000 |
| C | 10.295177000 | 4.805016000 | 1.176291000 |
| C | 11.221822000 | 5.853805000 | 1.152813000 |
| H | 10.883128000 | 6.875375000 | 1.327476000 |
| C | 10.712799000 | 3.484006000 | 0.965573000 |
| H | 9.994961000 | 2.659927000 | 0.992913000 |
| C | 12.058405000 | 3.220898000 | 0.737478000 |
| H | 12.383101000 | 2.197331000 | 0.550833000 |
| C | 1.818041000 | -0.169030000 | 0.685979000 |
| H | 1.111135000 | -0.975519000 | 0.479611000 |
| C | 3.162269000 | -0.468418000 | 0.902018000 |
| H | 3.499062000 | -1.505884000 | 0.875565000 |
| C | 12.980967000 | 4.266492000 | 0.706572000 |
| H | 14.034637000 | 4.057197000 | 0.509195000 |
| C | 12.565216000 | 5.580154000 | 0.917714000 |
| H | 13.294548000 | 6.391450000 | 0.896462000 |
| H | 8.076262000 | 1.121661000 | 2.799383000 |
| C | 8.805616000 | 0.310200000 | 2.820625000 |
| C | 10.149085000 | 0.583796000 | 3.055779000 |
| H | 10.487809000 | 1.605512000 | 3.230412000 |
| C | 8.389981000 | -1.003612000 | 2.609516000 |
| H | 7.336287000 | -1.212706000 | 2.412138000 |
| C | 9.312532000 | -2.049003000 | 2.640471000 |
| H | 8.987807000 | -3.072577000 | 2.453799000 |
| C | 10.657984000 | -1.785967000 | 2.868471000 |
| H | 11.375840000 | -2.609869000 | 2.895873000 |
| C | 11.075808000 | -0.465003000 | 3.079173000 |

| | | | |
|---|---|---|---|
| P | 12.811479000 | -0.132914000 | 3.441411000 |
| O | 12.969362000 | 1.331912000 | 3.948923000 |
| O | 13.249672000 | -1.269311000 | 4.494636000 |
| H | 14.131109000 | -1.824211000 | 4.242704000 |
| C | 13.881248000 | -0.395049000 | 1.944994000 |
| H | 13.447752000 | 0.152187000 | 1.092614000 |
| N | 15.257362000 | 0.005633000 | 2.217971000 |
| H | 13.846700000 | -1.463759000 | 1.693007000 |
| C | 15.596015000 | 1.401604000 | 1.964787000 |
| H | 16.284513000 | 1.519470000 | 1.112874000 |
| H | 14.685480000 | 1.966082000 | 1.721572000 |
| C | 16.295314000 | -0.983585000 | 1.948994000 |
| H | 16.049877000 | -1.625248000 | 1.087741000 |
| H | 17.241667000 | -0.477862000 | 1.712632000 |
| P | 16.585860000 | -2.052035000 | 3.441276000 |
| O | 15.232194000 | -2.648487000 | 3.931349000 |
| O | 17.342625000 | -1.113378000 | 4.508666000 |
| H | 17.369096000 | -0.068703000 | 4.273732000 |
| C | 17.743702000 | -3.386794000 | 3.077309000 |
| C | 17.299966000 | -4.713933000 | 3.050297000 |
| H | 16.246776000 | -4.932886000 | 3.229241000 |
| C | 18.208635000 | -5.738222000 | 2.804946000 |
| H | 17.871802000 | -6.775662000 | 2.778514000 |
| C | 19.552730000 | -5.438888000 | 2.588974000 |
| H | 20.259693000 | -6.245312000 | 2.382639000 |
| C | 19.996267000 | -4.117112000 | 2.624682000 |
| H | 21.043846000 | -3.885418000 | 2.433035000 |
| C | 19.095447000 | -3.085304000 | 2.862407000 |
| H | 19.449113000 | -2.051516000 | 2.893849000 |
| P | 16.350683000 | 2.186422000 | 3.470782000 |
| O | 17.526976000 | 1.305568000 | 3.989393000 |
| O | 15.139947000 | 2.386977000 | 4.512374000 |
| H | 14.226321000 | 1.885106000 | 4.261954000 |
| C | 16.942405000 | 3.850060000 | 3.102104000 |
| C | 18.315763000 | 4.116535000 | 3.059045000 |
| H | 19.026127000 | 3.308105000 | 3.235791000 |
| C | 18.757960000 | 5.409477000 | 2.798995000 |
| H | 19.826674000 | 5.626476000 | 2.761071000 |
| C | 17.833852000 | 6.430401000 | 2.582547000 |
| H | 18.184705000 | 7.441815000 | 2.366707000 |
| C | 16.465448000 | 6.165983000 | 2.631705000 |
| H | 15.746628000 | 6.962159000 | 2.438332000 |
| C | 16.012933000 | 4.876088000 | 2.884941000 |
| H | 14.939406000 | 4.674366000 | 2.926637000 |
| C | 10.868542000 | 1.152771000 | 6.430523000 |
| H | 11.916190000 | 1.384404000 | 6.238869000 |
| C | 9.967766000 | 2.184609000 | 6.668298000 |
| H | 10.321437000 | 3.218372000 | 6.699744000 |
| C | 8.615963000 | 1.883083000 | 6.883326000 |
| C | 8.172242000 | 0.555991000 | 6.856167000 |
| H | 7.118956000 | 0.336956000 | 7.035224000 |
| P | 7.458159000 | 3.217969000 | 7.247161000 |
| O | 6.104582000 | 2.621414000 | 7.737355000 |
| O | 8.214900000 | 4.156620000 | 8.314545000 |
| H | 8.241424000 | 5.201169000 | 8.079607000 |
| C | 7.167562000 | 4.286337000 | 5.754884000 |

| | | | |
|---|---|---|---|
| H | 6.922204000 | 3.644604000 | 4.893718000 |
| H | 8.113907000 | 4.791939000 | 5.518535000 |
| N | 6.129671000 | 5.275526000 | 6.023878000 |
| C | 6.468293000 | 6.671481000 | 5.770673000 |
| H | 7.156740000 | 6.789391000 | 4.918887000 |
| H | 5.557873000 | 7.235969000 | 5.527476000 |
| C | 4.753587000 | 4.874880000 | 5.750856000 |
| H | 4.320004000 | 5.422001000 | 4.898591000 |
| H | 4.718935000 | 3.806121000 | 5.498928000 |
| P | 7.223062000 | 7.456388000 | 7.276580000 |
| O | 8.399134000 | 6.575647000 | 7.795247000 |
| O | 6.012285000 | 7.656746000 | 8.318174000 |
| H | 5.098649000 | 7.155028000 | 8.067853000 |
| C | 7.814723000 | 9.120050000 | 6.908092000 |
| C | 9.188007000 | 9.386363000 | 6.864898000 |
| H | 9.898424000 | 8.578086000 | 7.041656000 |
| C | 6.885247000 | 10.145976000 | 6.690810000 |
| H | 5.811698000 | 9.944284000 | 6.732538000 |
| C | 7.337790000 | 11.435792000 | 6.437603000 |
| H | 6.618929000 | 12.232087000 | 6.244219000 |
| P | 3.683692000 | 5.137048000 | 7.247269000 |
| O | 3.841581000 | 6.601760000 | 7.754811000 |
| O | 4.121954000 | 4.000711000 | 8.300576000 |
| H | 5.003439000 | 3.445708000 | 8.048621000 |
| C | 1.947968000 | 4.805014000 | 6.885143000 |
| C | 1.021321000 | 5.853797000 | 6.861660000 |
| H | 1.360014000 | 6.875371000 | 7.036322000 |
| C | -0.322068000 | 5.580153000 | 6.626562000 |
| H | -1.051409000 | 6.391452000 | 6.605309000 |
| C | -0.737824000 | 4.266490000 | 6.415422000 |
| H | -1.791492000 | 4.057196000 | 6.218045000 |
| C | 0.184742000 | 3.220894000 | 6.446330000 |
| H | -0.139960000 | 2.197332000 | 6.259685000 |
| C | 1.530343000 | 3.484010000 | 6.674422000 |
| H | 2.248175000 | 2.659932000 | 6.701764000 |
| C | 8.706113000 | 11.700273000 | 6.388387000 |
| H | 9.057026000 | 12.711849000 | 6.172559000 |
| C | 9.630285000 | 10.679326000 | 6.604896000 |
| H | 10.698905000 | 10.896434000 | 6.566925000 |
| C | 10.425102000 | -0.169035000 | 6.394827000 |
| H | 11.132009000 | -0.975522000 | 6.188462000 |
| C | 9.080874000 | -0.468420000 | 6.610871000 |
| H | 8.744081000 | -1.505883000 | 6.584419000 |
| C | 9.312467000 | 8.490806000 | 10.252161000 |
| H | 8.987816000 | 7.467333000 | 10.065530000 |
| C | 8.389889000 | 9.536232000 | 10.221415000 |
| H | 7.336307000 | 9.327126000 | 10.023977000 |
| C | 8.805617000 | 10.849998000 | 10.432516000 |
| H | 8.076318000 | 11.661374000 | 10.411359000 |
| C | 10.658027000 | 8.753792000 | 10.480276000 |
| H | 11.375819000 | 7.929939000 | 10.507580000 |
| C | 10.149103000 | 11.123590000 | 10.667632000 |
| H | 10.487772000 | 12.145283000 | 10.842344000 |
| C | 11.075741000 | 10.074768000 | 10.691017000 |
| P | 12.811426000 | 10.406862000 | 11.053257000 |
| O | 12.969391000 | 11.871652000 | 11.560676000 |

| | | | |
|---|---|---|---|
| O | 13.249732000 | 9.270588000 | 12.106337000 |
| H | 14.131069000 | 8.715596000 | 11.854621000 |
| C | 13.881157000 | 10.144746000 | 9.556913000 |
| H | 13.447806000 | 10.691864000 | 8.704504000 |
| H | 13.846702000 | 9.076131000 | 9.304821000 |
| N | 15.257335000 | 10.545305000 | 9.829542000 |
| C | 15.595996000 | 11.941301000 | 9.576659000 |
| H | 16.284406000 | 12.059219000 | 8.724760000 |
| H | 14.685540000 | 12.505836000 | 9.333360000 |
| C | 16.295349000 | 9.556087000 | 9.560941000 |
| H | 16.049853000 | 8.914609000 | 8.699694000 |
| H | 17.241563000 | 10.061854000 | 9.324408000 |
| P | 16.585822000 | 8.487703000 | 11.053123000 |
| O | 15.232284000 | 7.891415000 | 11.543188000 |
| O | 17.342534000 | 9.426427000 | 12.120339000 |
| H | 17.369165000 | 10.471079000 | 11.885579000 |
| C | 17.743698000 | 7.153050000 | 10.689213000 |
| C | 17.299900000 | 5.825986000 | 10.662084000 |
| H | 16.246675000 | 5.606878000 | 10.841099000 |
| C | 18.208555000 | 4.801593000 | 10.416755000 |
| H | 17.871706000 | 3.764017000 | 10.390311000 |
| C | 19.552749000 | 5.100955000 | 10.200787000 |
| H | 20.259688000 | 4.294342000 | 9.994348000 |
| C | 19.996159000 | 6.422670000 | 10.236414000 |
| H | 21.043781000 | 6.654305000 | 10.044786000 |
| C | 19.095497000 | 7.454501000 | 10.474194000 |
| H | 19.449070000 | 8.488182000 | 10.505650000 |
| P | 16.350786000 | 12.726240000 | 11.082571000 |
| O | 17.526891000 | 11.845336000 | 11.601106000 |
| O | 15.140051000 | 12.926631000 | 12.124114000 |
| H | 14.226280000 | 12.424865000 | 11.873767000 |
| C | 16.942427000 | 14.389855000 | 10.713952000 |
| C | 18.315725000 | 14.656196000 | 10.670818000 |
| H | 19.026093000 | 13.847937000 | 10.847601000 |
| C | 18.758018000 | 15.949134000 | 10.410845000 |
| H | 19.826685000 | 16.166259000 | 10.372927000 |
| C | 17.833903000 | 16.970151000 | 10.194435000 |
| H | 18.184750000 | 17.981710000 | 9.978496000 |
| C | 16.465476000 | 16.705730000 | 10.243426000 |
| H | 15.746556000 | 17.501990000 | 10.050085000 |
| C | 16.012875000 | 15.415831000 | 10.496719000 |
| H | 14.939376000 | 15.214100000 | 10.538403000 |