Supporting Information

Homolysis/Mesolysis of Alkoxyamines Activated by Chemical Oxidation and Photochemical-triggered Radical Reactions at Room Temperature

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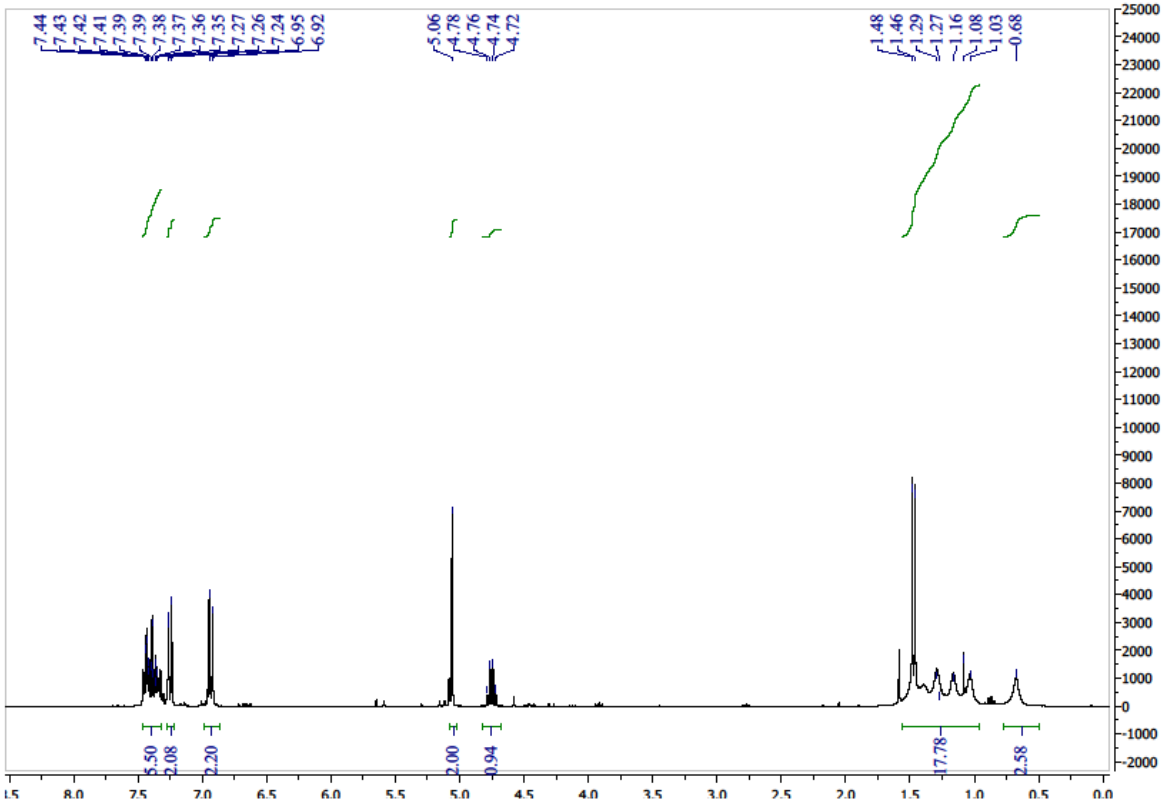
Content

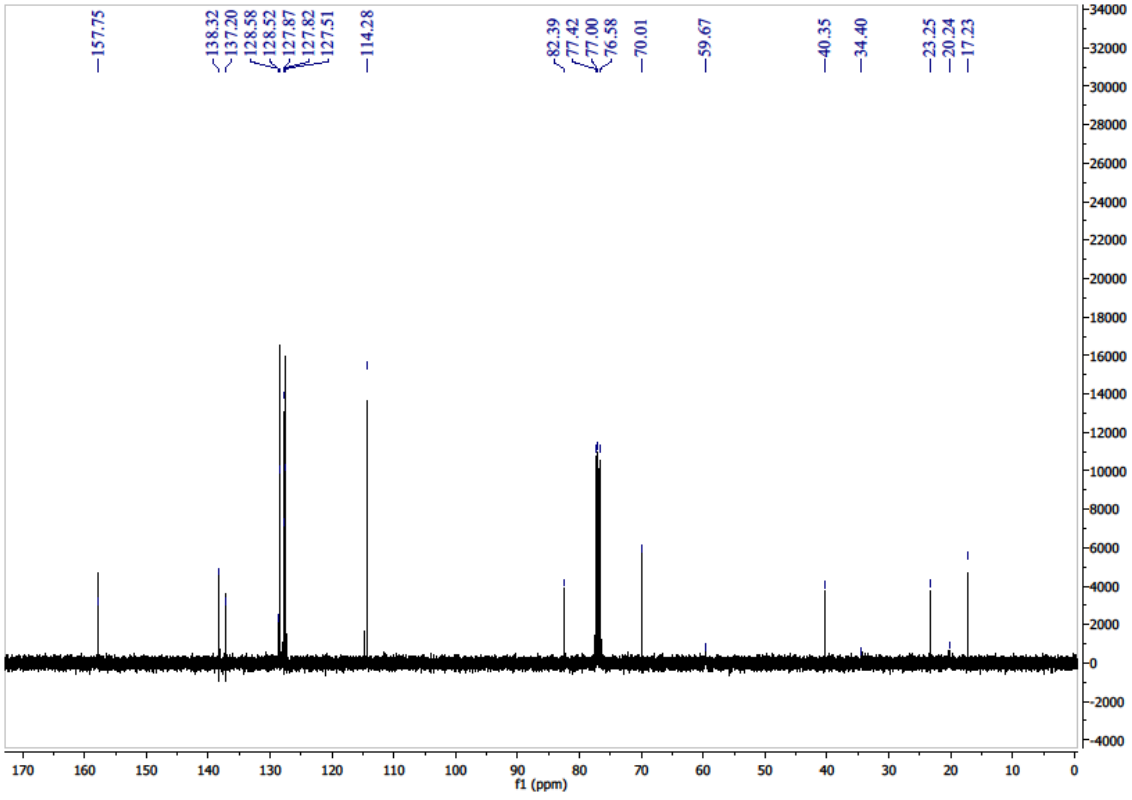
1. NMR spectra (1H, 13C, 31P, DEPT 135) and HRMS of alkoxyamines 1a,b-5a,b, 1d, 3d and 3e.

1-(1-(4-(benzyloxy)phenyl)ethoxy)-2,2,6,6-tetramethylpiperidine **(1b).**

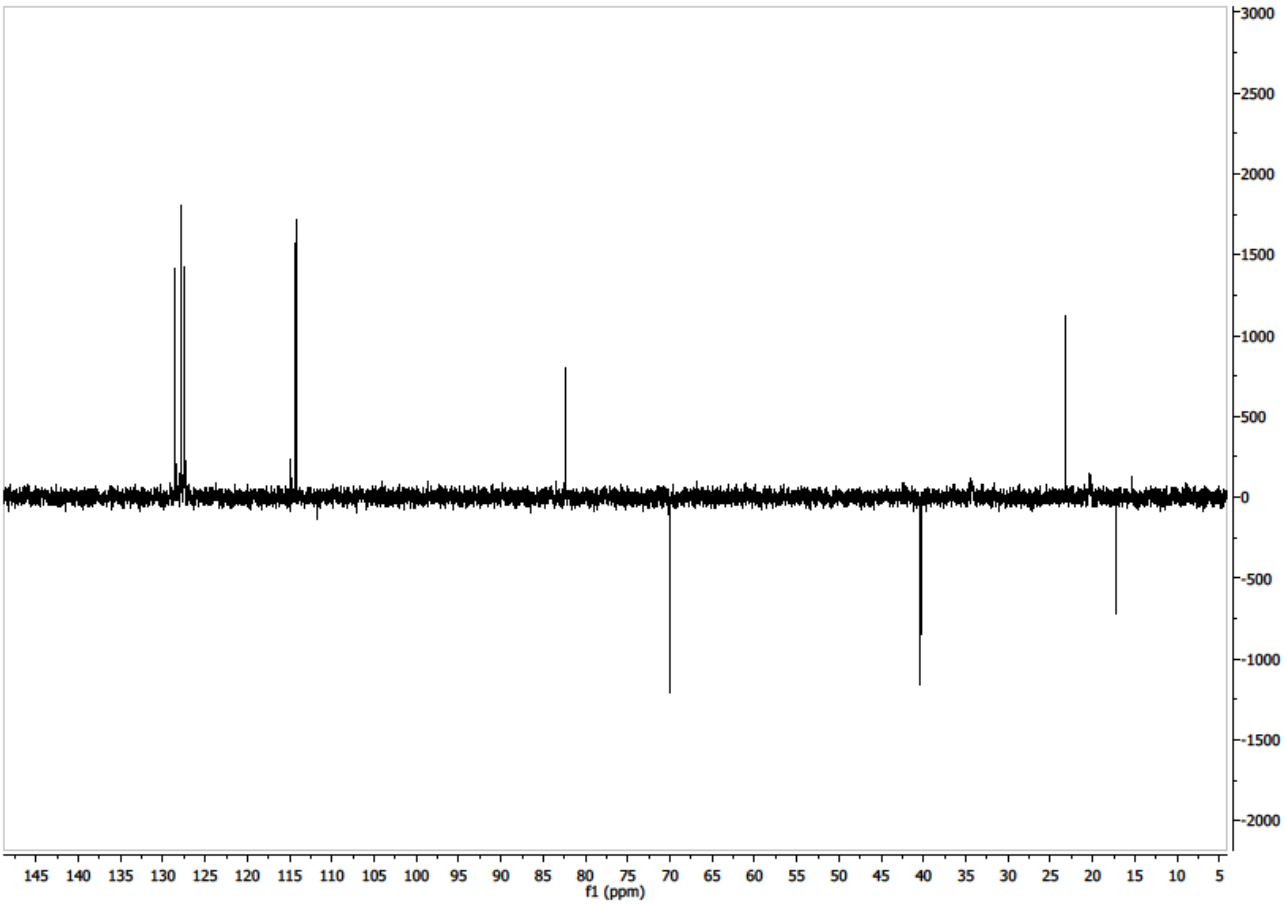
^{1}H NMR (300 MHz, $CDCl_3$)



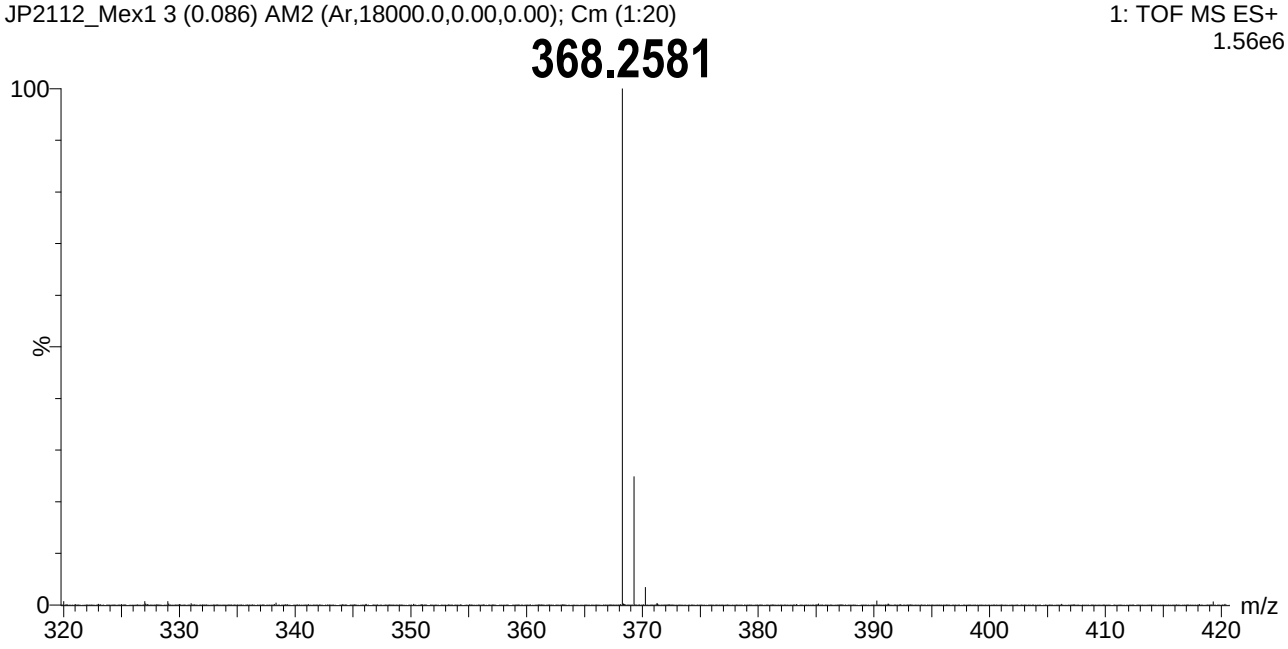
^{13}C NMR (75 MHz, $CDCl_3$)



DEPT 135 (75 MHz, $CDCl_3$)

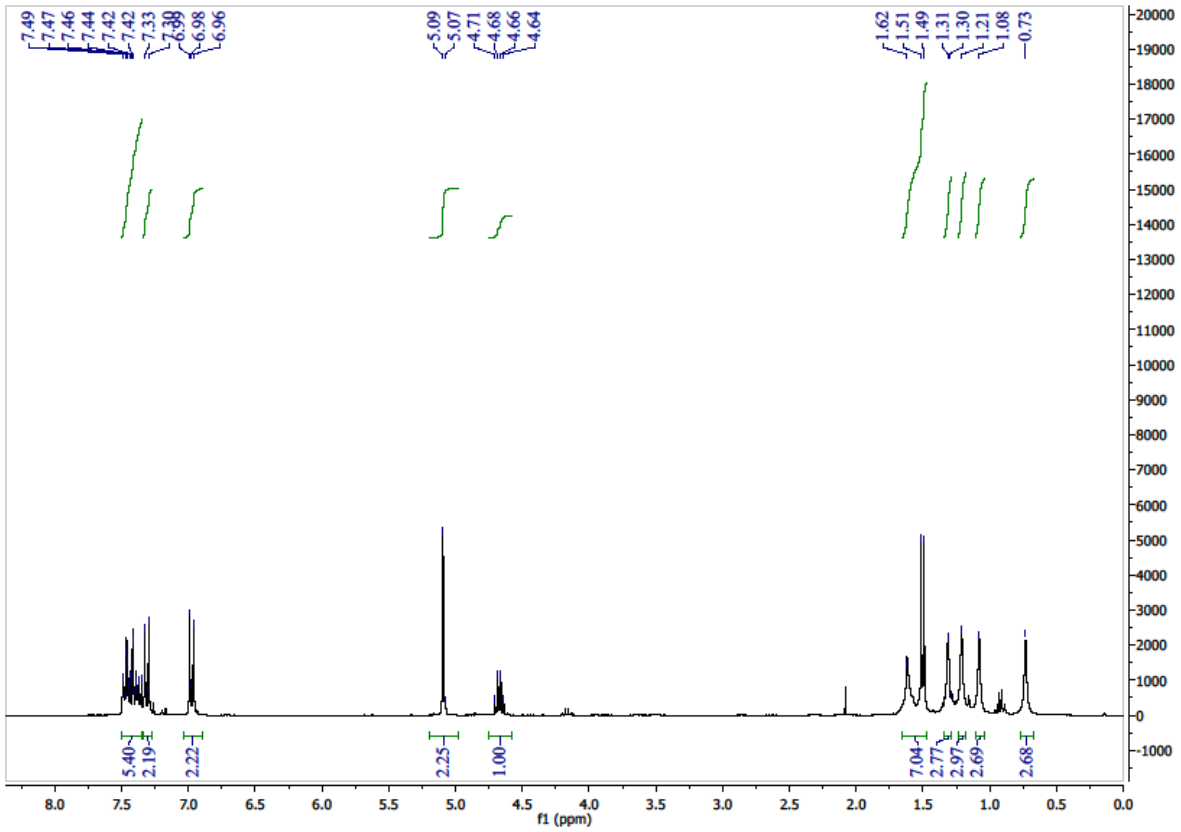


HRMS

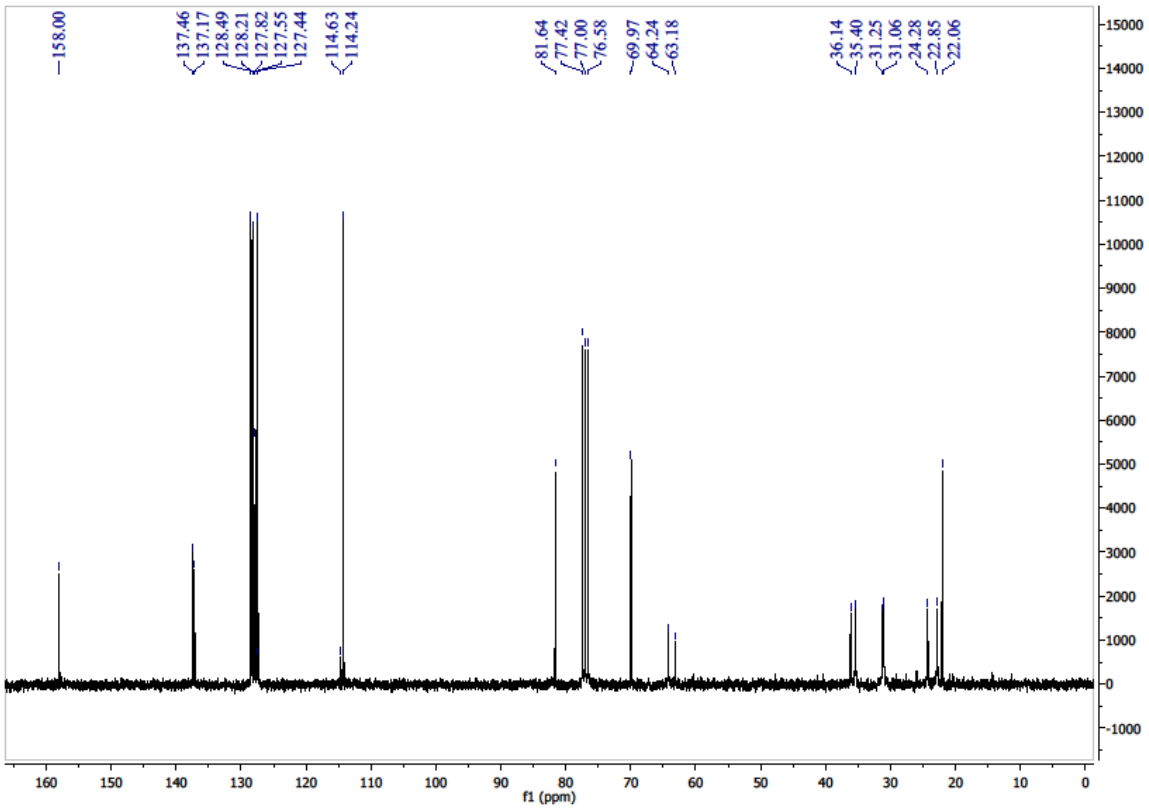


***1-(1-(4-(benzyloxy)phenyl)ethoxy)-2,2,5,5-tetramethylpyrrolidine* (2b)**

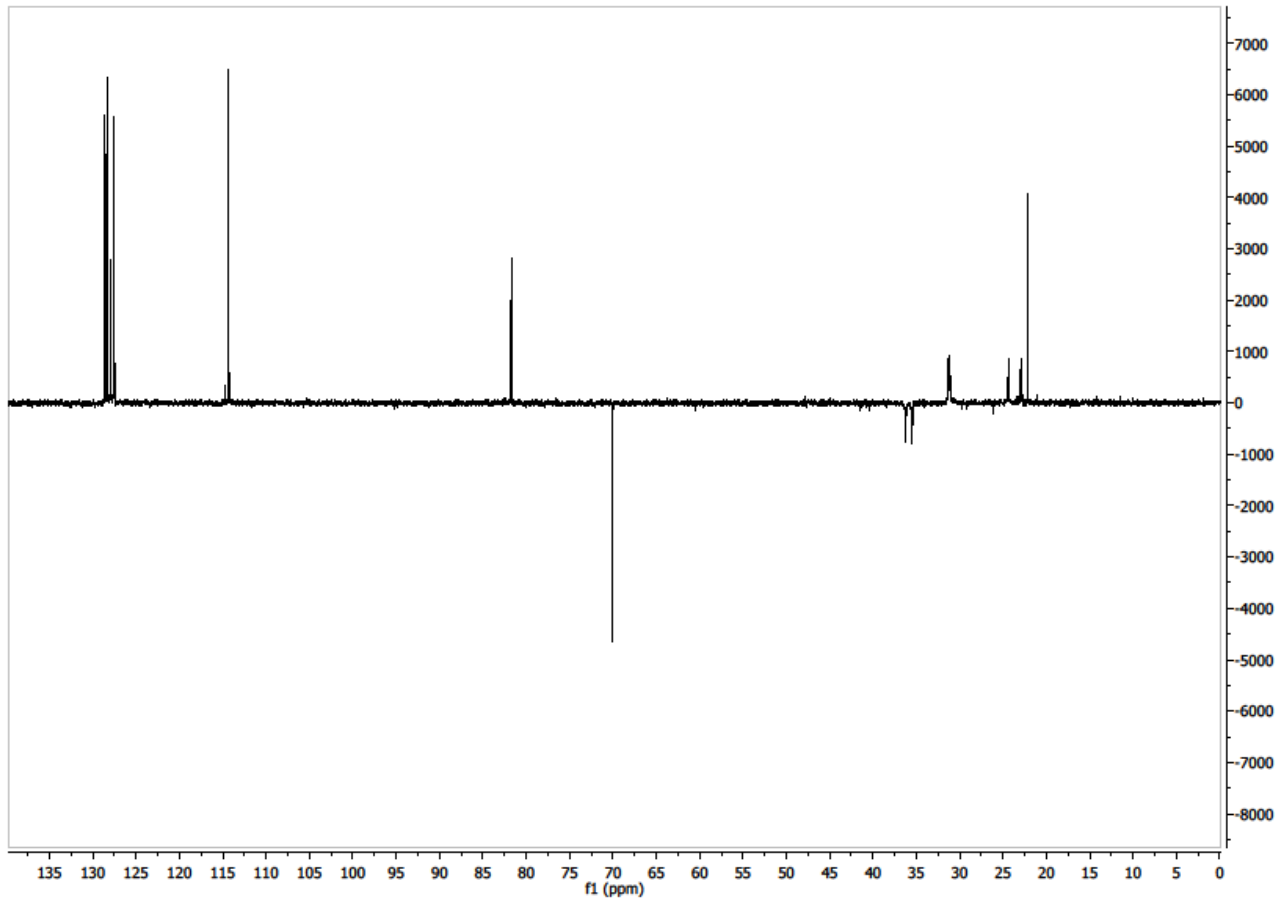
^{1}H NMR (300 MHz, $CDCl_3$)



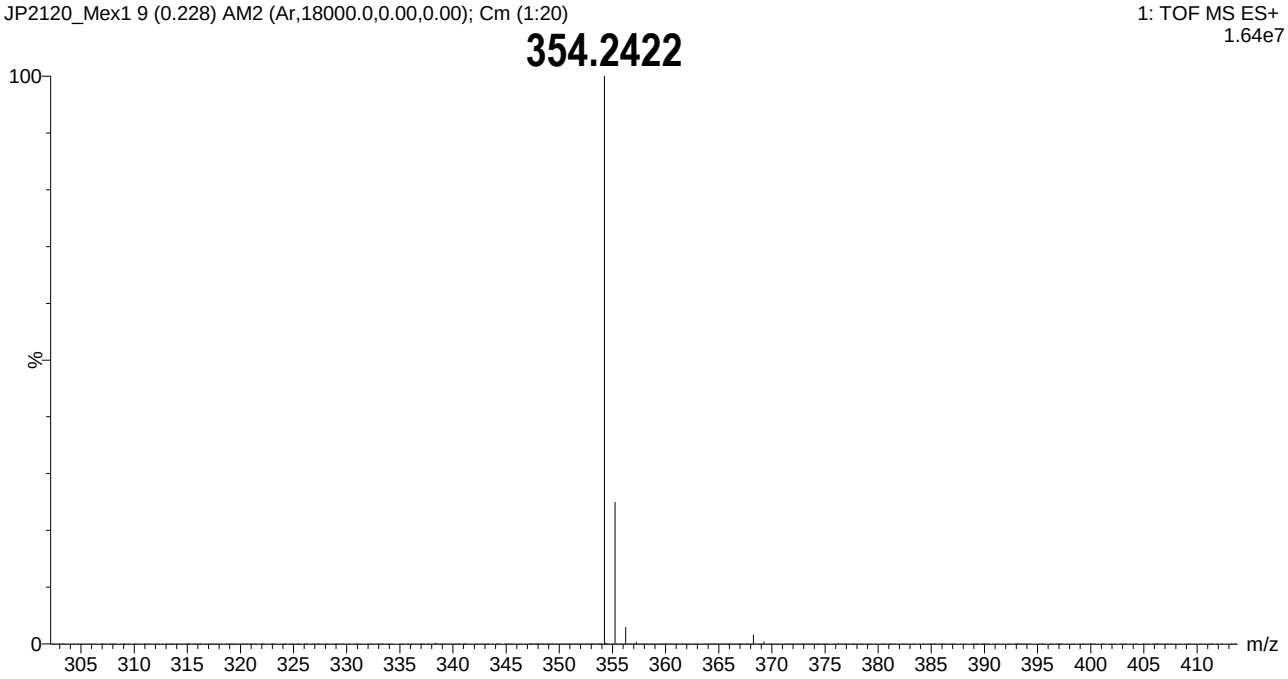
^{13}C NMR (75 MHz, $CDCl_3$)



DEPT 135 (75 MHz, $CDCl_3$)

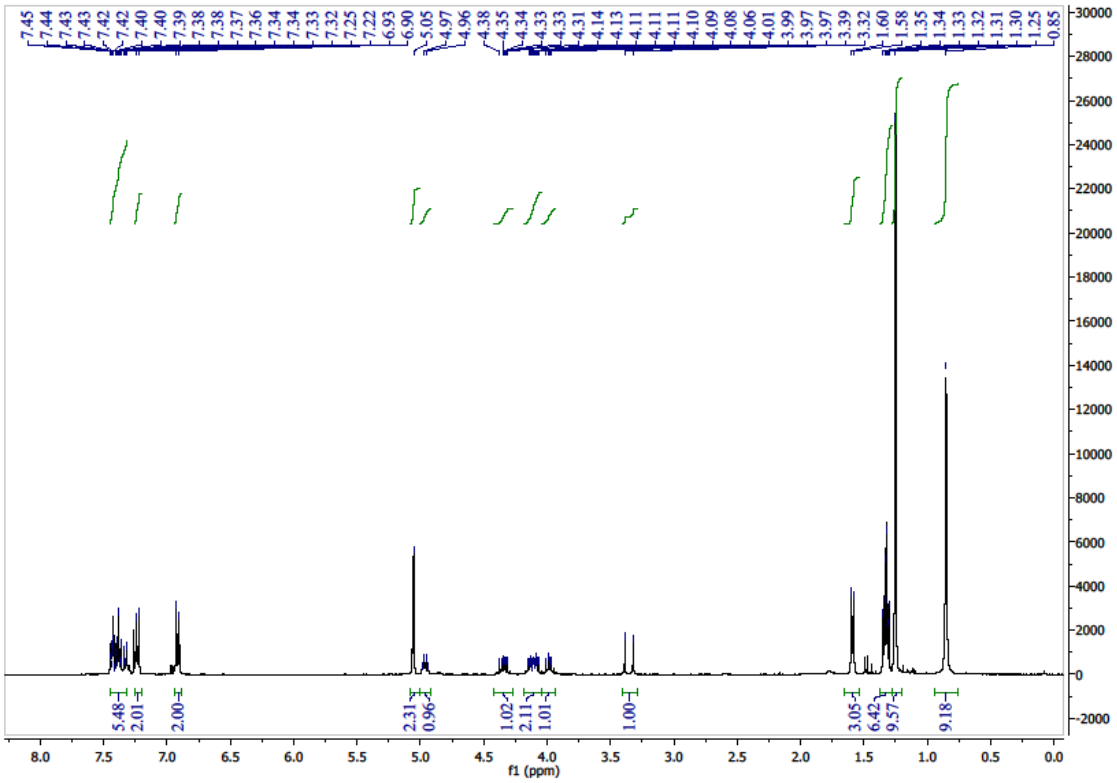


HRMS

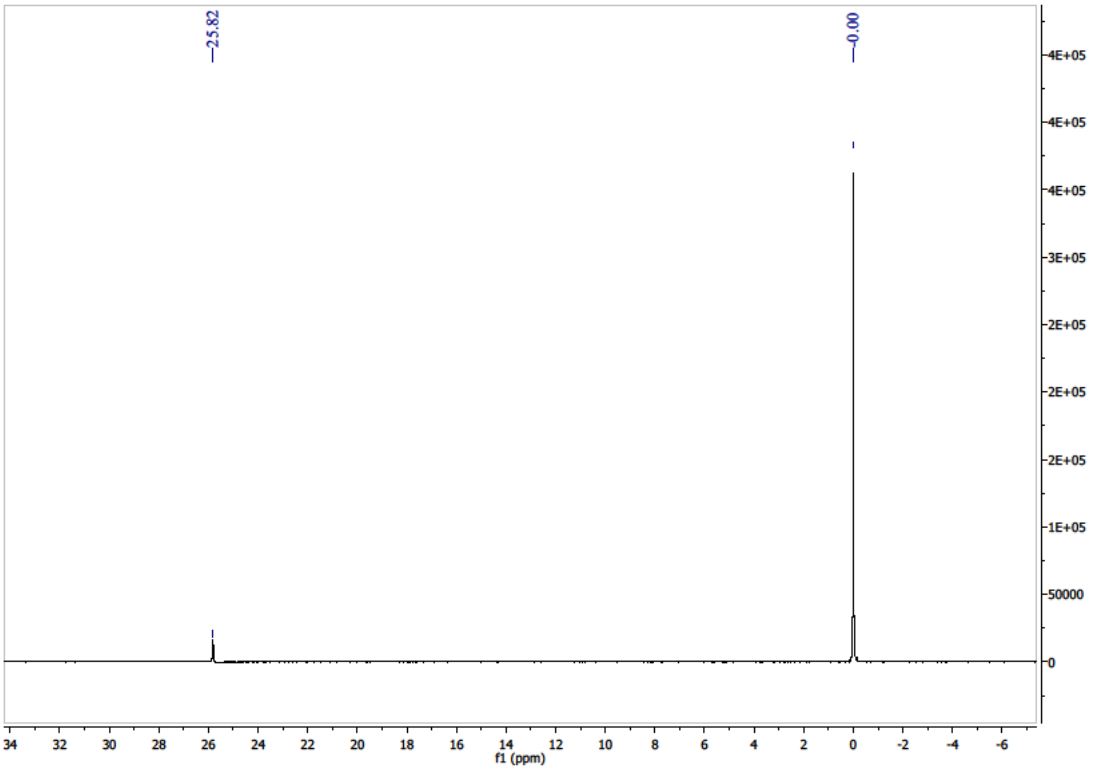


***diethyl(1-((1-(4-(benzyloxy)phenyl)ethoxy)(tert-butyl)amino)-2,2-dimethylpropyl)phosphonate* (3b)**

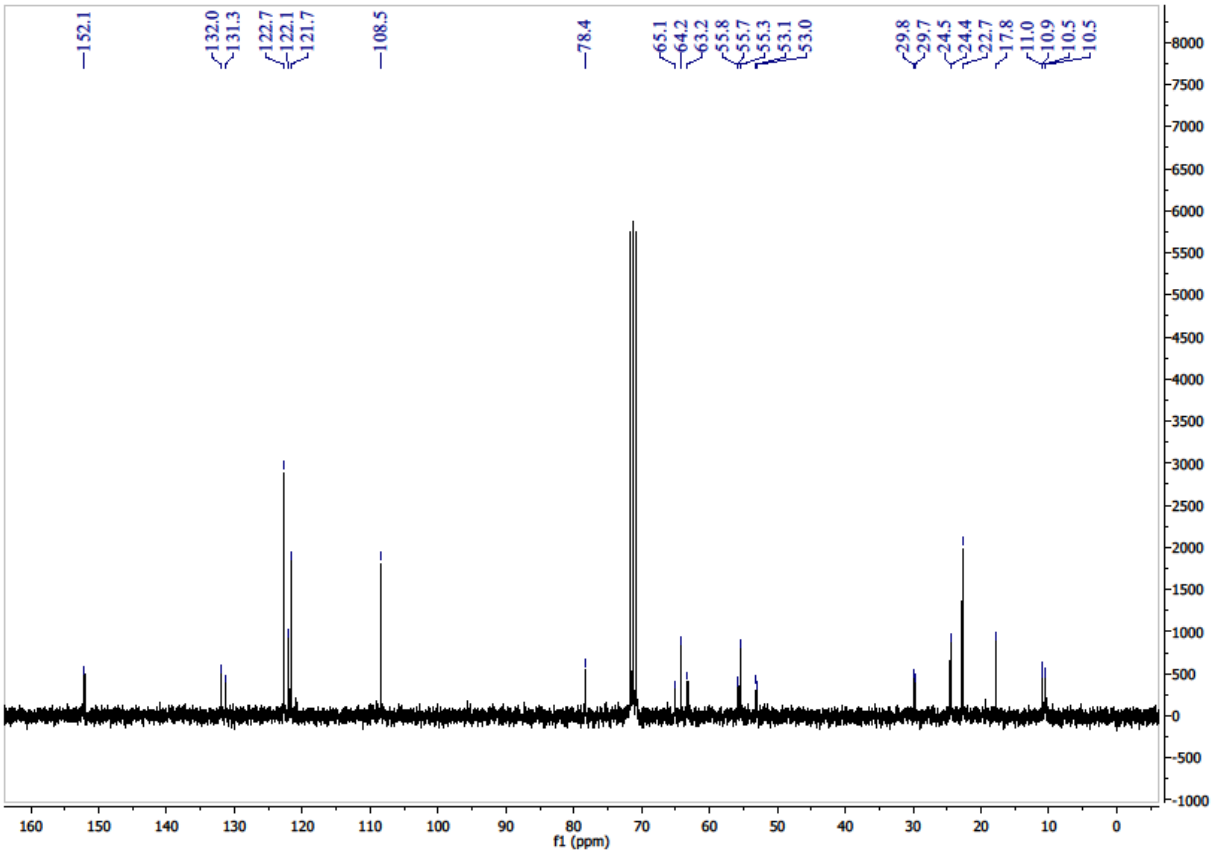
(*RR/SS*)-**3b** ^{1}H NMR (400 MHz, $CDCl_3$)



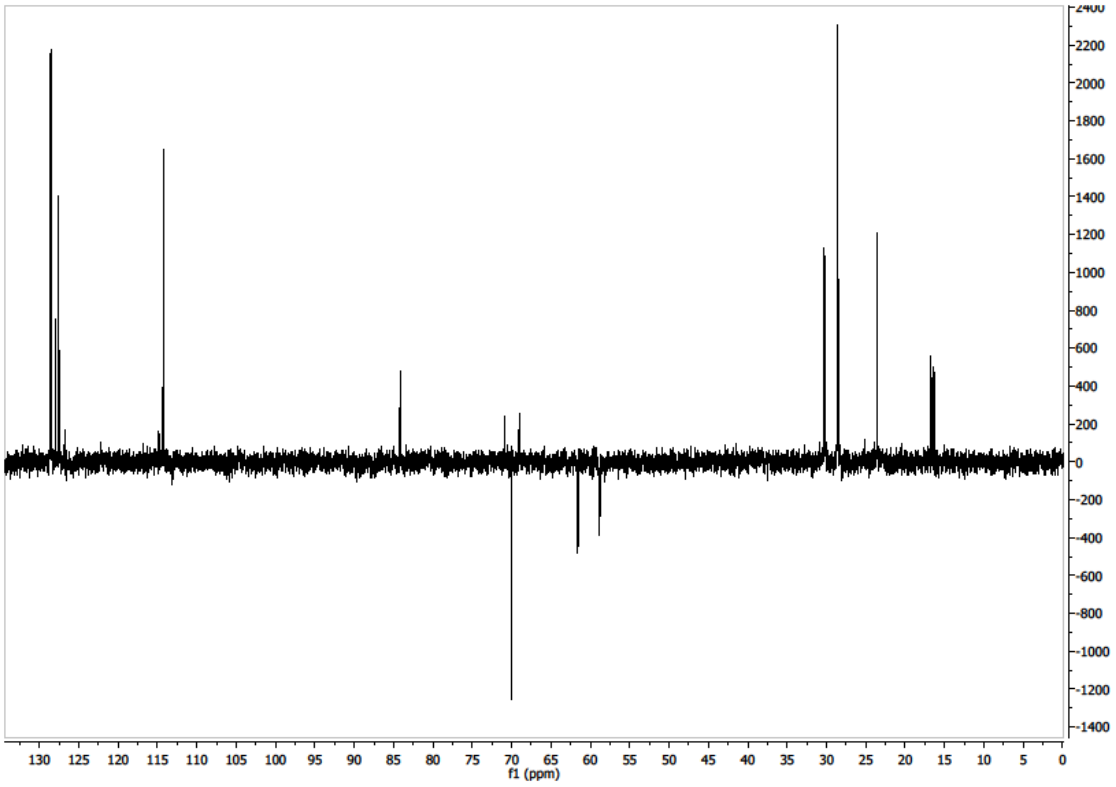
(*RR/SS*)-**3b** ^{31}P NMR (121 MHz, $CDCl_3$)



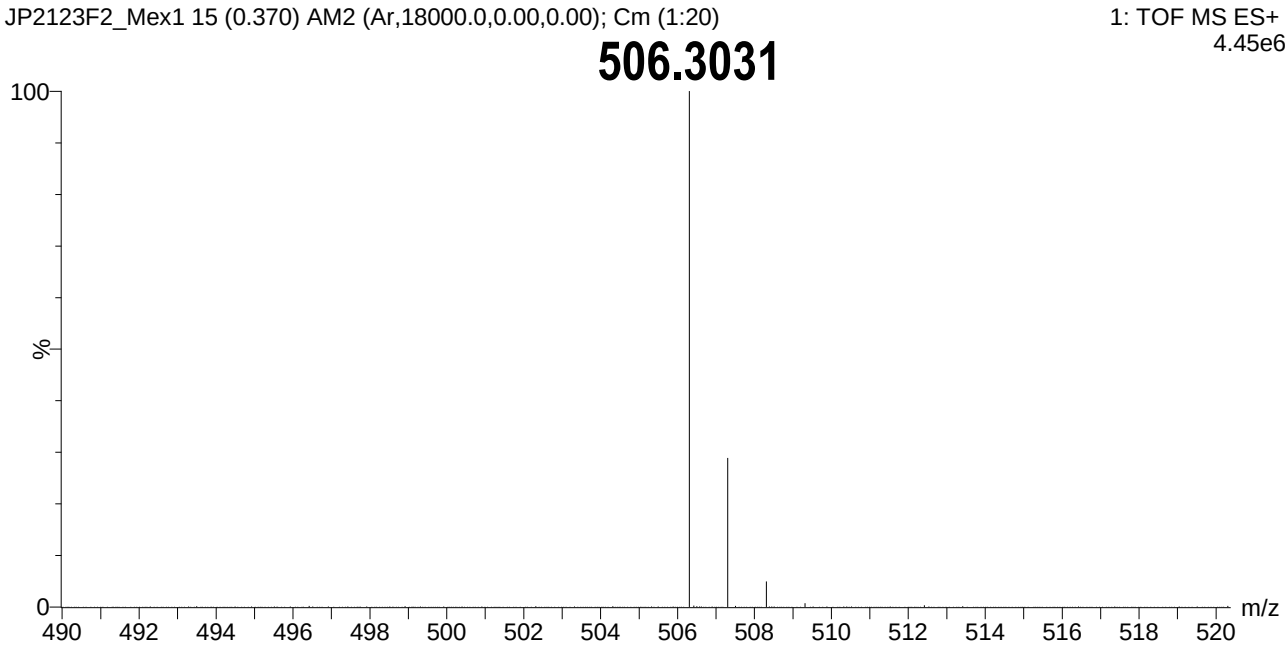
(*RR/SS*)-**3b** ^{13}C NMR (75 MHz, Acetone-d_6)



(*RR/SS*)-**3b** DEPT 135 (75 MHz, Acetone-d_6)



HRMS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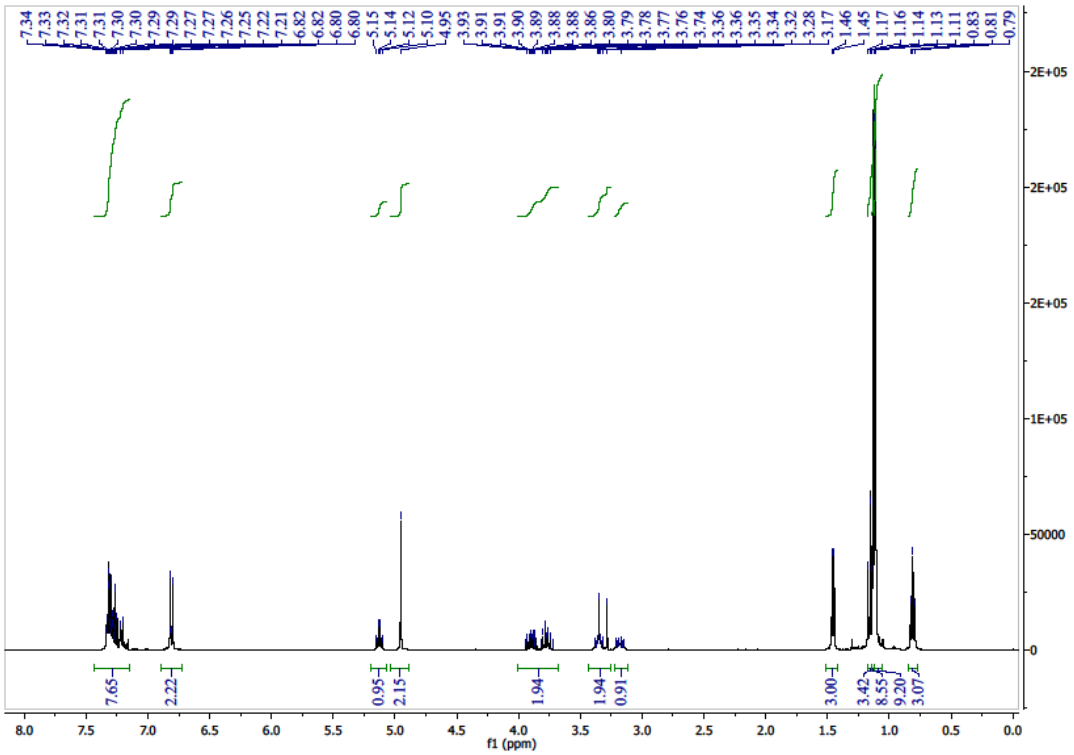
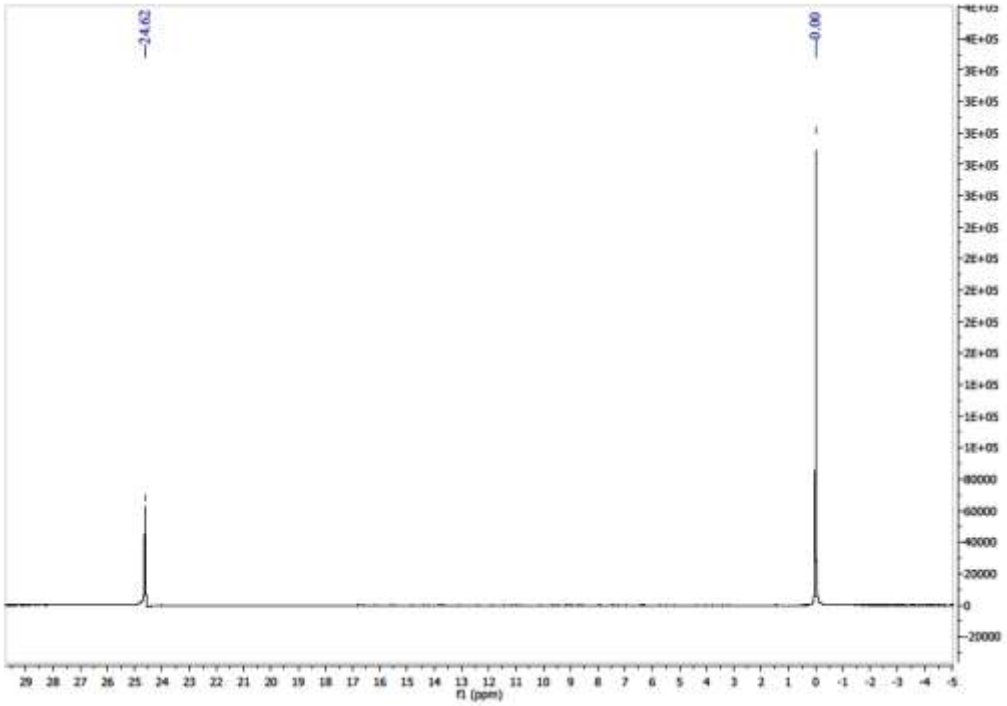
506.3031
100
%
0
490
492
494
496
498
500
502
504
506
508
510
512
514
516
518
520
m/z

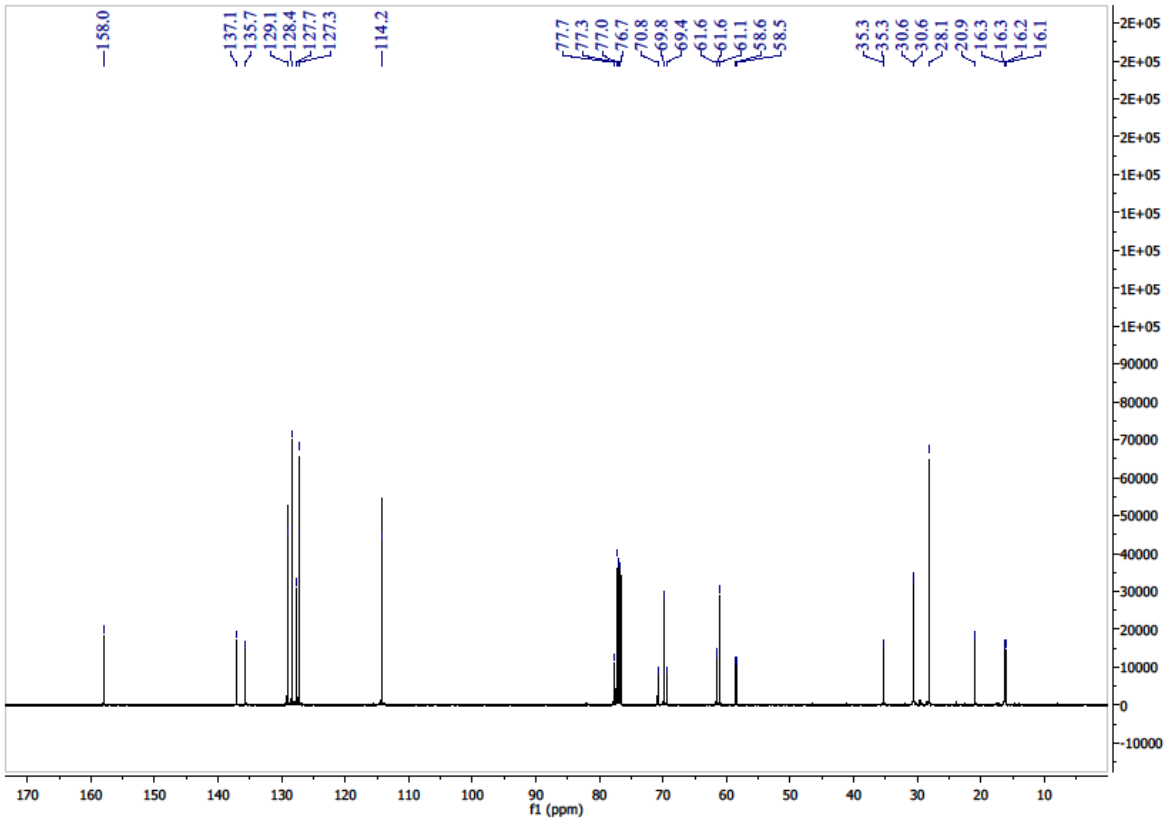
(*RS/SR*)-**3b** ^{1}H NMR (400 MHz, $CDCl_3$)



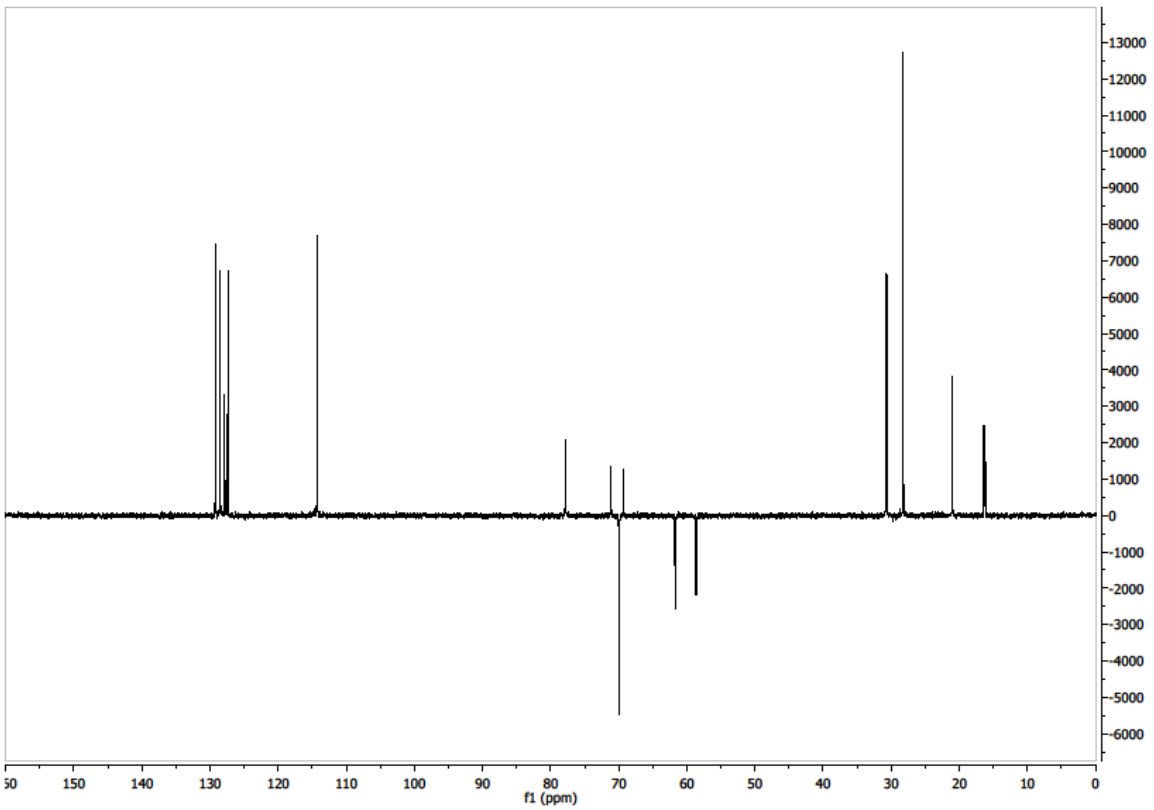
(*RS/SR*)-**3b** ^{31}P NMR (121 MHz, $CDCl_3$)



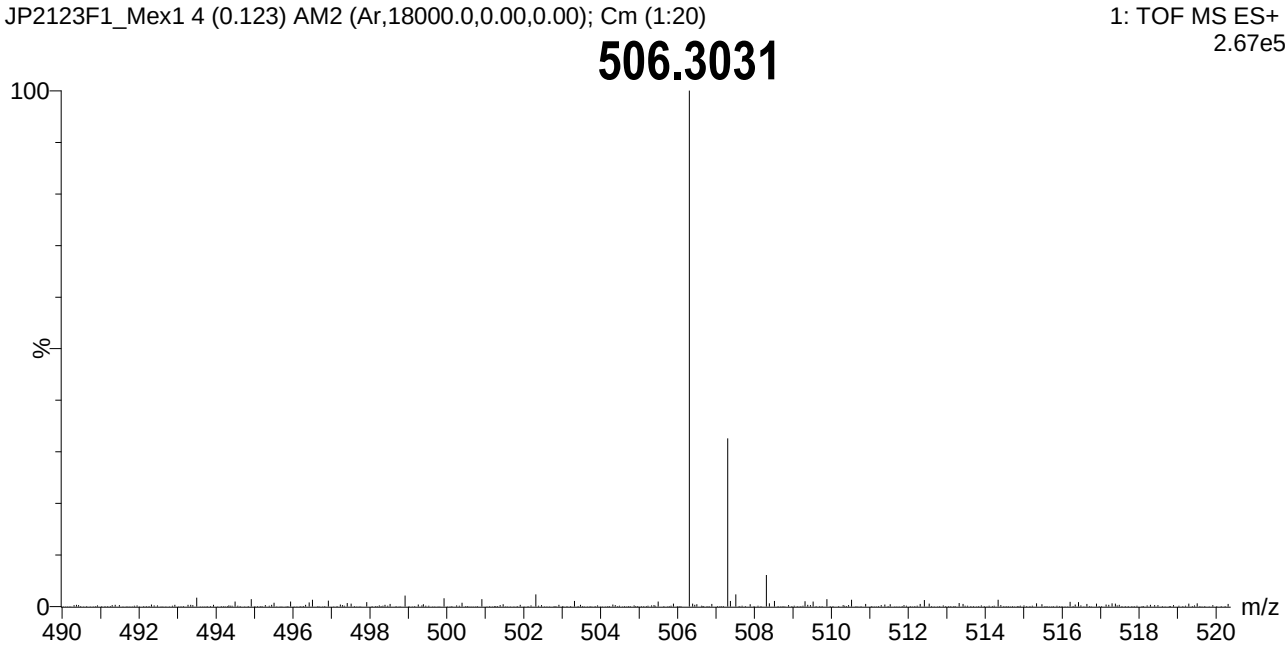
(*RS/SR*)-**3b** ^{13}C NMR (121 MHz, $CDCl_3$)



(*RR/SS*)-**3b** DEPT 135 (121 MHz, $CDCl_3$)



HRMS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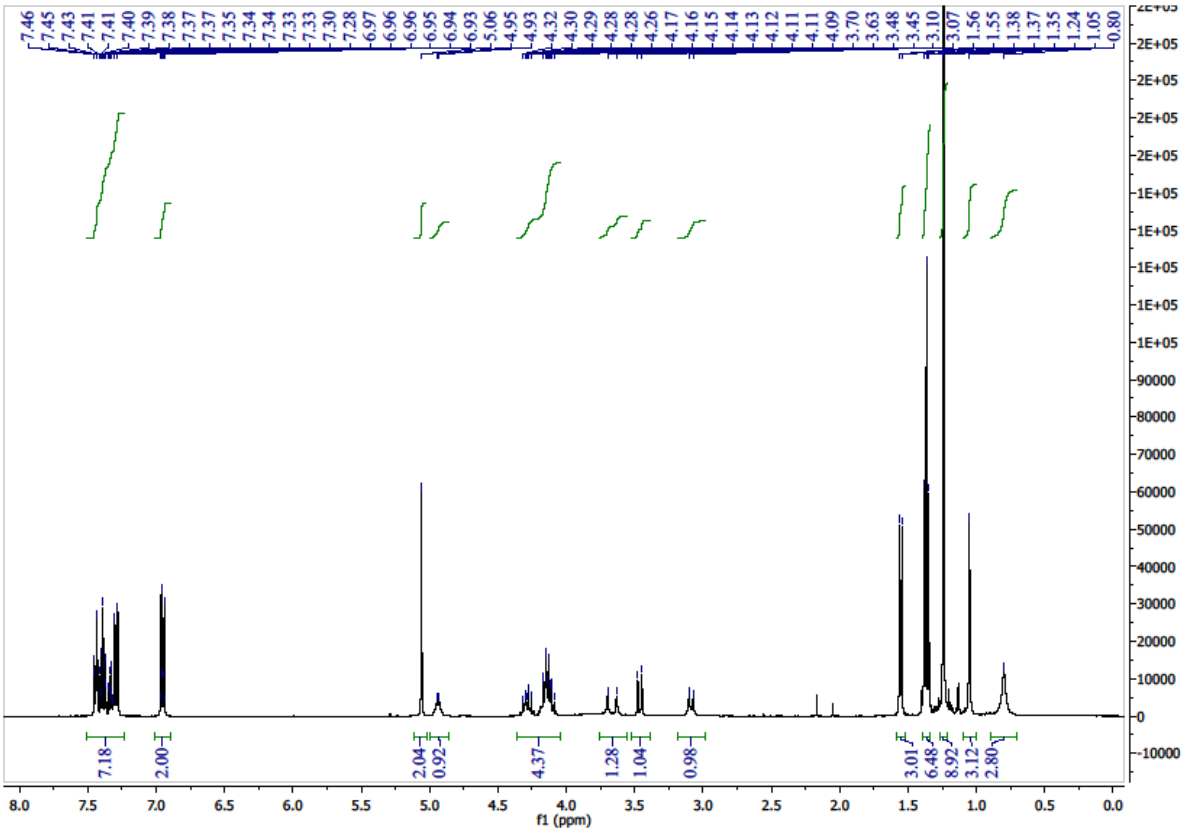
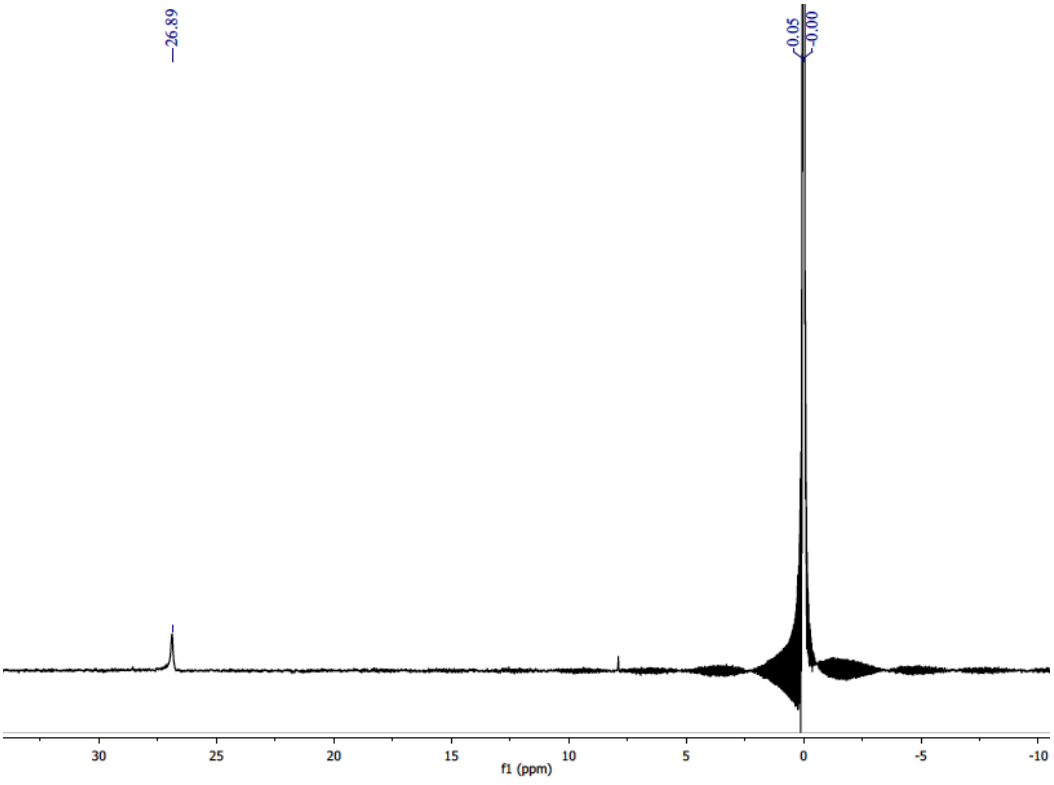
100
%
0
m/z
490
492
494
496
498
500
502
504
506
508
510
512
514
516
518
520

***diethyl(1-((1-(4-(benzyloxy)phenyl)ethoxy)(1-hydroxy-2-methylpropan-2-yl)amino)-2,2-dimethylpropyl)phosphonate* (4b)**

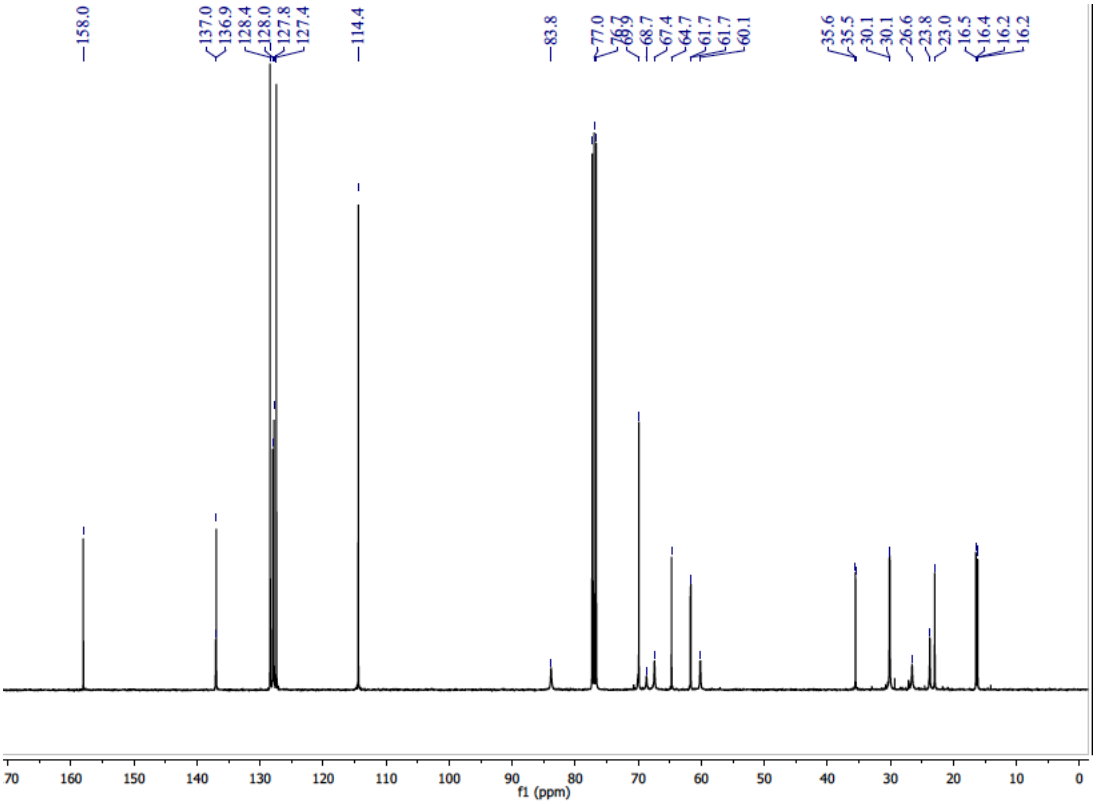
(*RR/SS*)-**4b** ^{1}H NMR (400 MHz, $CDCl_3$)



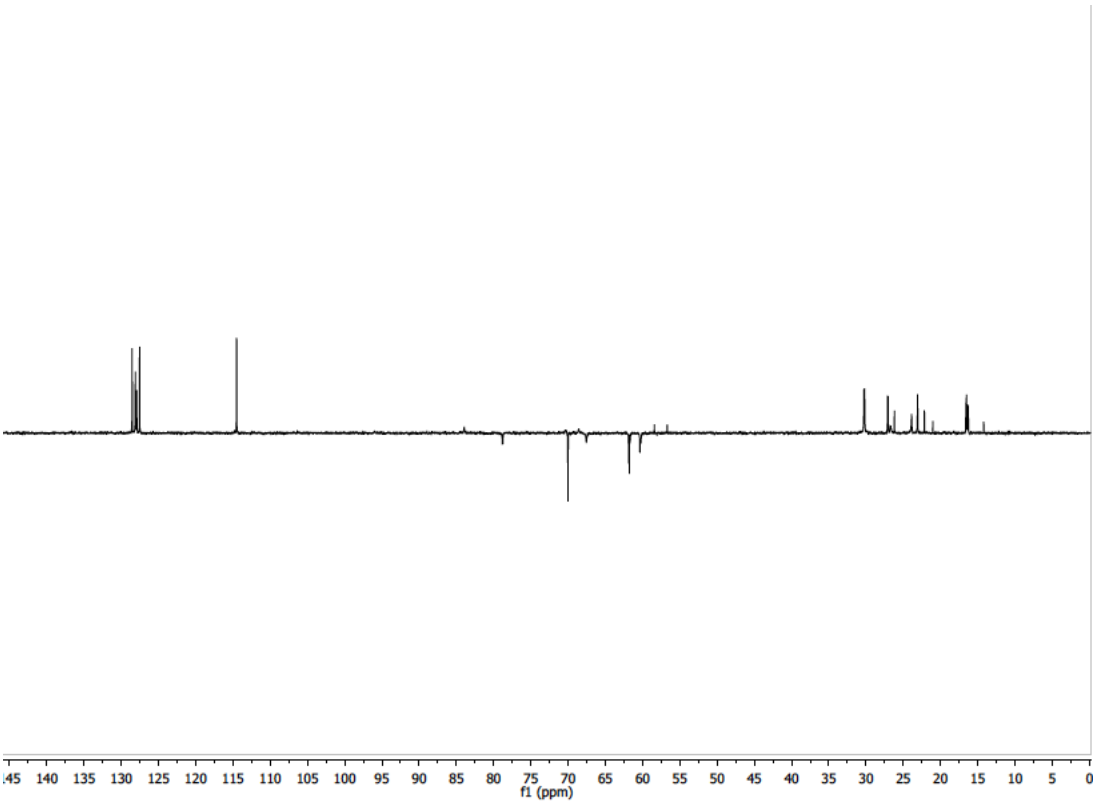
(*RR/SS*)-**4b** ^{31}P NMR (121 MHz, $CDCl_3$)



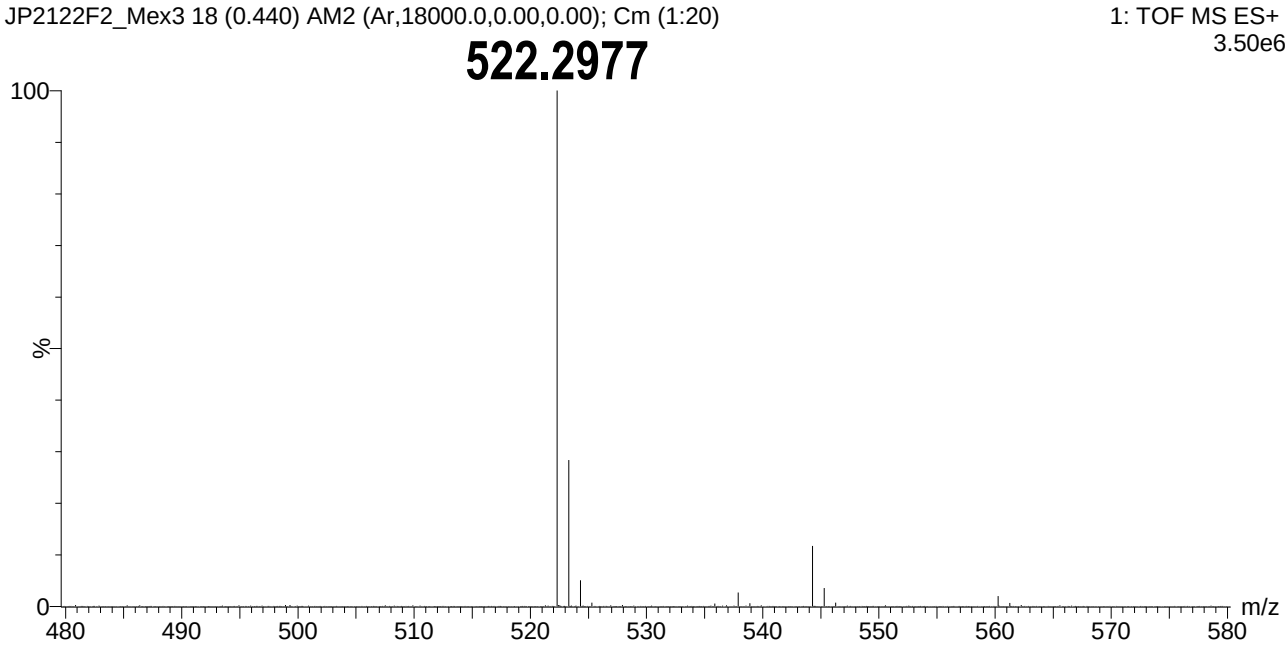
(*RR/SS*)-**4b** ^{13}C NMR (75 MHz, $CDCl_3$)



(*RR/SS*)-**4b** DEPT 135 (75 MHz, $CDCl_3$)



HRMS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522.2977
100
%
0
480
490
500
510
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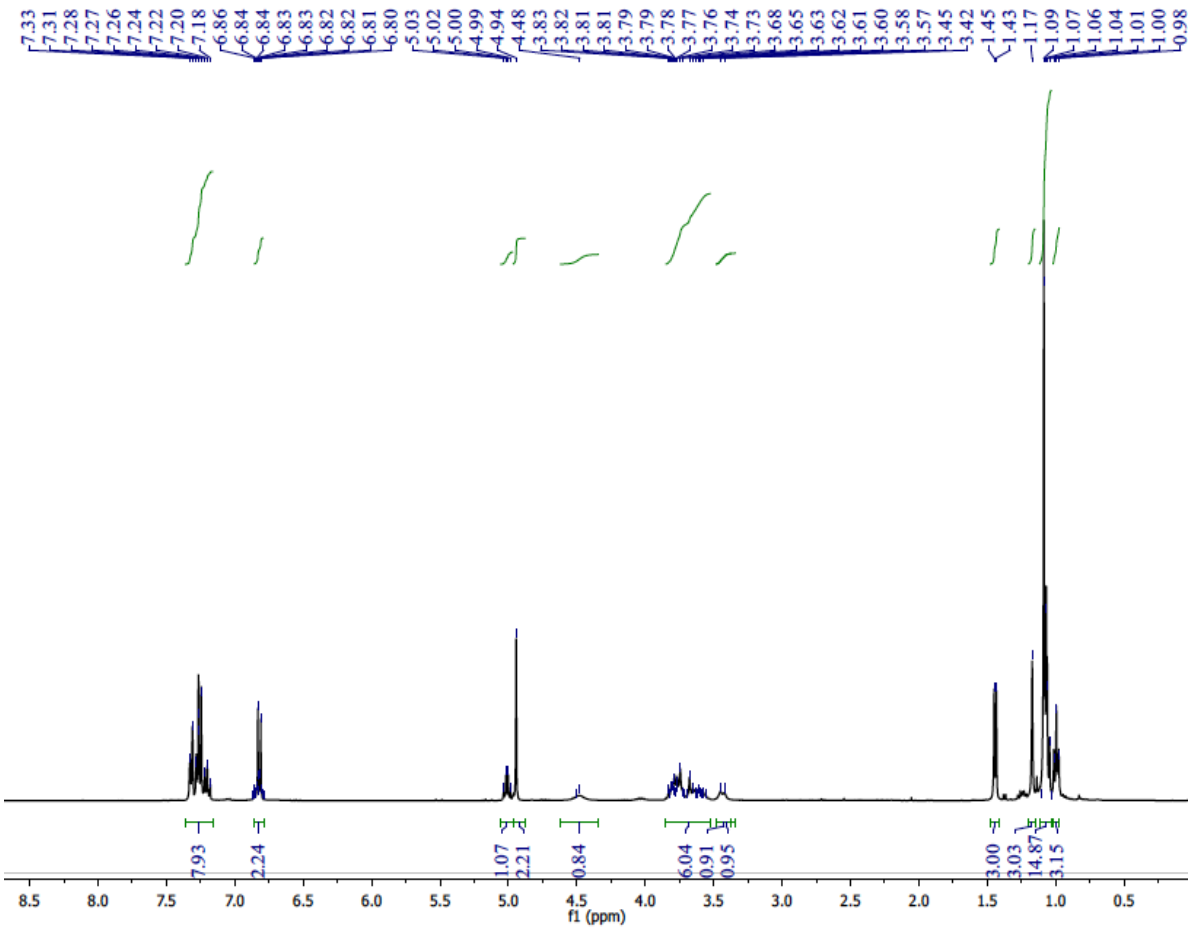
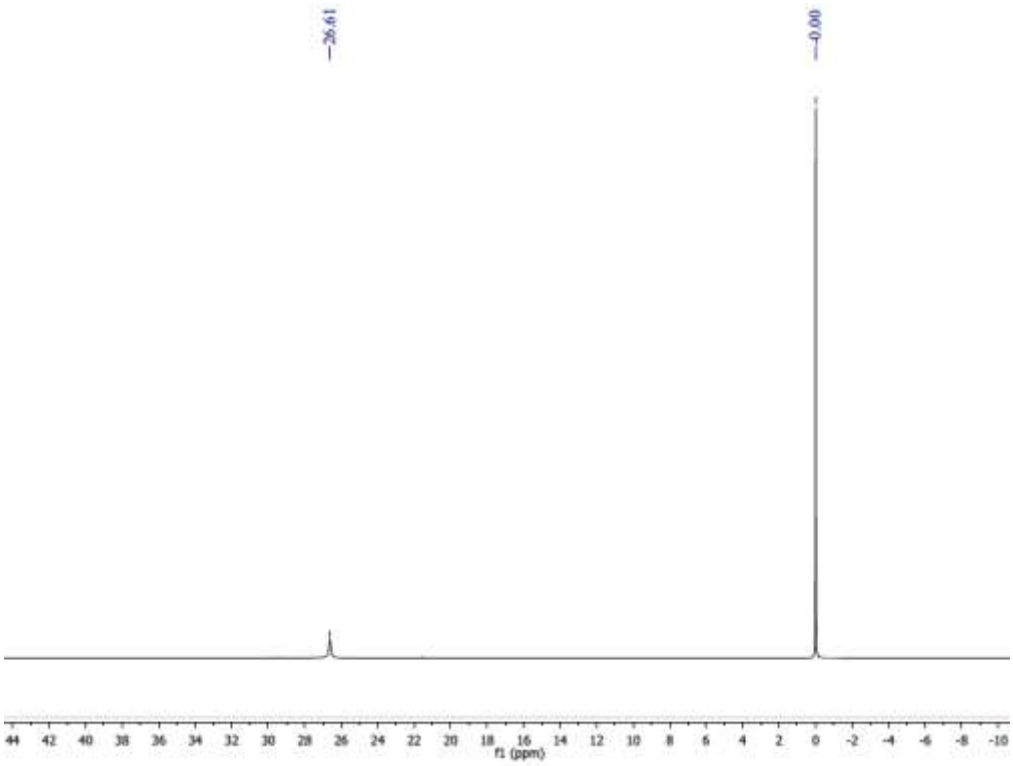
540
550
560
570
580
m/z

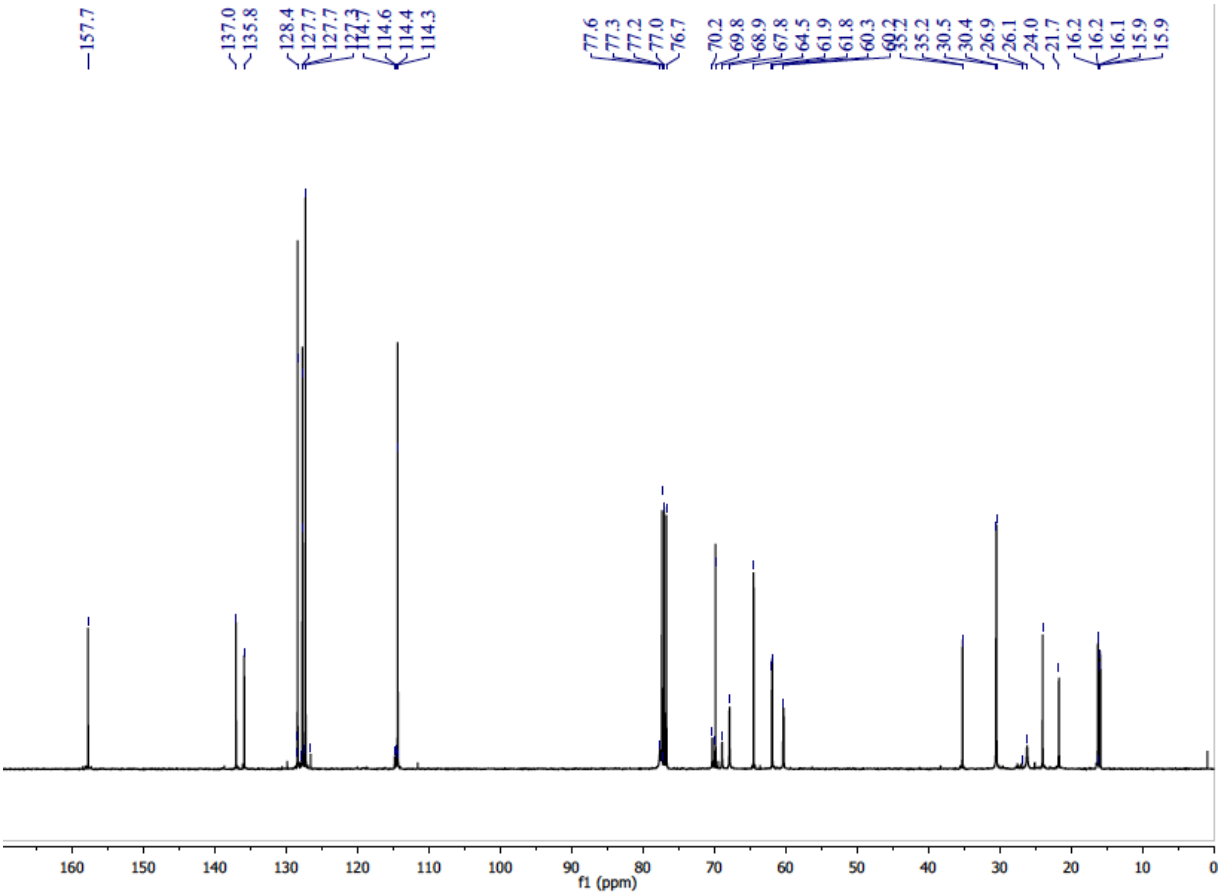
(*RS/SR*)-**4b** ^{1}H NMR (400 MHz, $CDCl_3$)



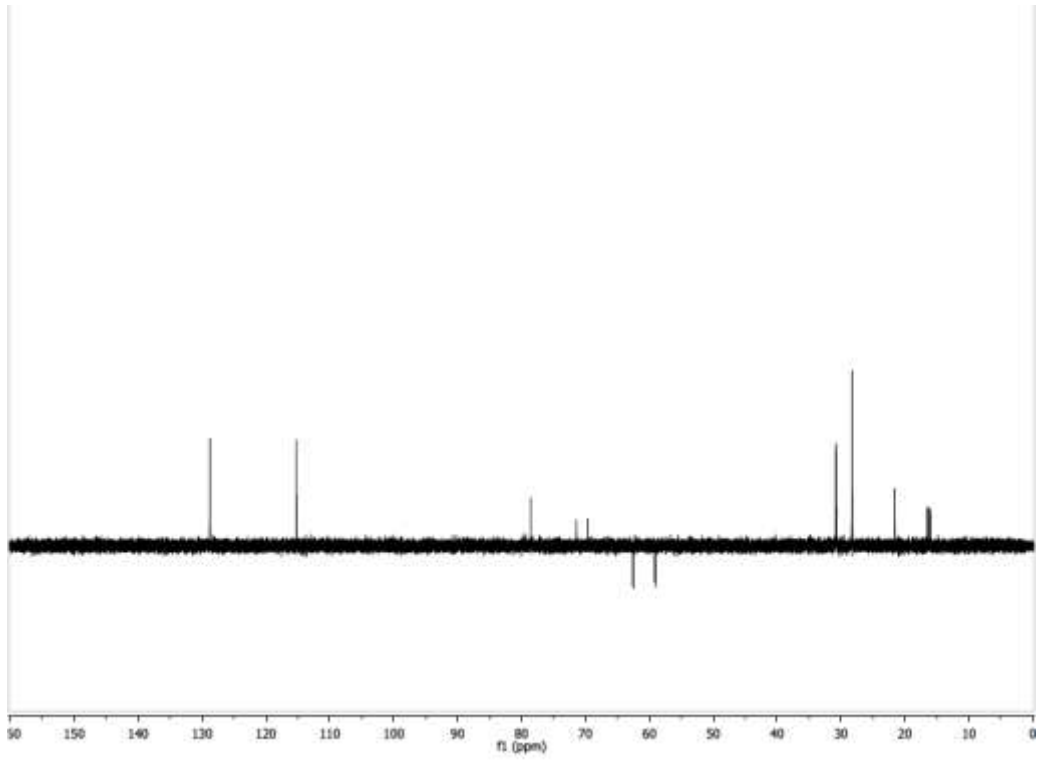
(*RS/SR*)-**4b** ^{31}P NMR (121 MHz, $CDCl_3$)



(*RS/SR*)-**4b** ^{13}C NMR (101 MHz, $CDCl_3$)



(*RS/SR*)-**4b** DEPT 135 (101 MHz, $CDCl_3$)



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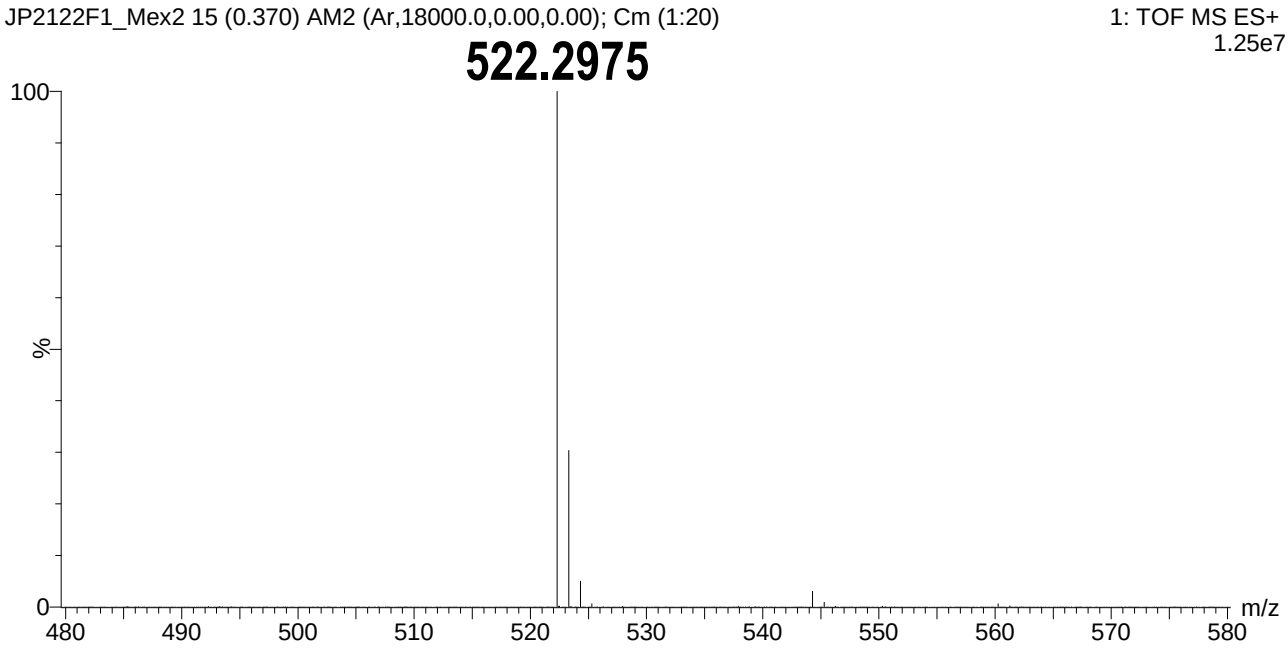
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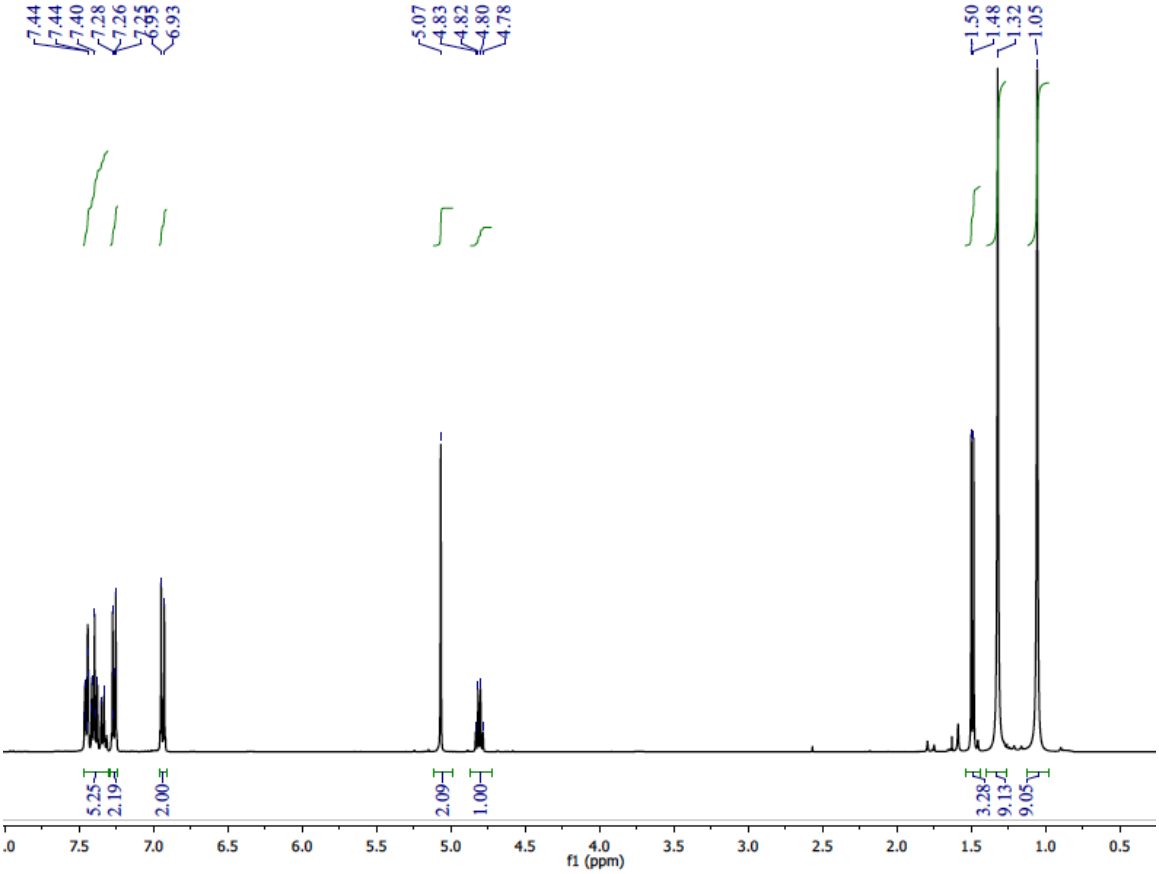
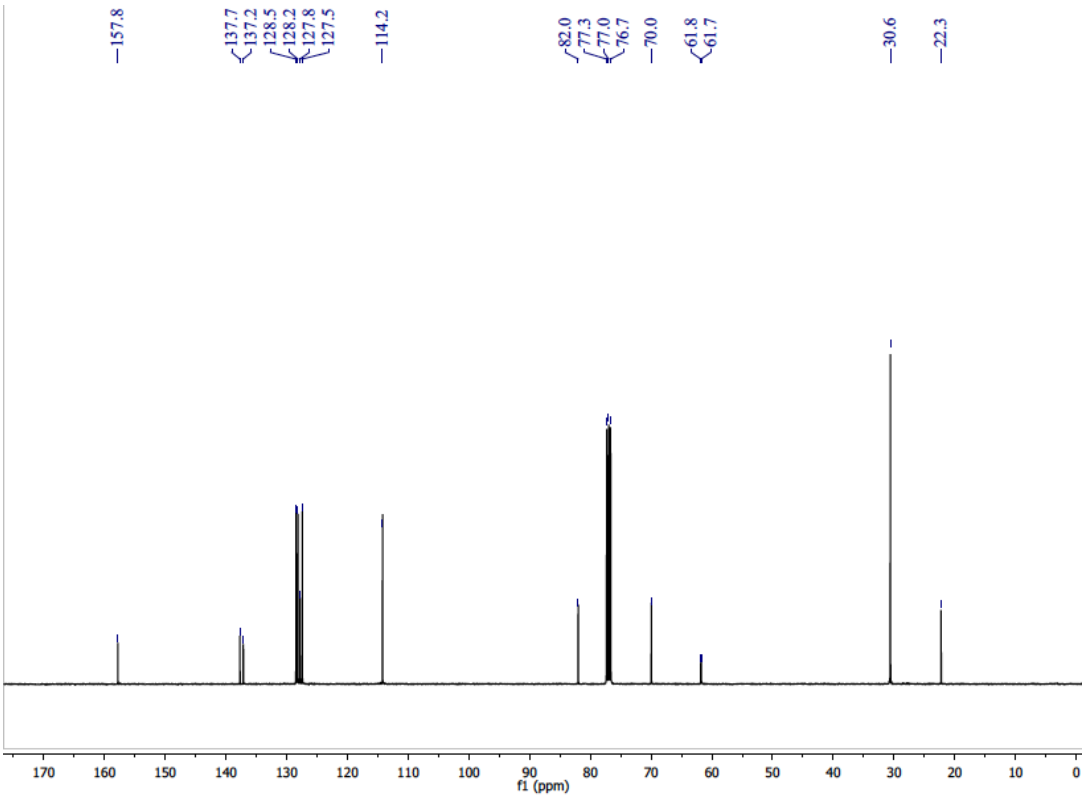
1.25e7
522.2975
100
%
0
480
490
500
510
520
530
540
550
560
570
580
m/z

***O-(1-(4-(benzyloxy)phenyl)ethyl)-N,N-di-tert-butylhydroxylamine* (5b).**

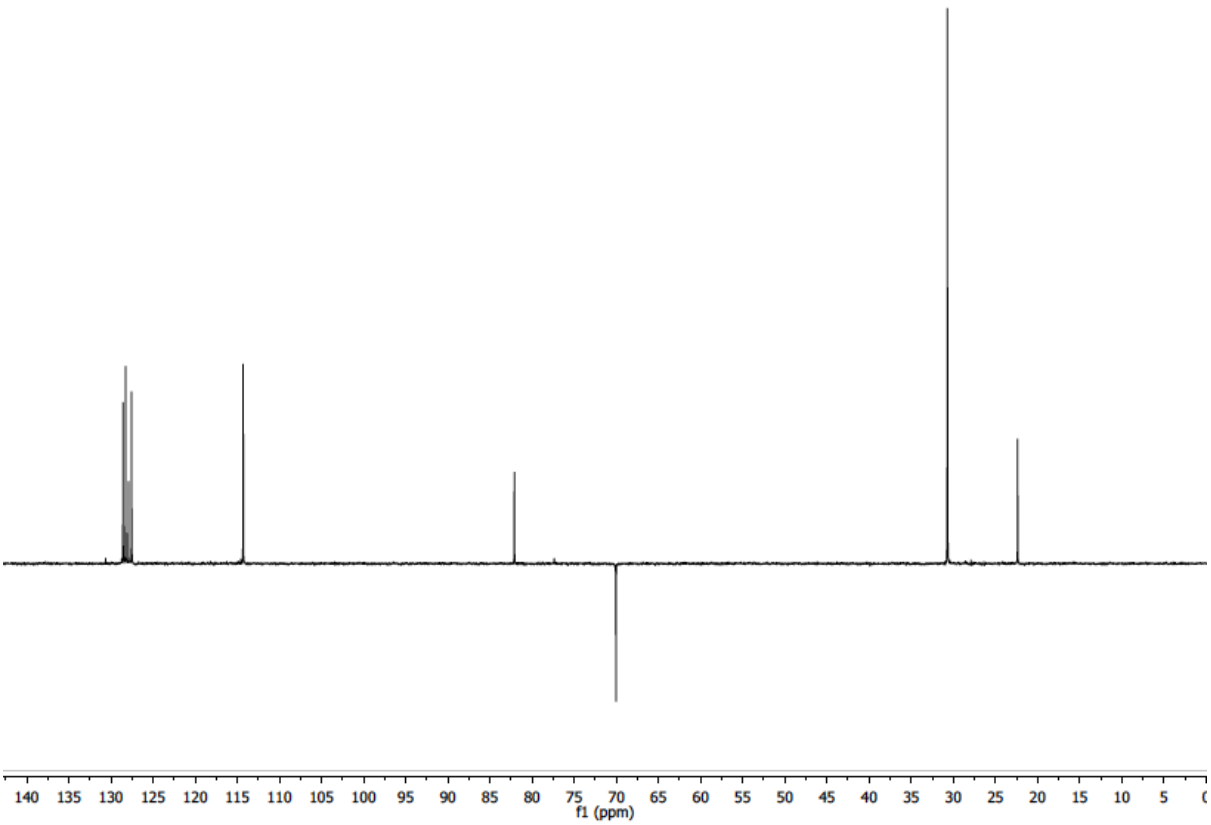
5b ^{1}H NMR (400 MHz, $CDCl_3$)



5b ^{13}C NMR (101 MHz, $CDCl_3$)



5b DEPT 135 (101 MHz, $CDCl_3$)



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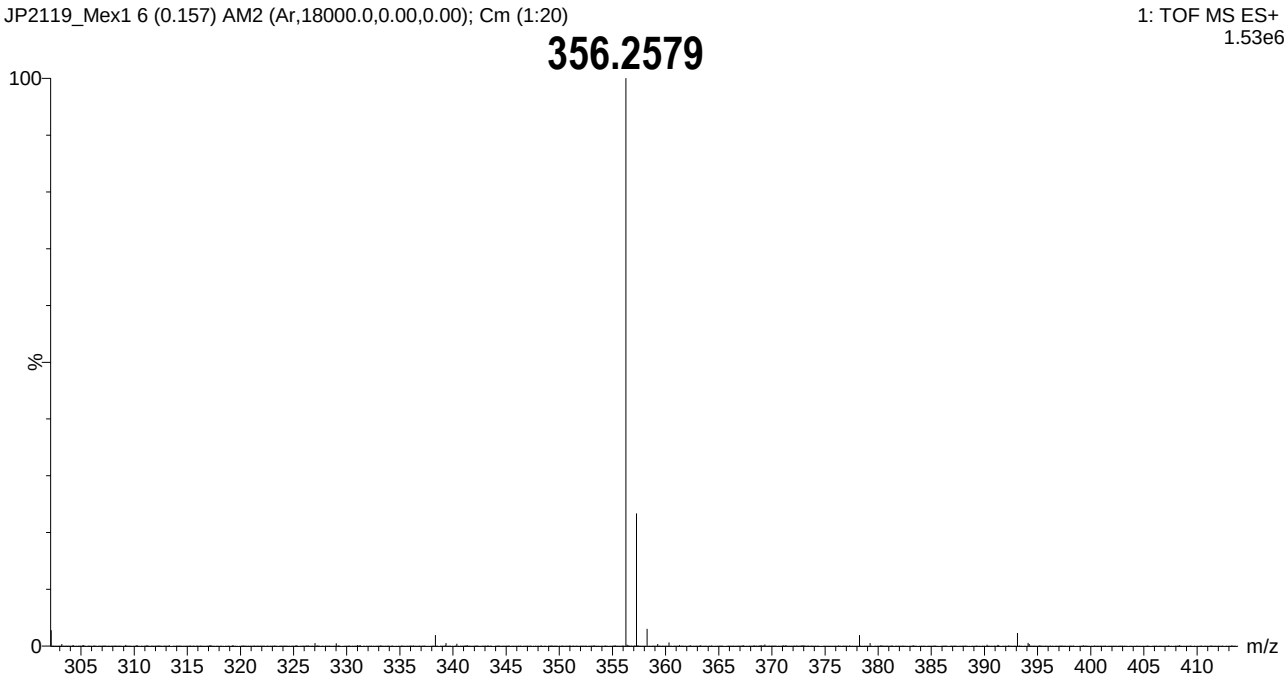
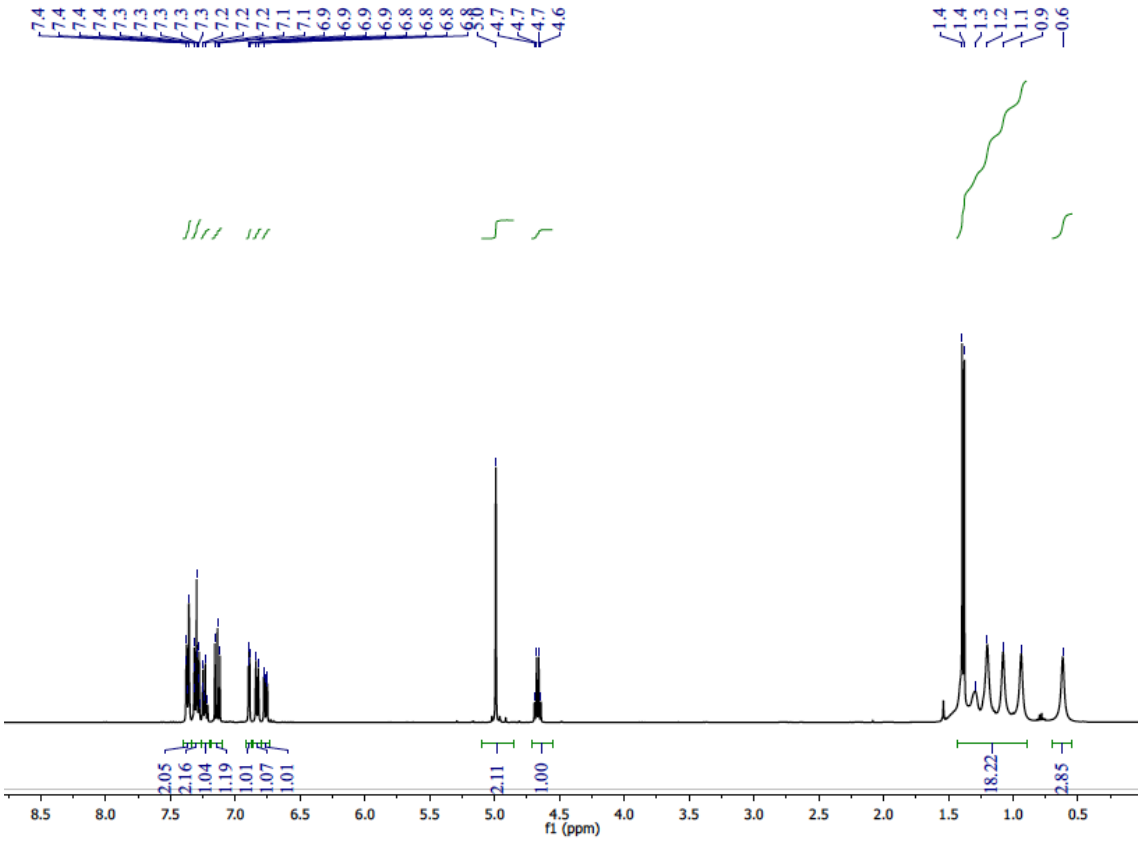
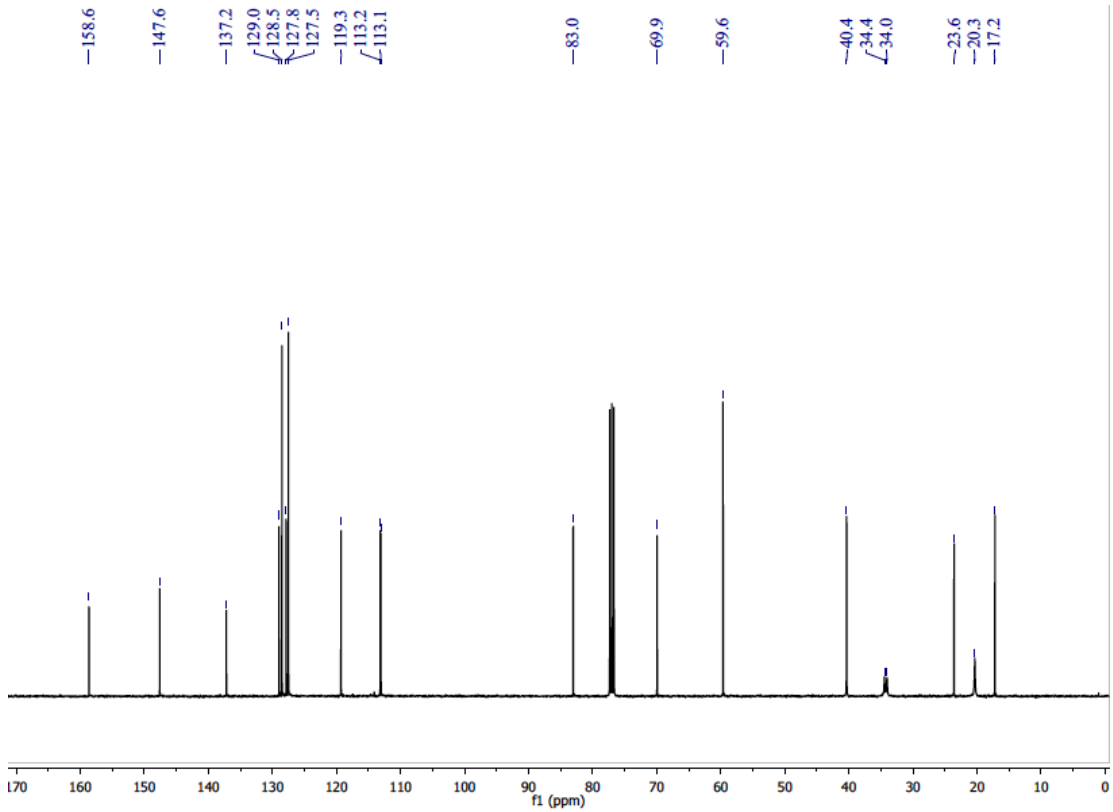


***1-(1-(3-(benzyloxy)phenyl)ethoxy)-2,2,6,6-tetramethylpiperidine* (1d).**

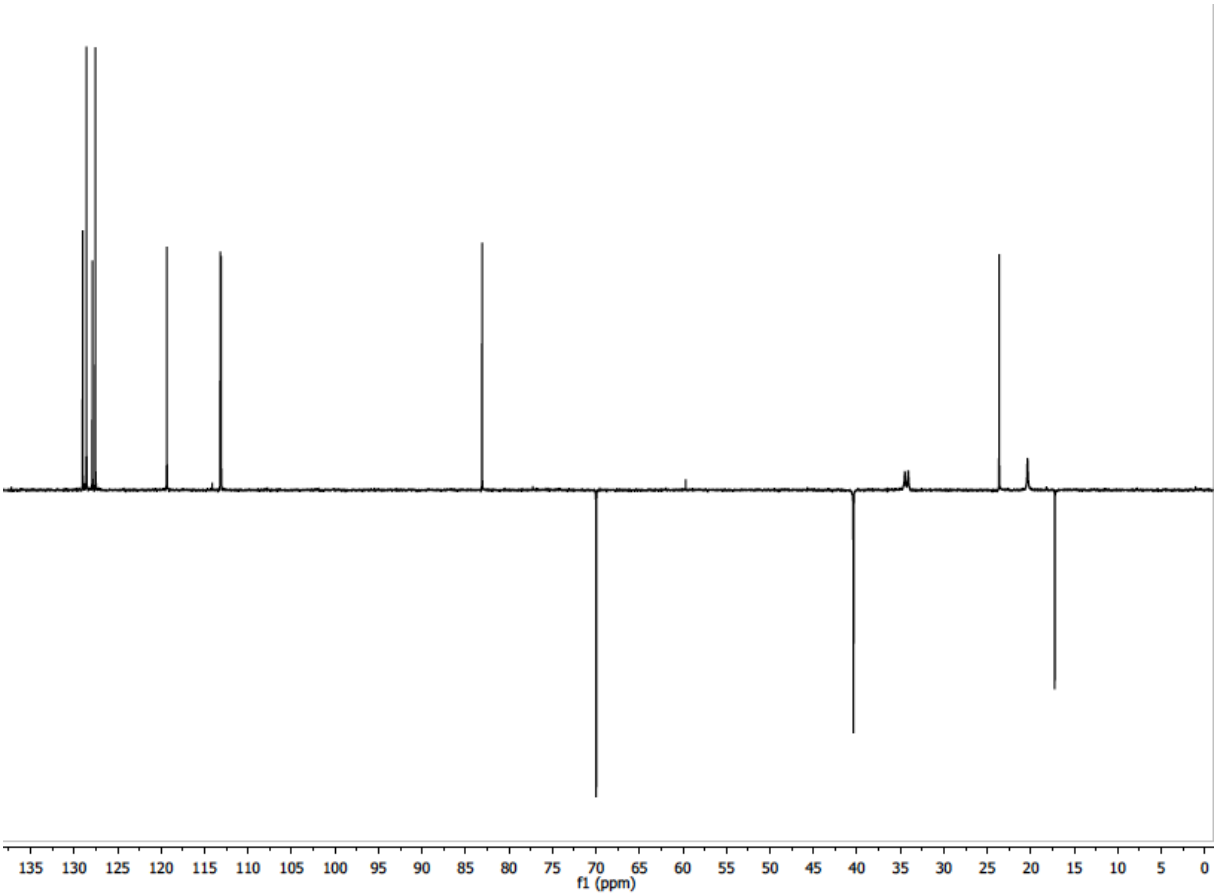
1d ^{1}H NMR (400 MHz, $CDCl_3$)



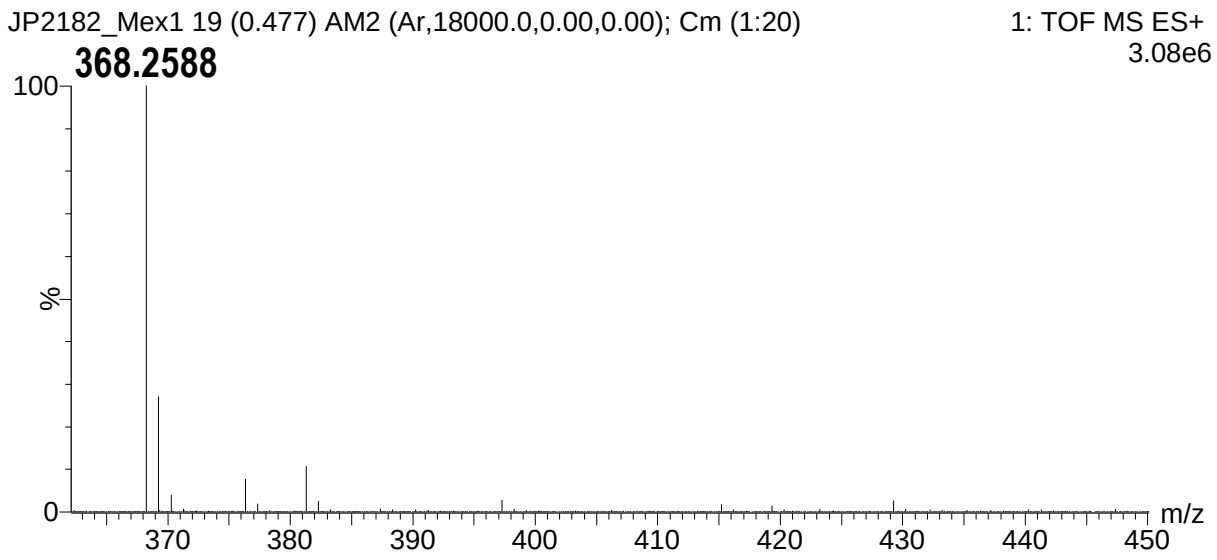
1d ^{13}C NMR (101 MHz, $CDCl_3$)



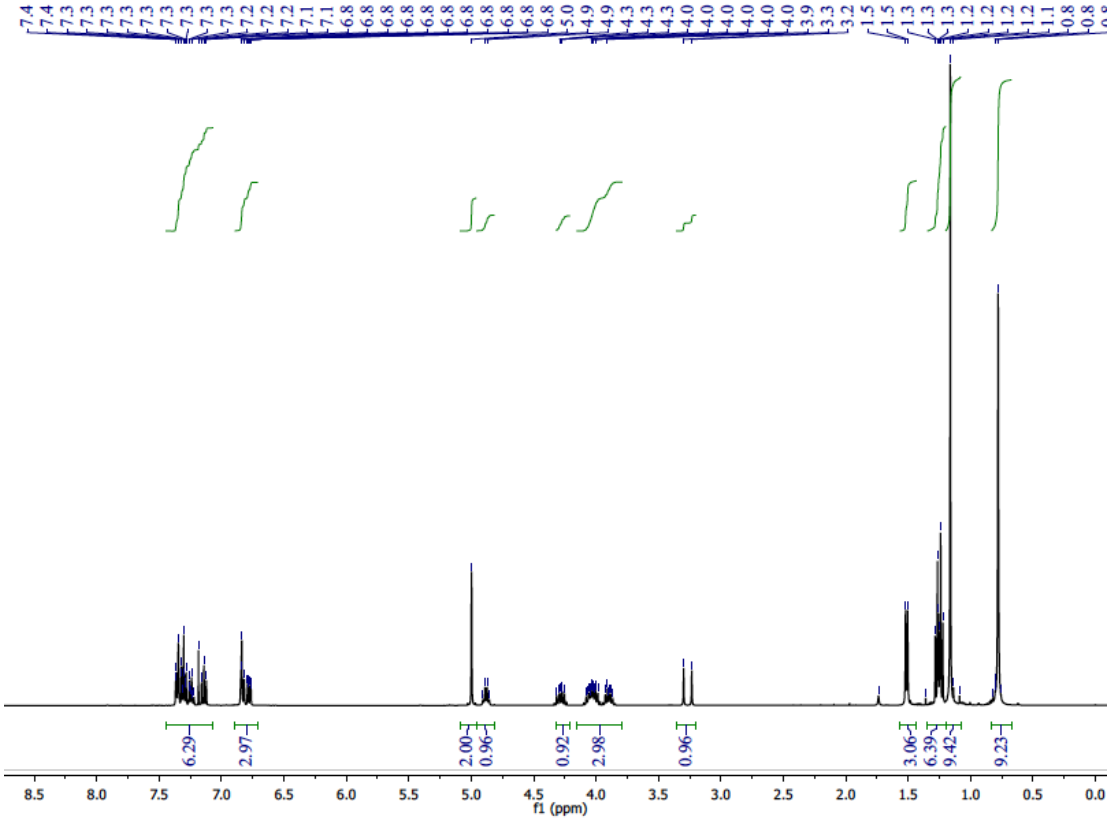
1dDEPT 135 (101 MHz, $CDCl_3$)



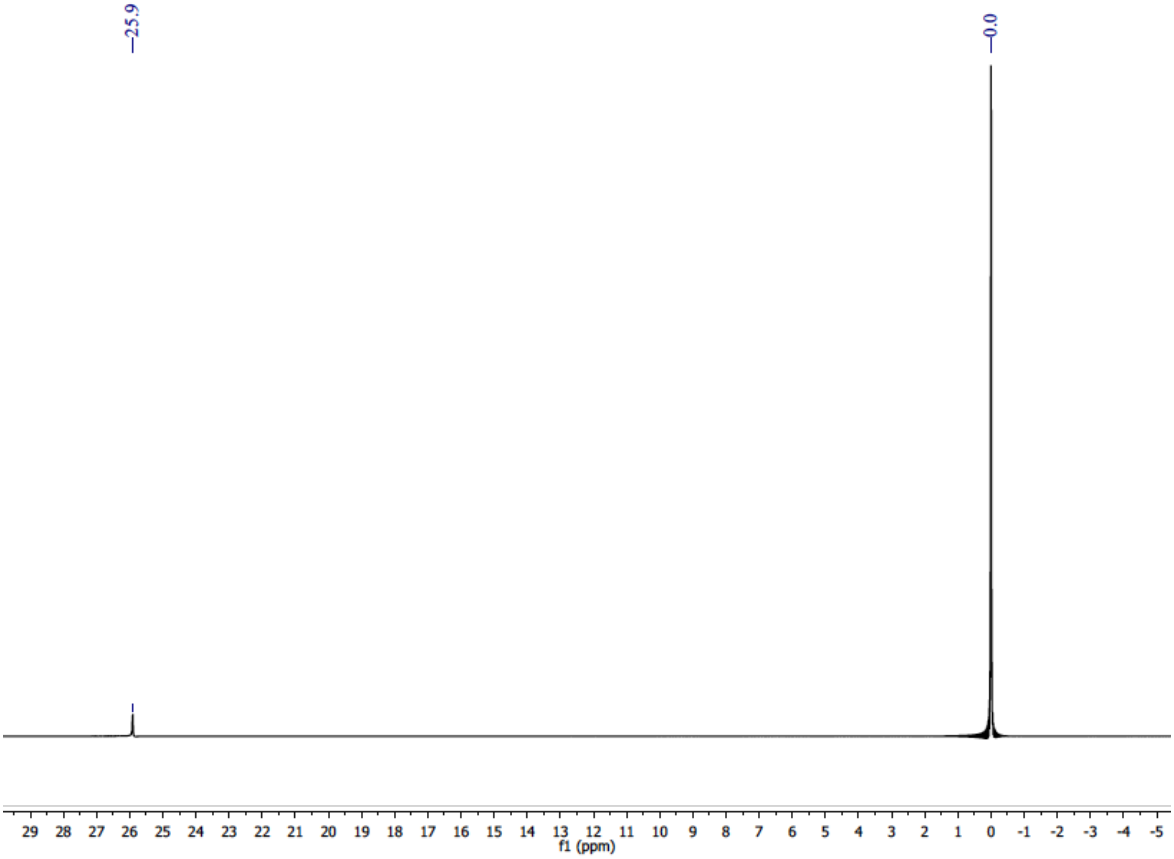
HRMS



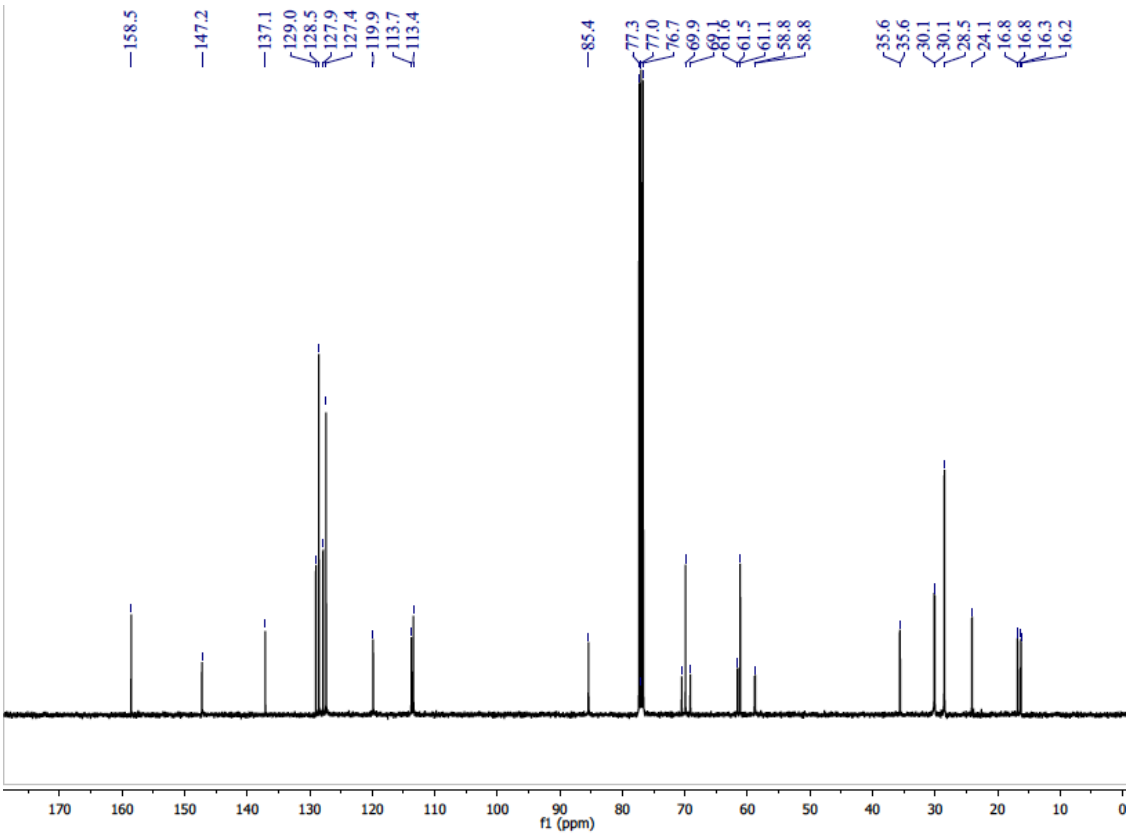
diethyl(1-((1-(3-(benzyloxy)phenyl)ethoxy)(tert-butyl)amino)-2,2-dimethylpropyl)phosphonate **(3d).**
(RR/SS)-**3d** ^{1}H NMR (400 MHz, $CDCl_3$)



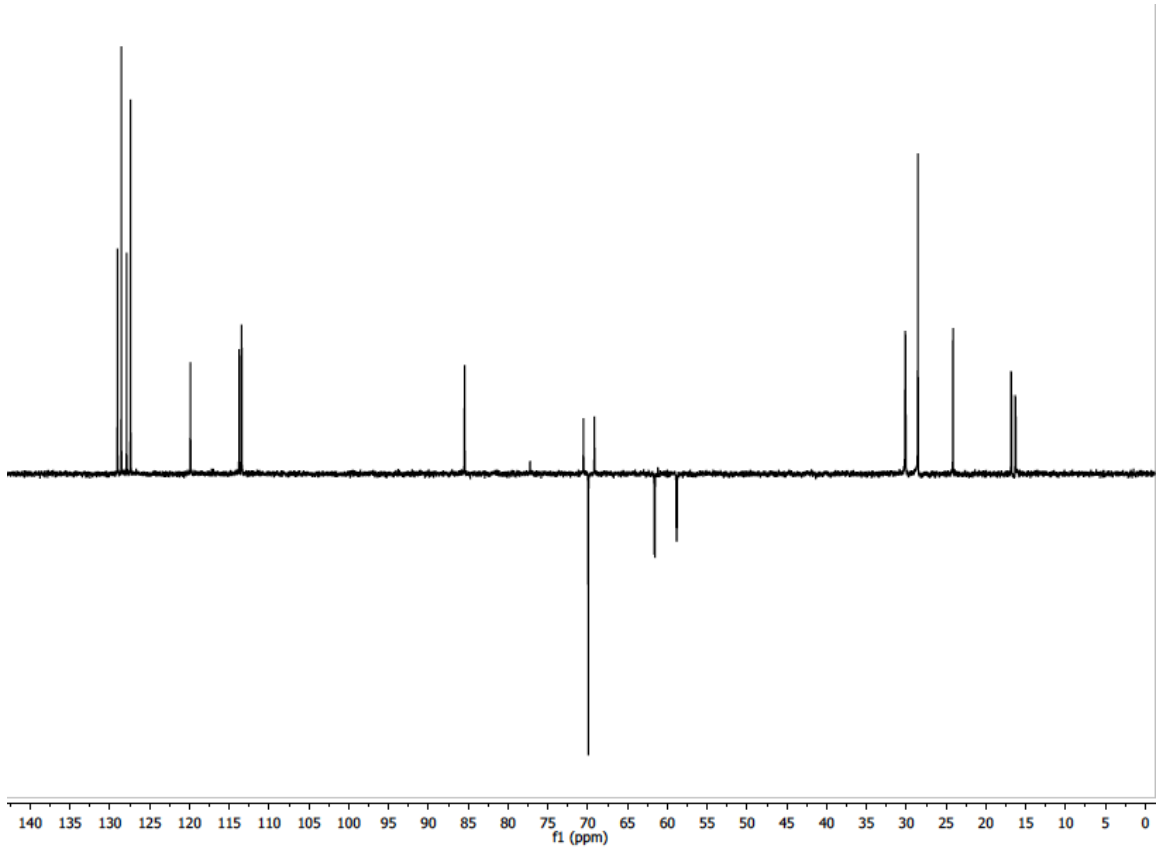
(RR/SS)-**3d** ^{31}P NMR (121 MHz, $CDCl_3$)



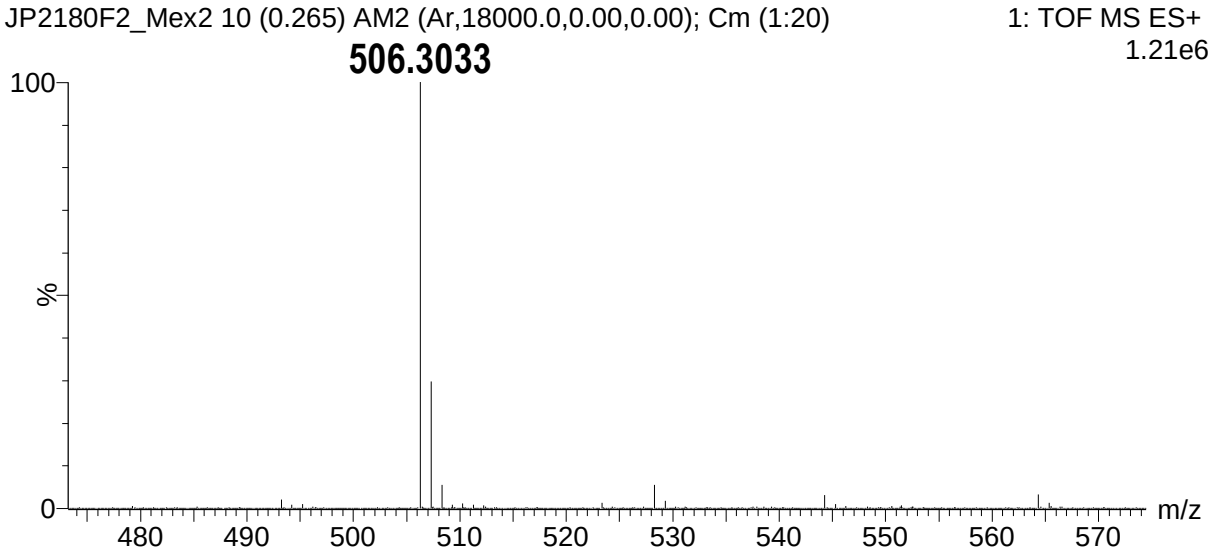
(RR/SS)-**3d** ^{13}C NMR (101 MHz, $CDCl_3$)



(RR/SS)-**3d** DEPT 135 (101 MHz, $CDCl_3$)



HRMS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506.3033
100
%
0
480
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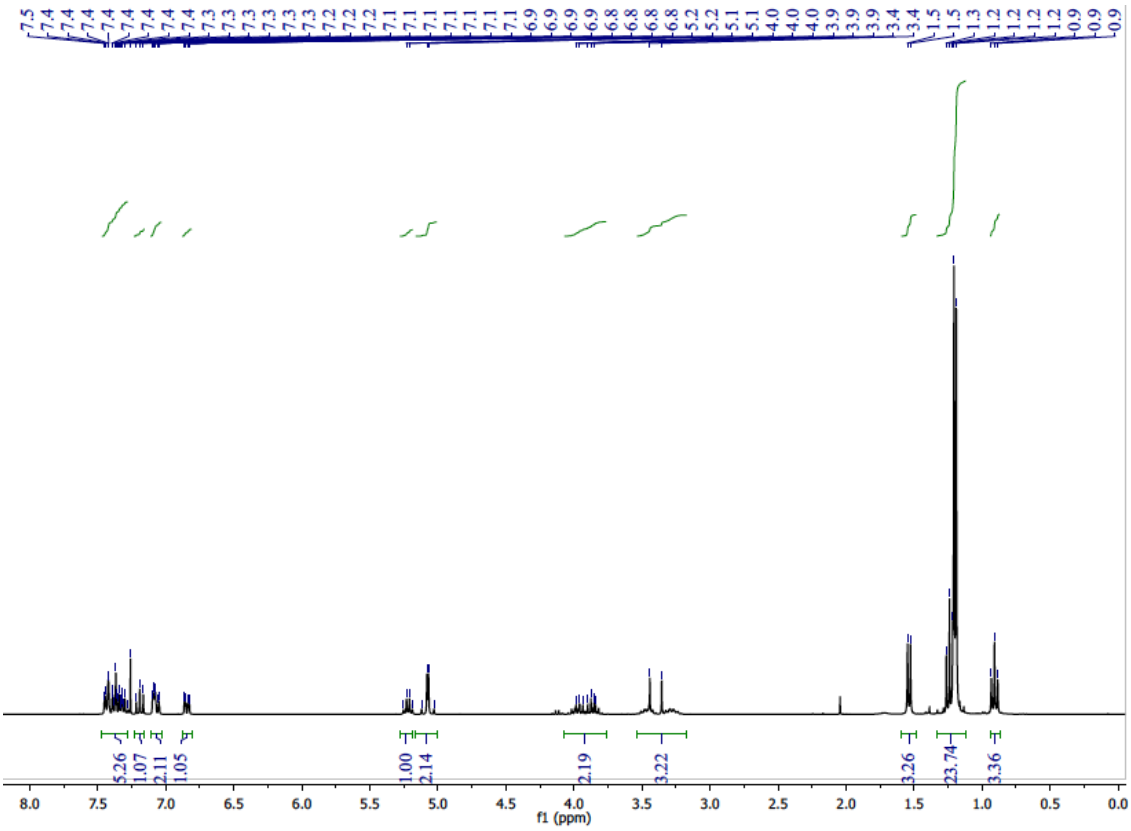
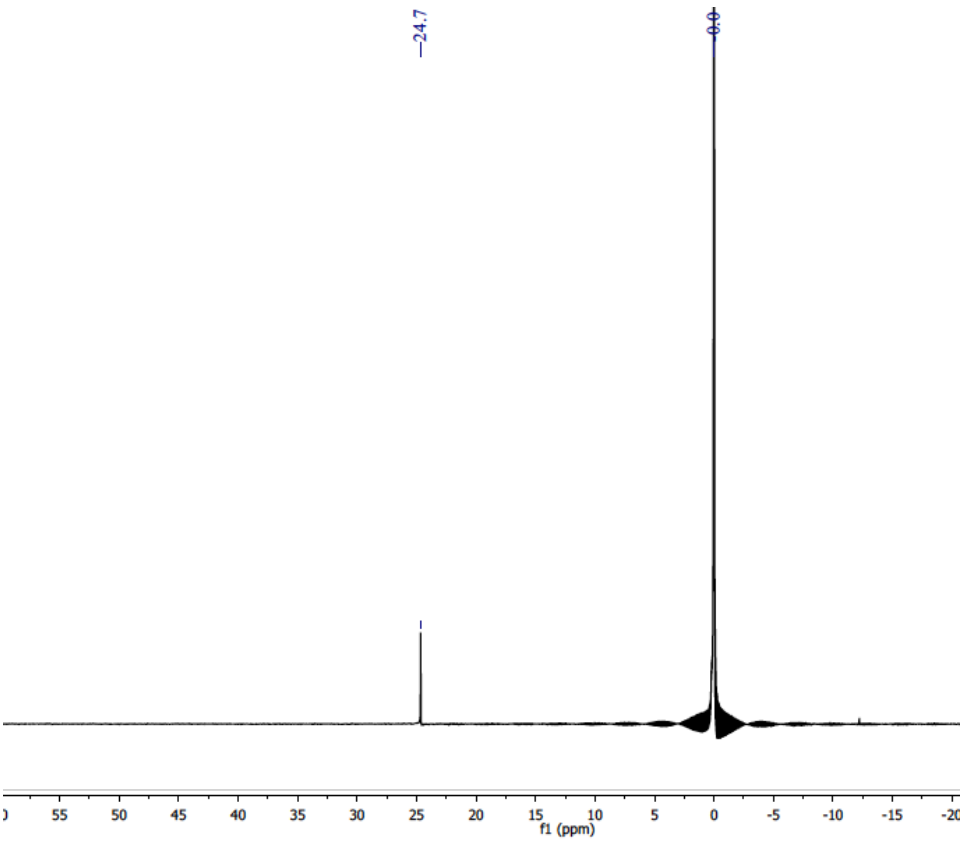
520
530
540
550
560
570
m/z

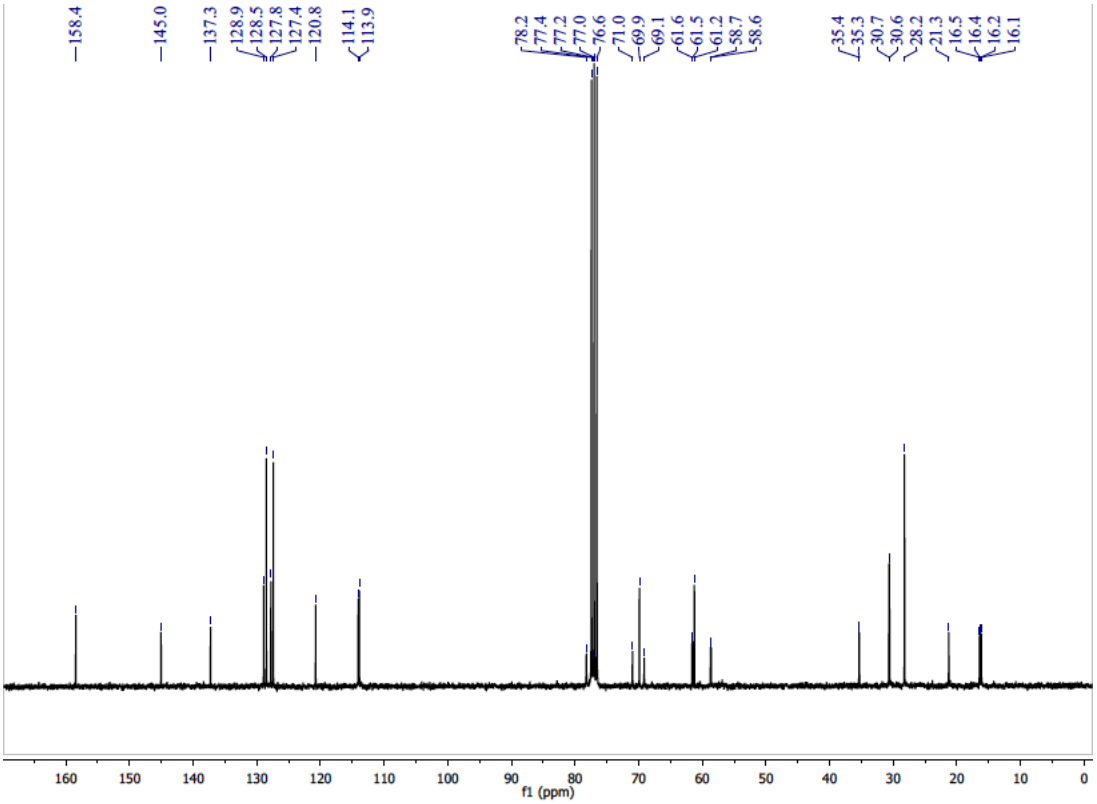
(RS/SR)-**3d** ^{1}H NMR (300 MHz, $CDCl_3$)



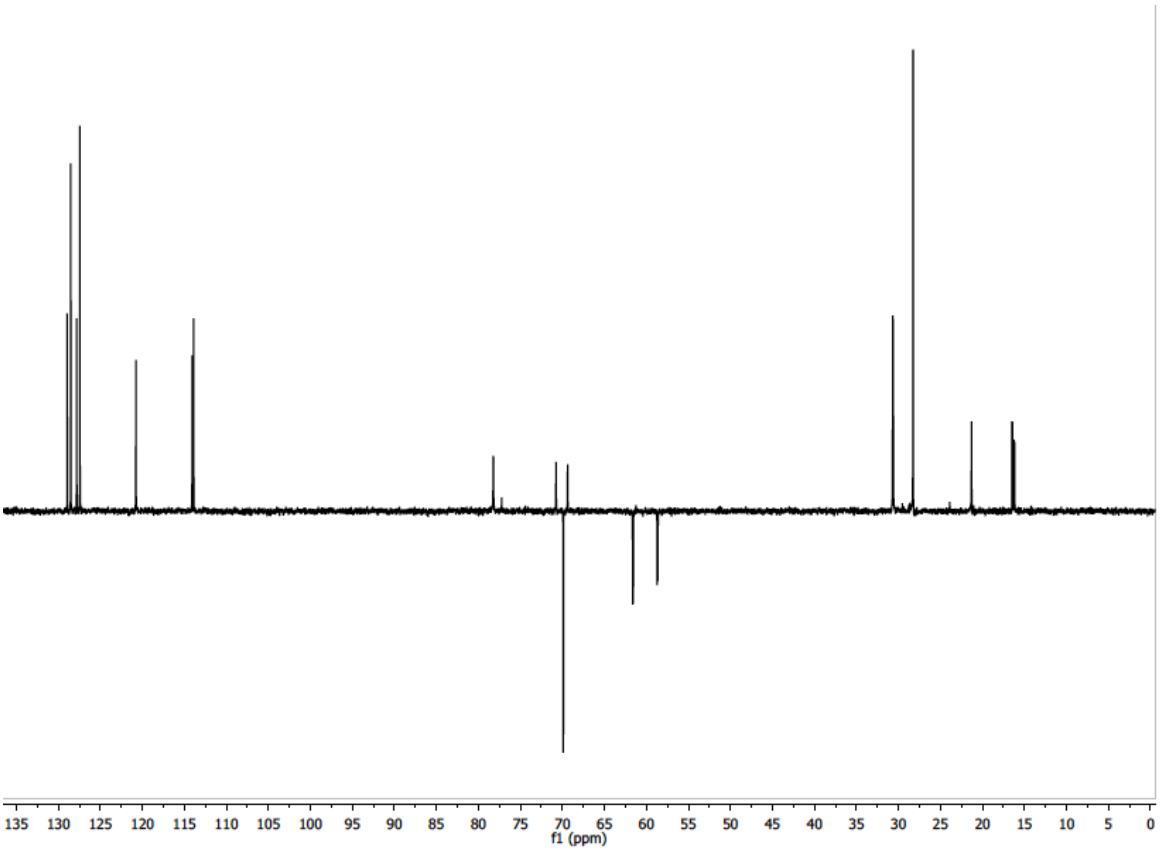
(RS/SR)-**3d** ^{31}P NMR (121 MHz, $CDCl_3$)



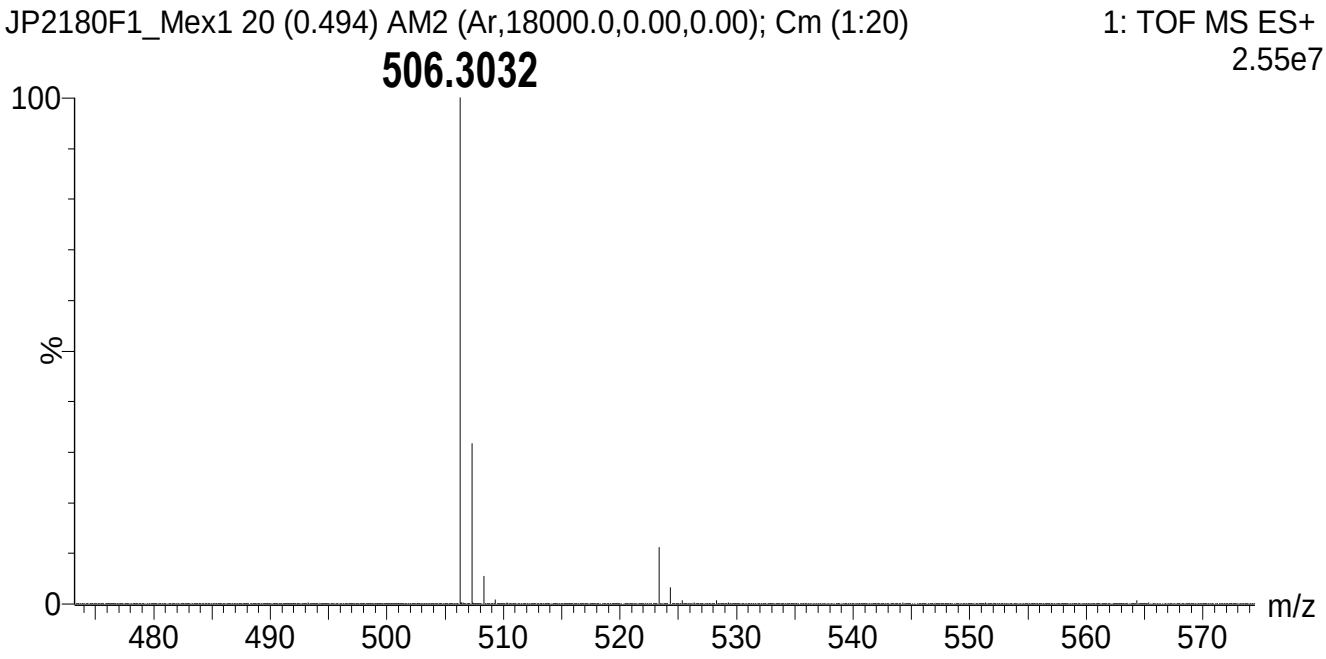
(RS/SR)-**3d** ^{13}C NMR (75 MHz, $CDCl_3$)



(RS/SR)-**3d** DEPT 135 (75 MHz, $CDCl_3$)



HRMS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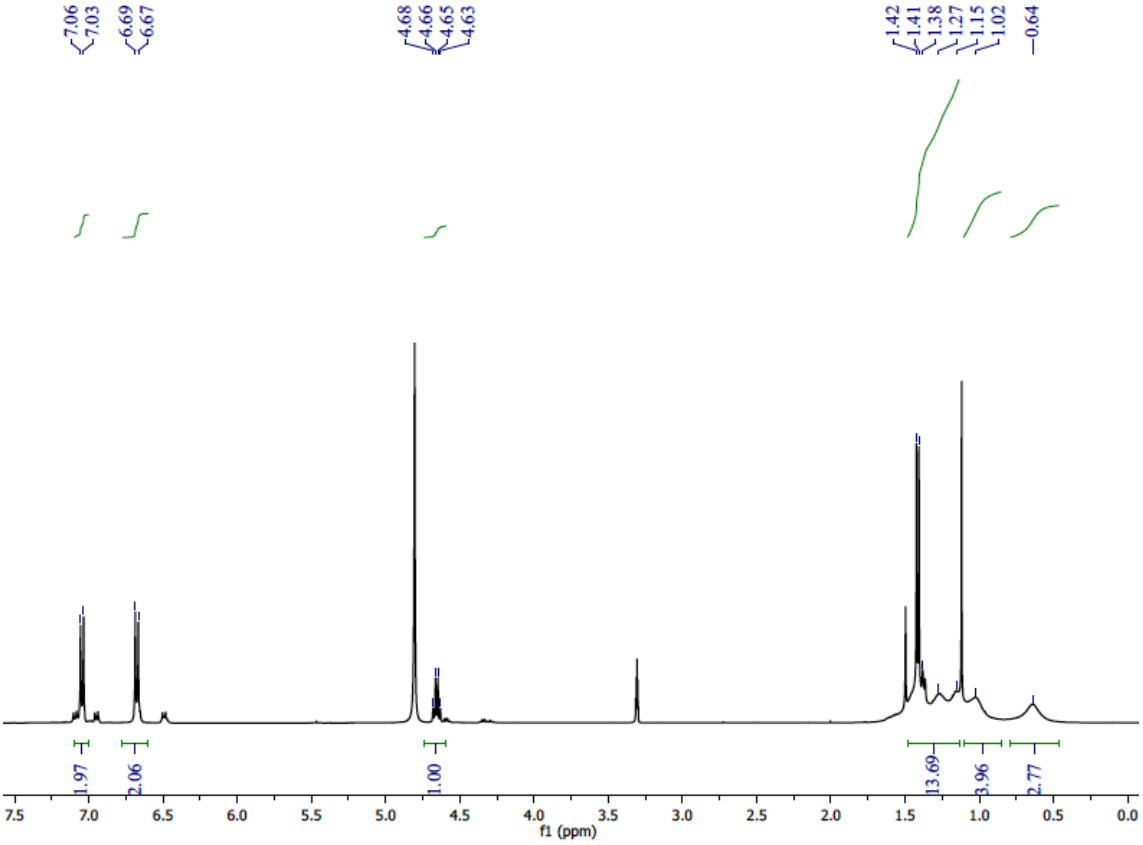
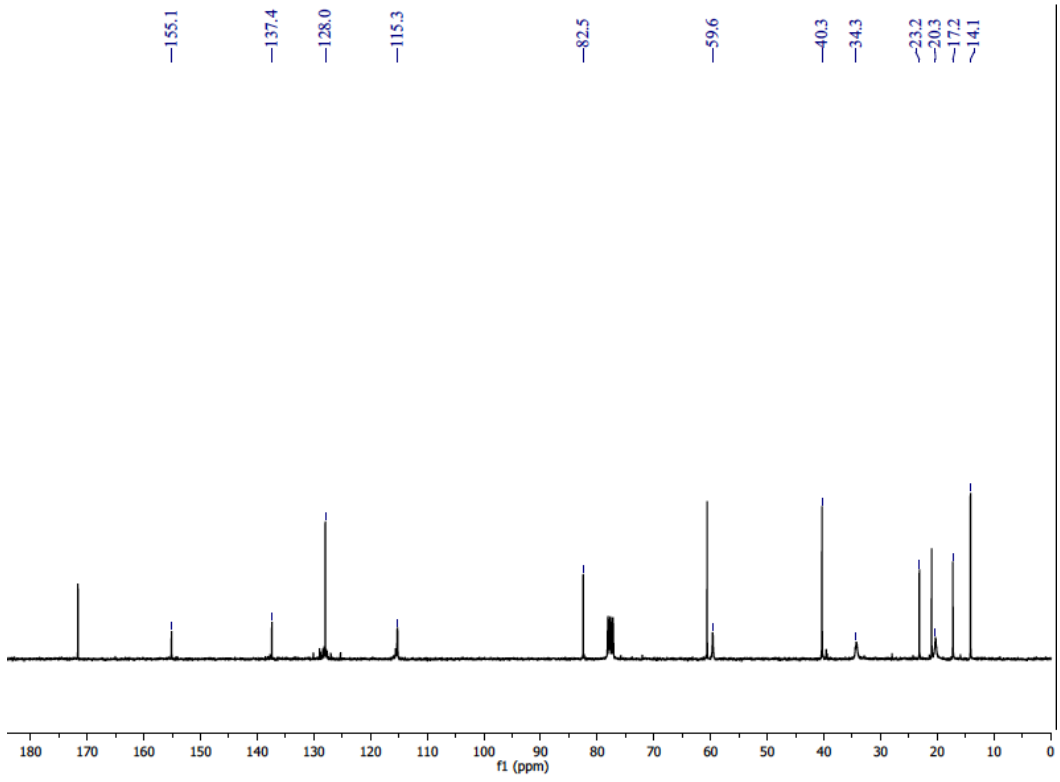
1: TOF MS ES+
2.55e7
506.3032
100
%
0
480
490
500
510
520
530
540
550
560
570
m/z

***4-(1-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)ethyl)phenol* (1a).**

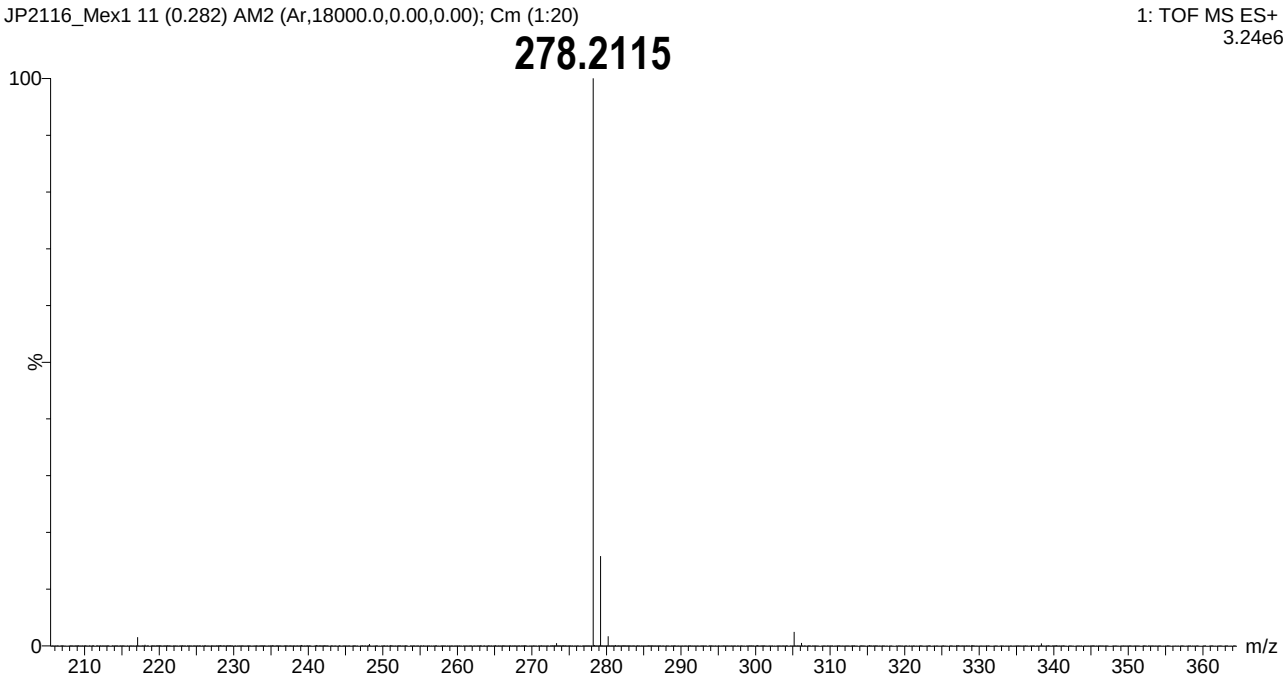
1a ^{1}H NMR (400 MHz, CD_3OD)



1a ^{13}C NMR (75 MHz, $CDCl_3$ with EtOAc)

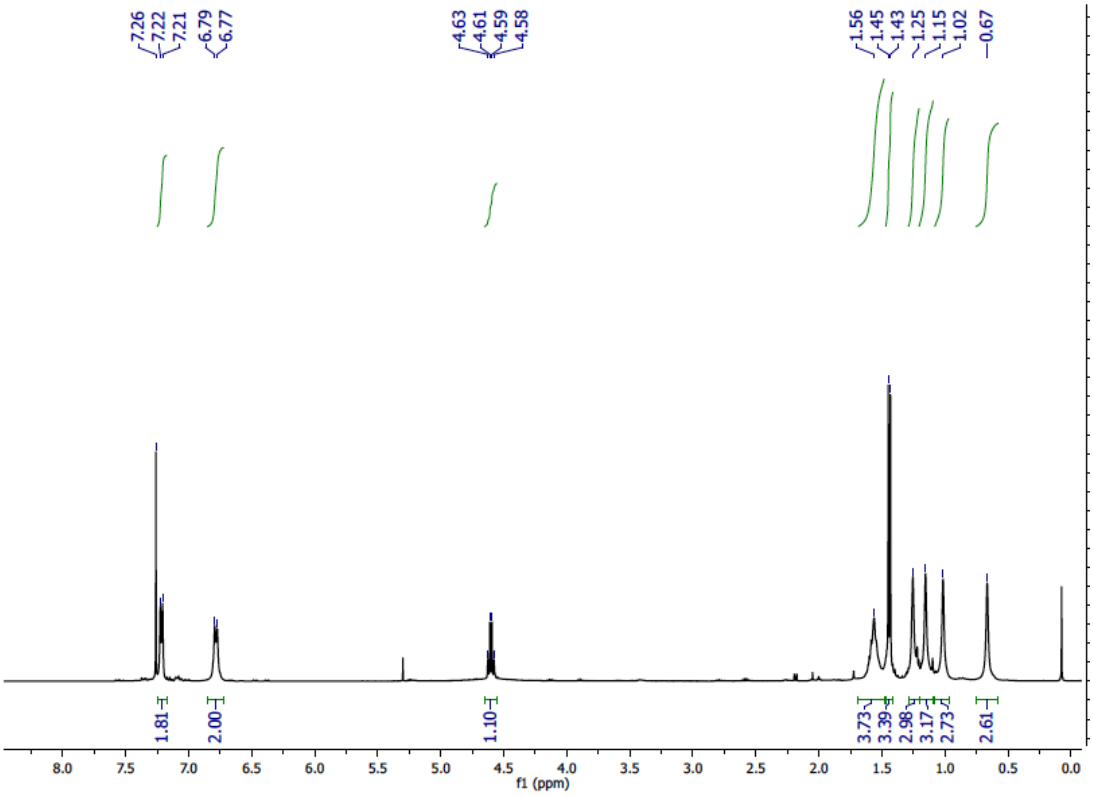


HRMS

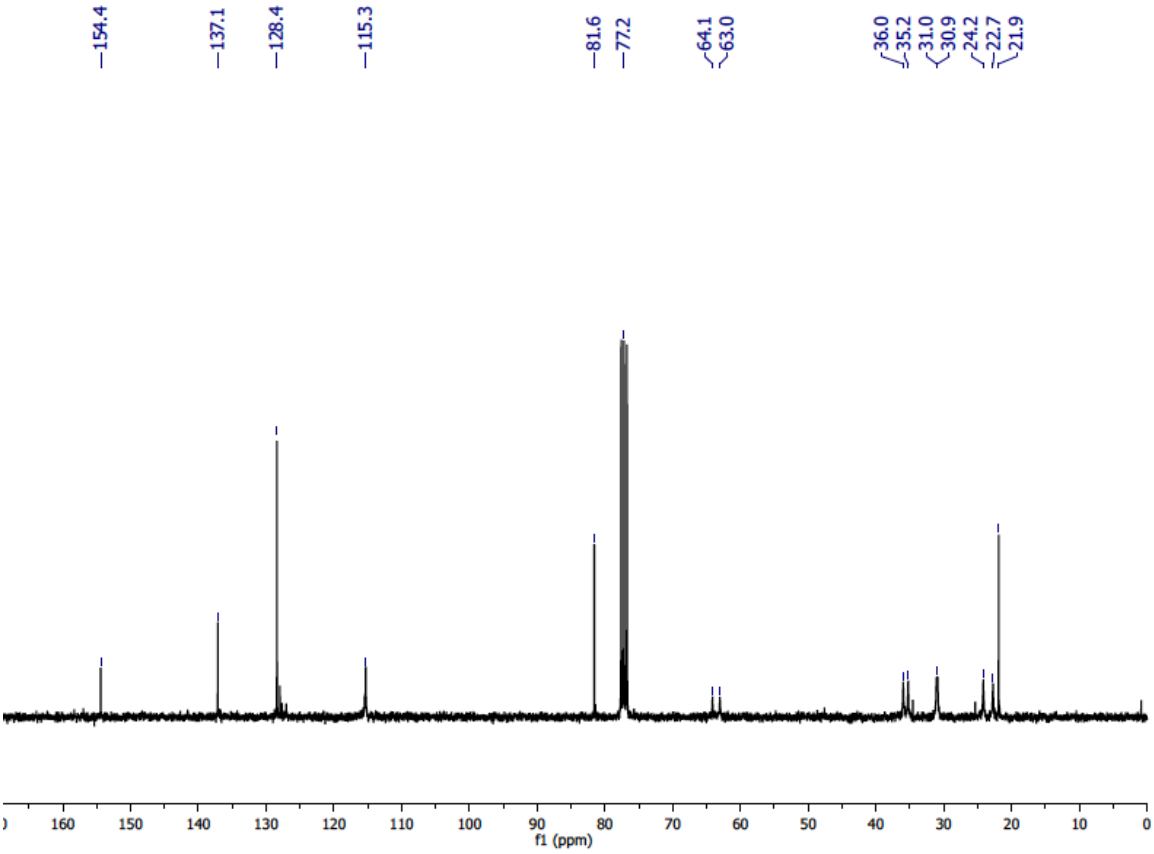

JP2116_Mex1 11 (0.282) AM2 (Ar,18000.0,0.00,0.00); Cm (1:20)
1: TOF MS ES+
3.24e6
278.2115
100
%
0
210
220
230
240
250
260
270
280
290
300
310
320
330
340
350
360
m/z

***4-(1-((2,2,5,5-tetramethylpyrrolidin-1-yl)oxy)ethyl)phenol* (2a).**

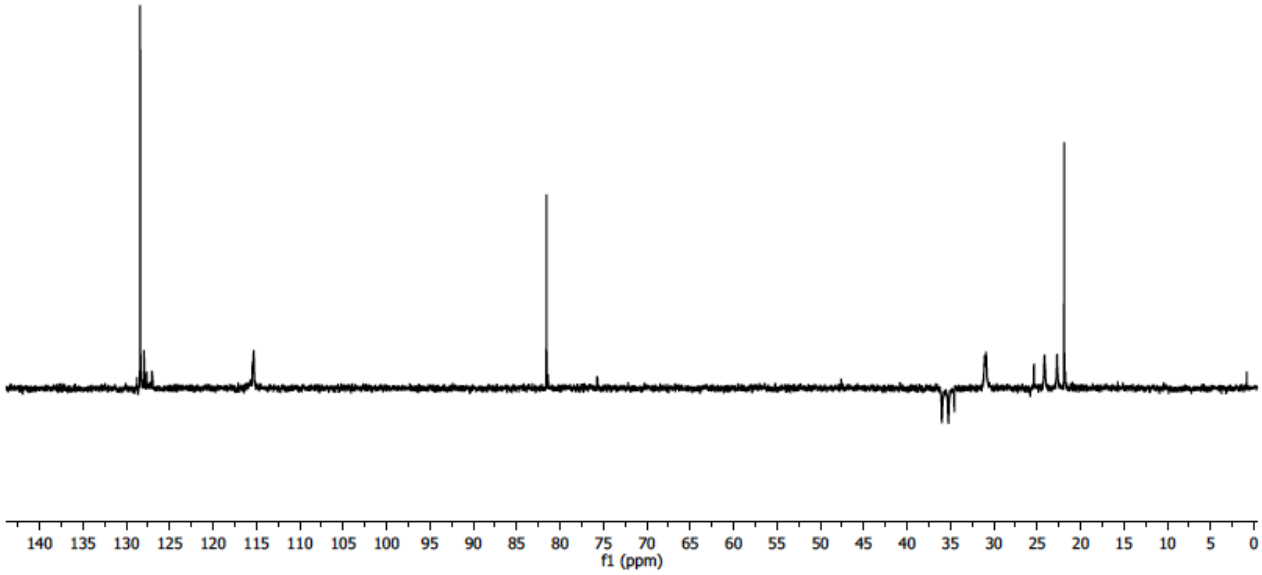
2a ^{1}H NMR (400 MHz, $CDCl_3$)



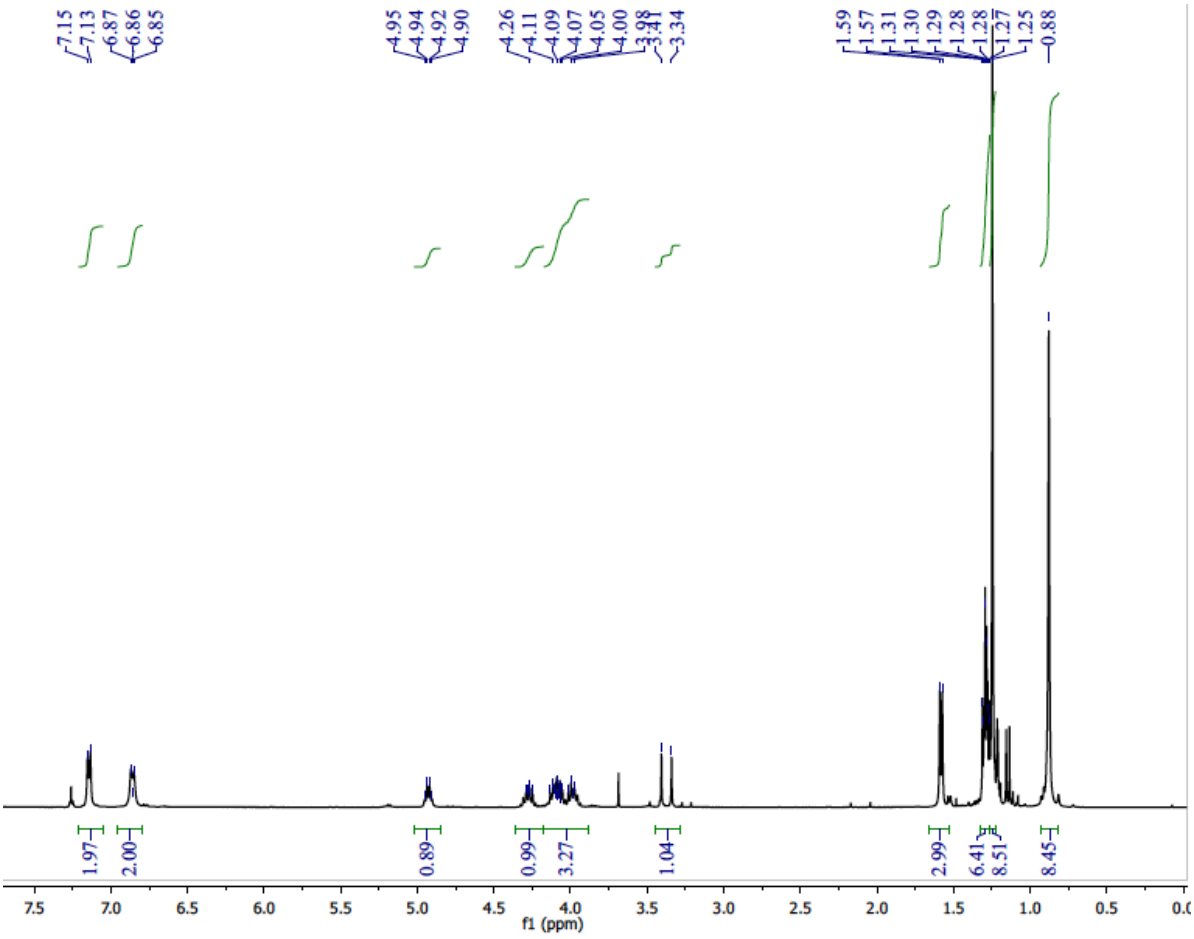
2a ^{13}C NMR (75 MHz, $CDCl_3$)



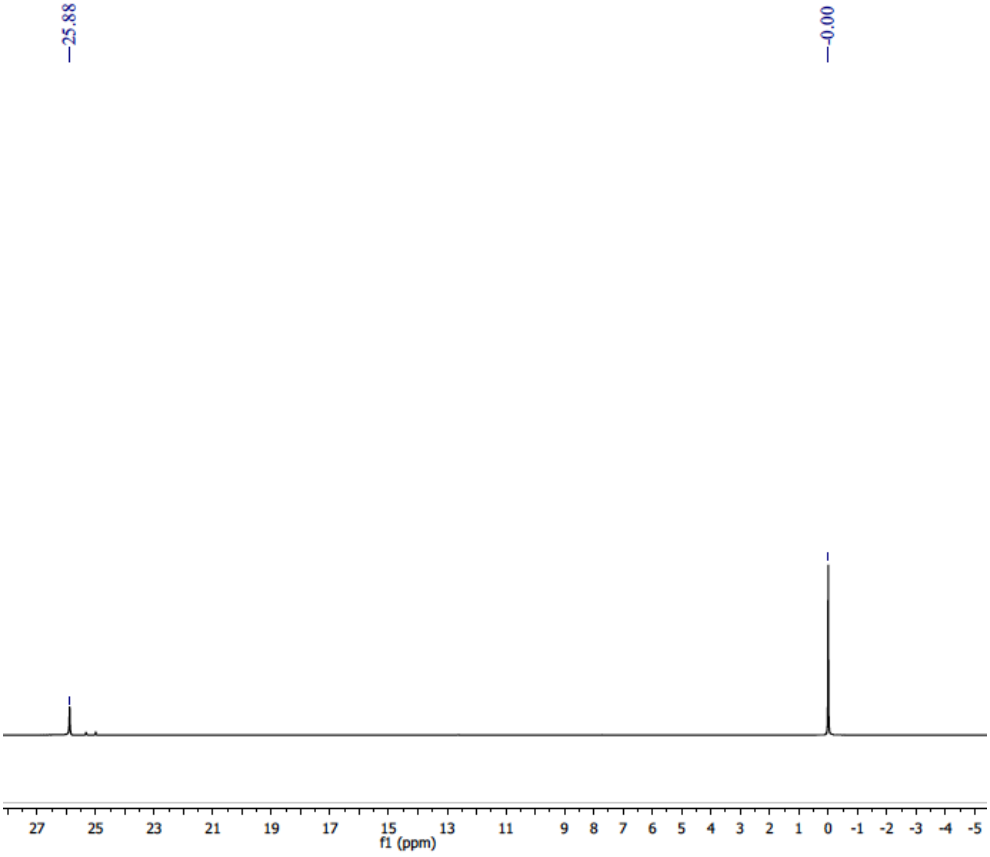
2a DEPT 135 (75 MHz, $CDCl_3$)



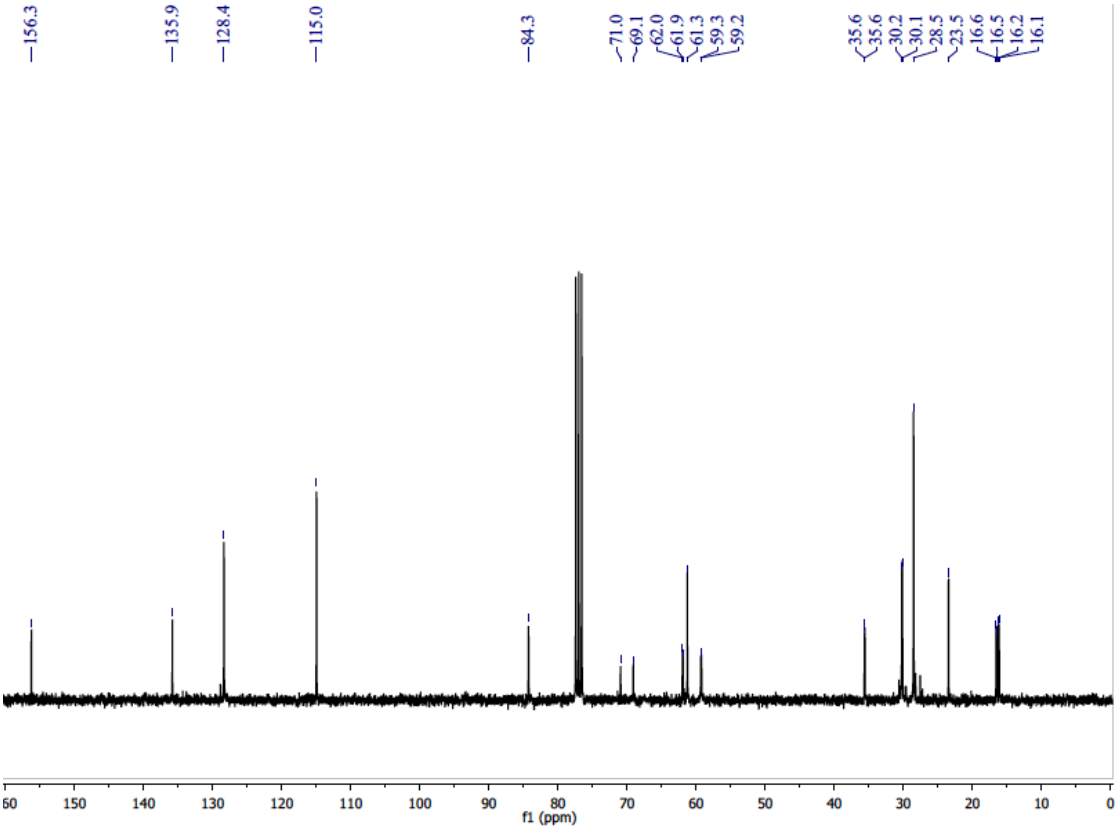
diethyl (1-(tert-butyl(1-(4-hydroxyphenyl)ethoxy)amino)-2,2-dimethylpropyl)phosphonate **(3a)**.
(RR/SS)-**3a** ^{1}H NMR (400 MHz, $CDCl_3$)



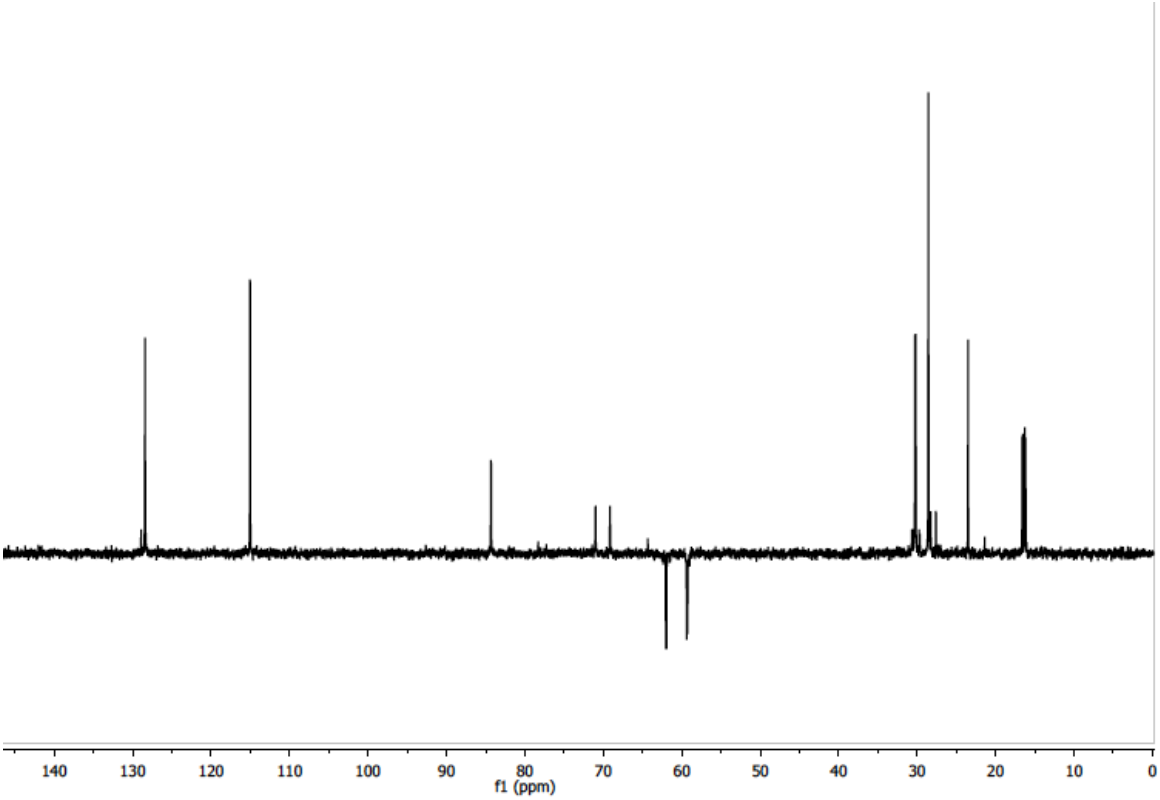
(RR/SS)-**3a** ^{31}P NMR (121 MHz, $CDCl_3$)



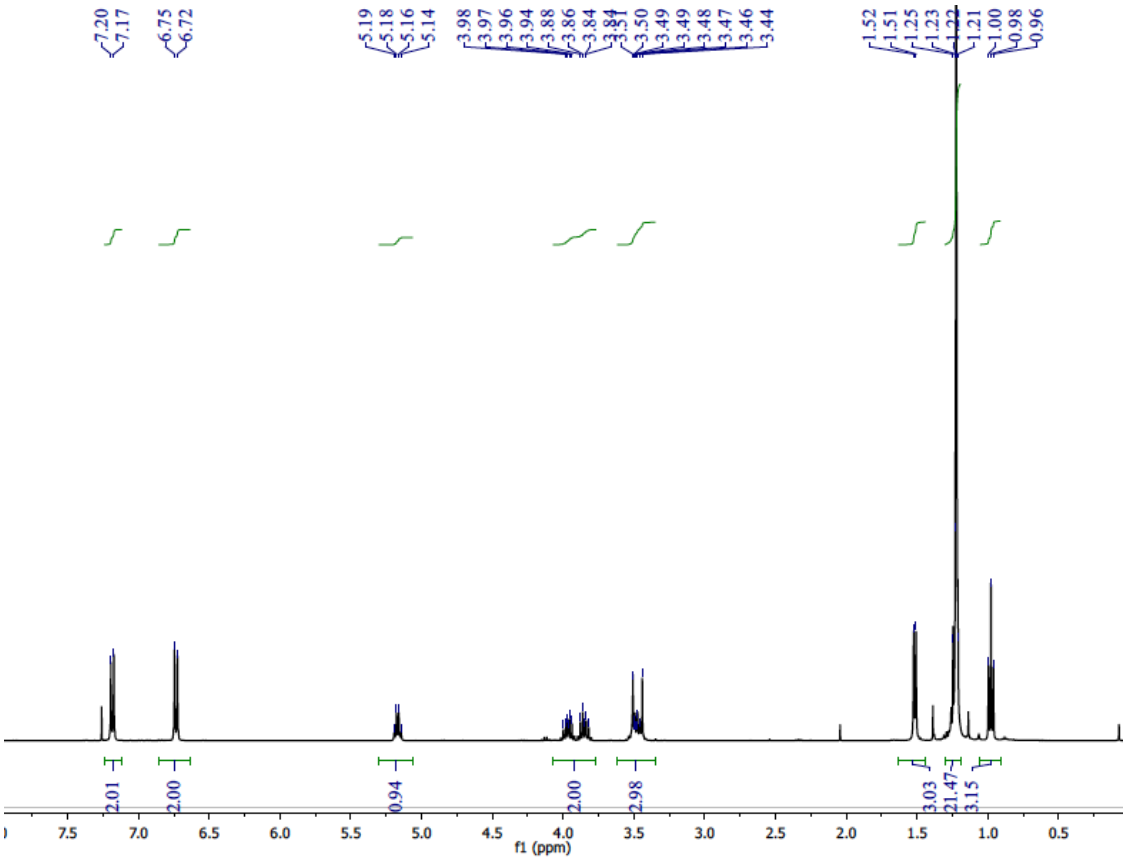
(RR/SS)-**3a** ^{13}C NMR (75 MHz, $CDCl_3$)



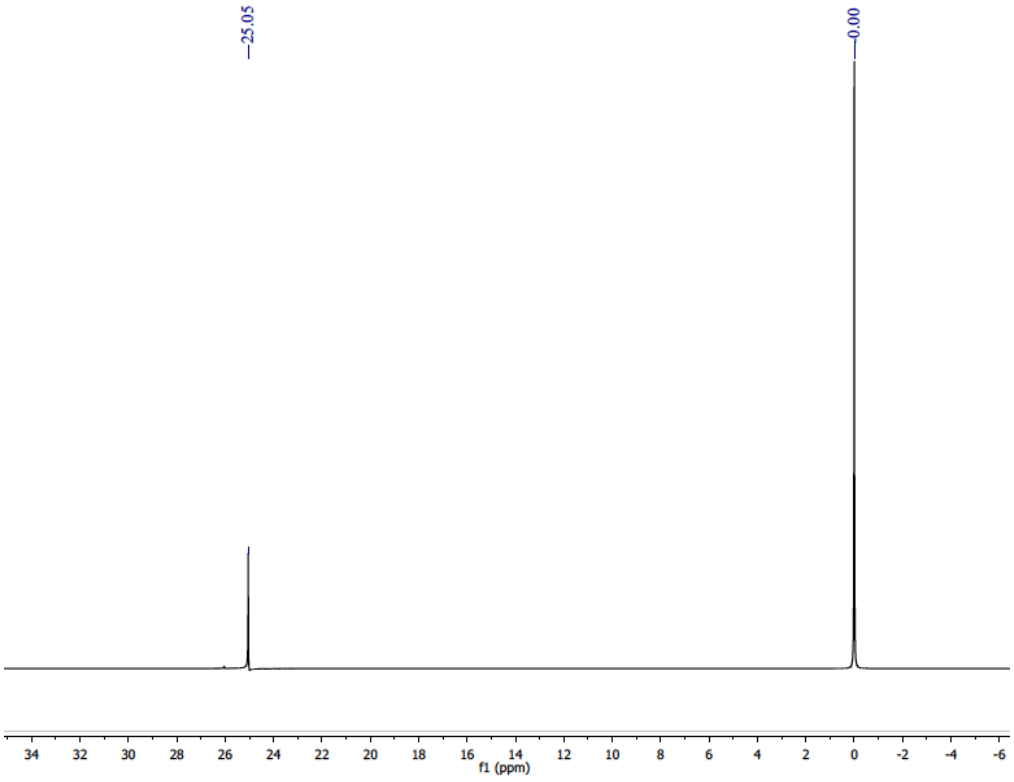
(RR/SS)-**3a** DEPT 135 (75 MHz, $CDCl_3$)



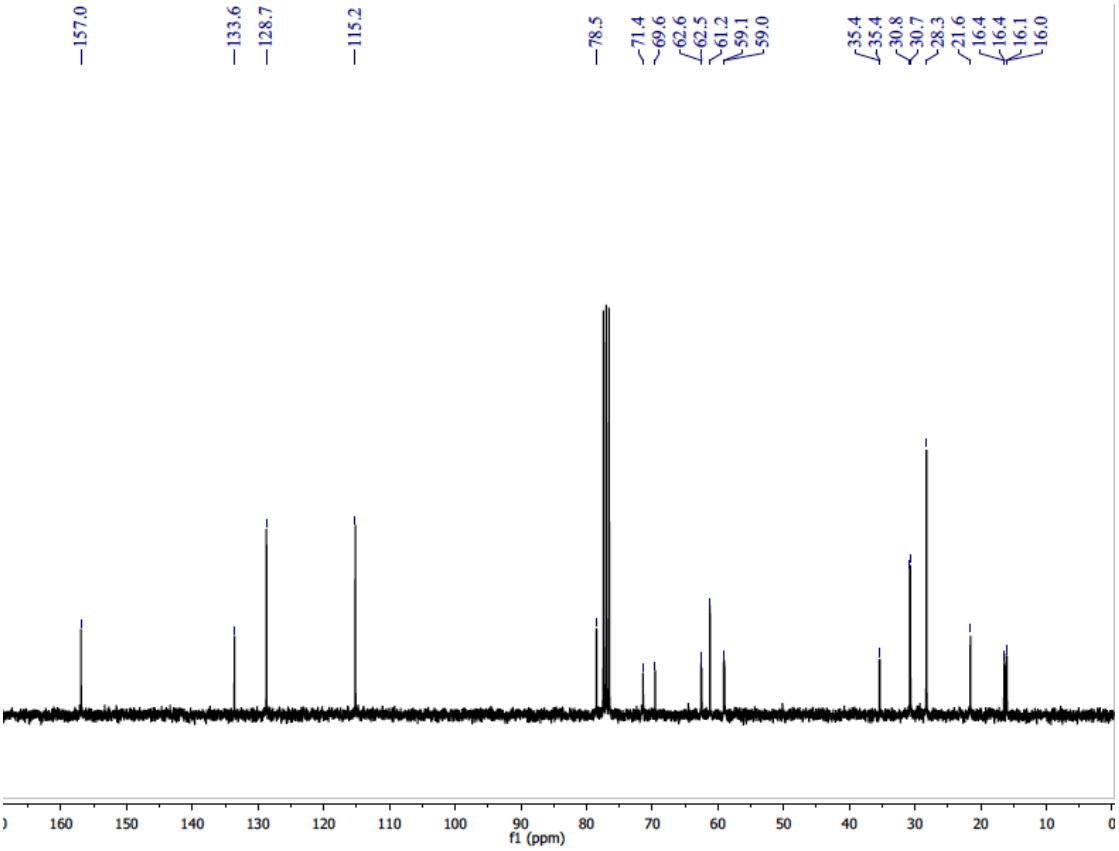
(RS/SR)-**3a** ^{1}H NMR (400 MHz, $CDCl_3$)



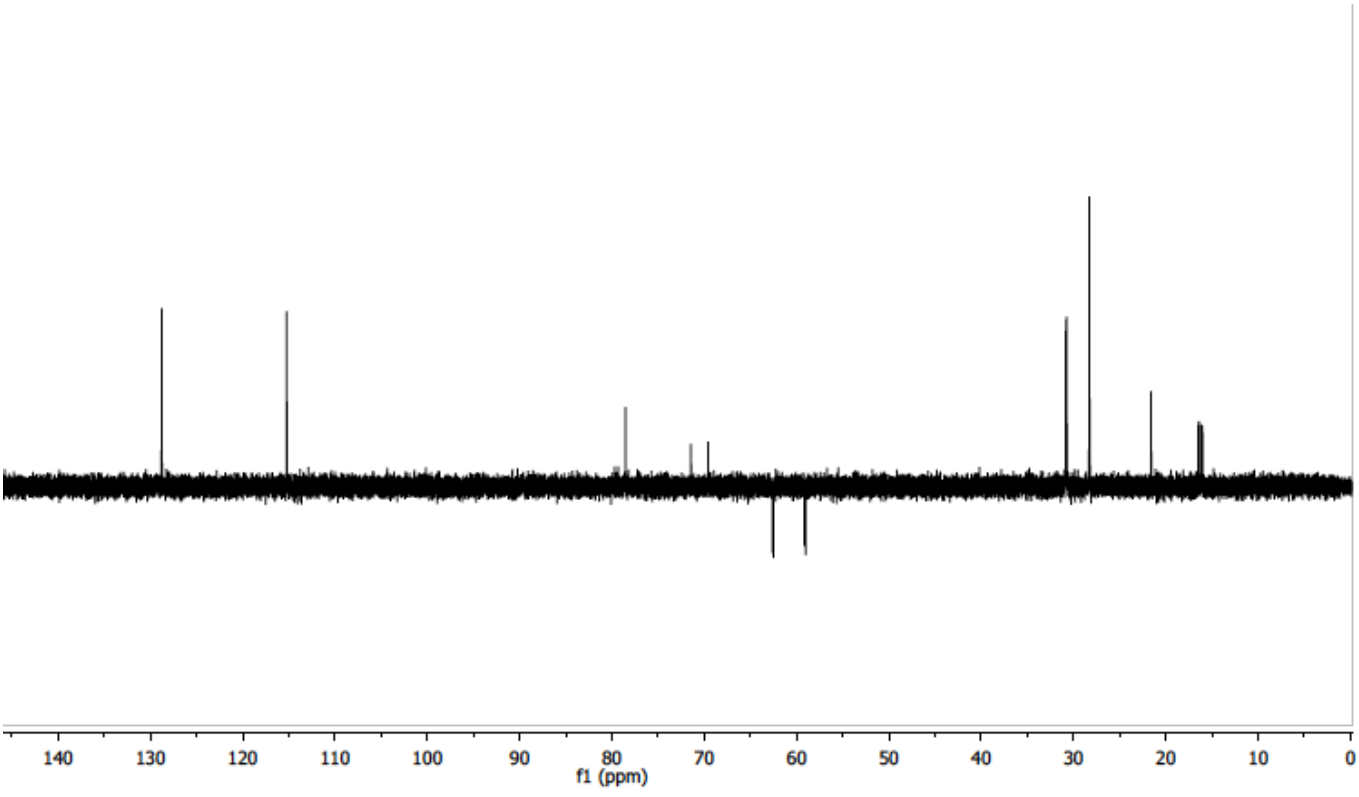
(RS/SR)-**3a** ^{31}P NMR (121 MHz, $CDCl_3$)



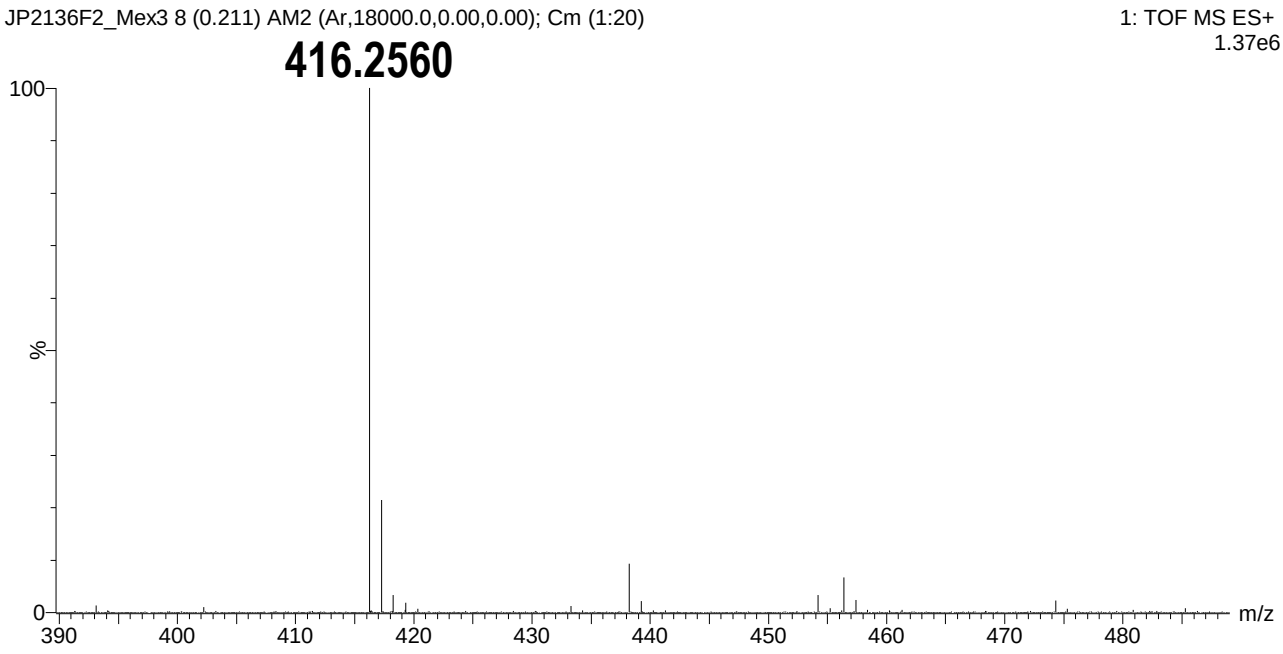
(RS/SR)-**3a** ^{13}C NMR (75 MHz, $CDCl_3$)



(RS/SR)-**3a** DEPT 135 (75 MHz, $CDCl_3$)

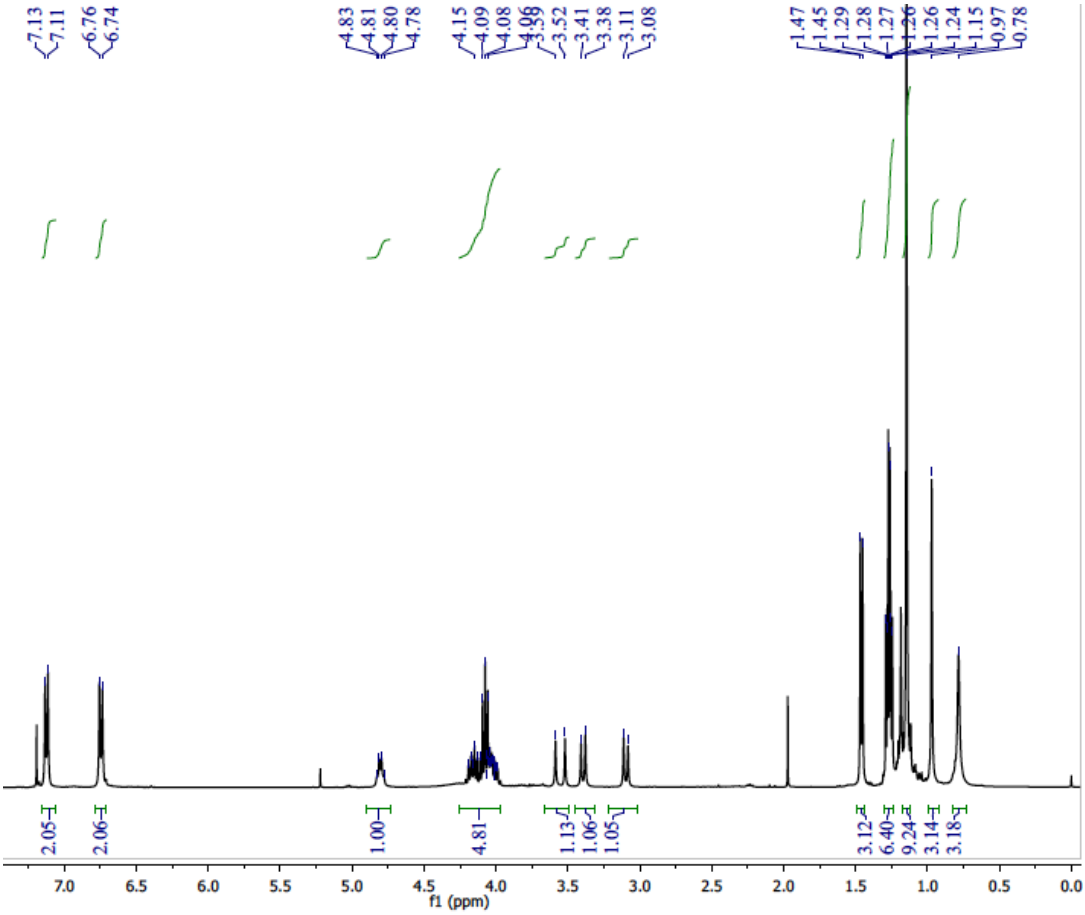


HRMS (mixture of diastereoisomers)

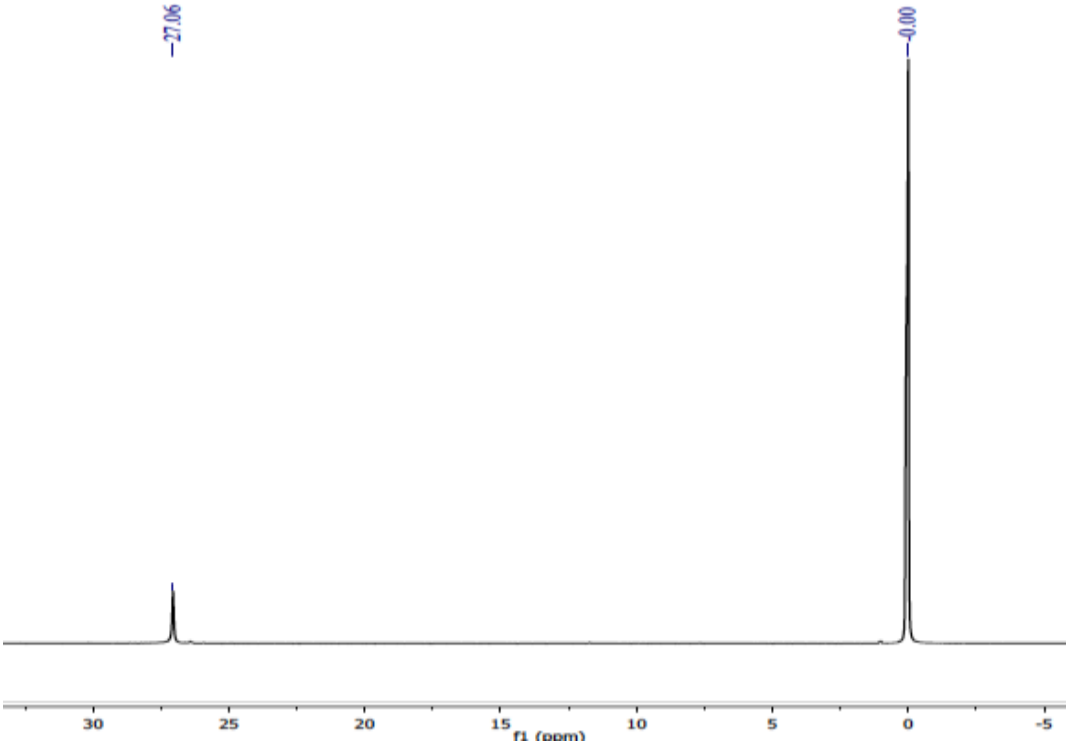


***diethyl(1-((1-hydroxy-2-methylpropan-2-yl)(1-(4-hydroxyphenyl)ethoxy)amino)-2,2 dimethylpropyl)phosphonate* (4a).**

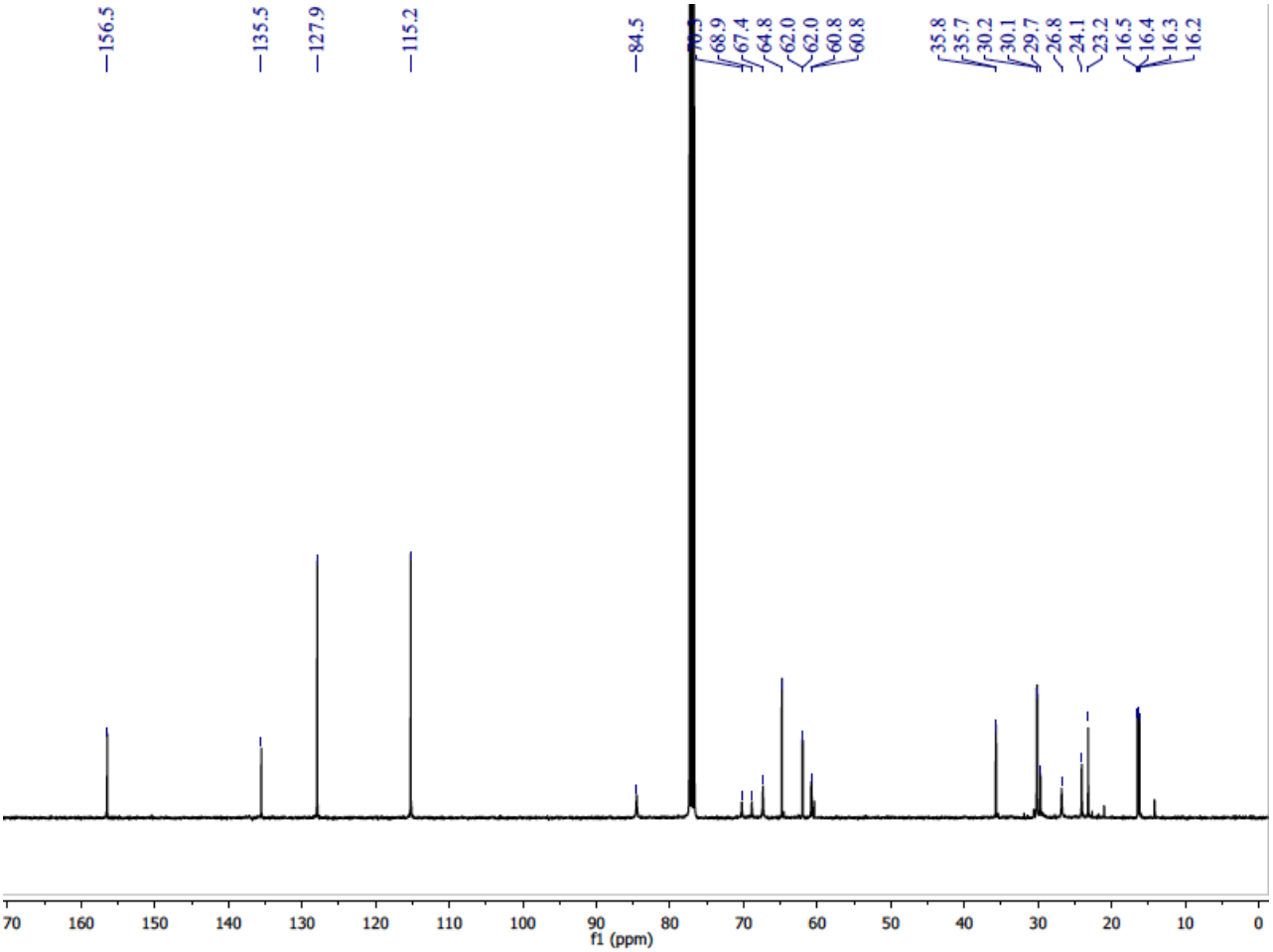
(RR/SS)-**4a** ^{1}H NMR (400 MHz, $CDCl_3$)



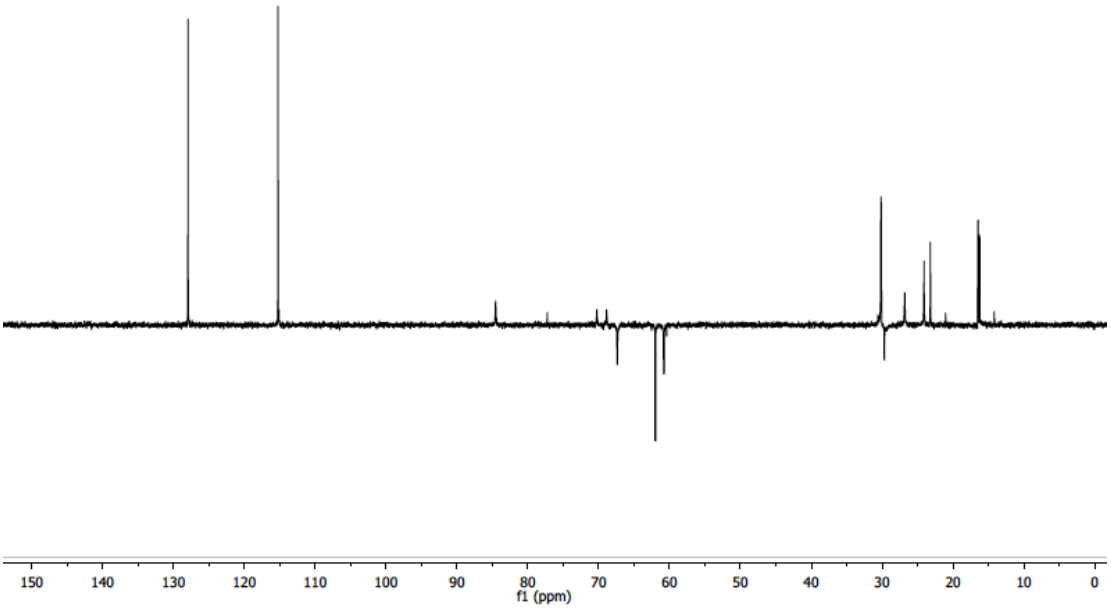
(RR/SS)-**4a** ^{31}P NMR (121 MHz, $CDCl_3$)



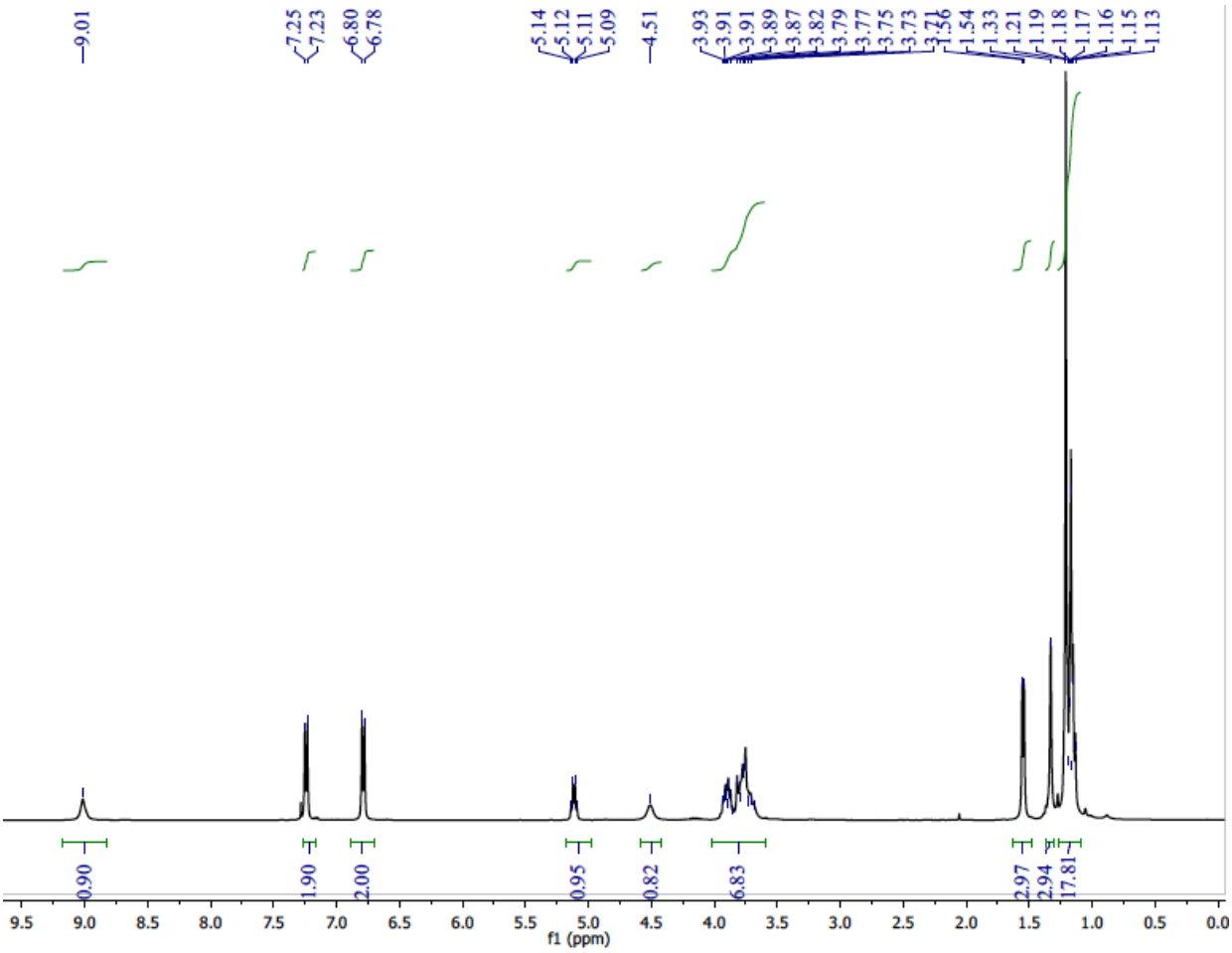
(RR/SS)-**4a** ^{13}C NMR (101 MHz, $CDCl_3$)



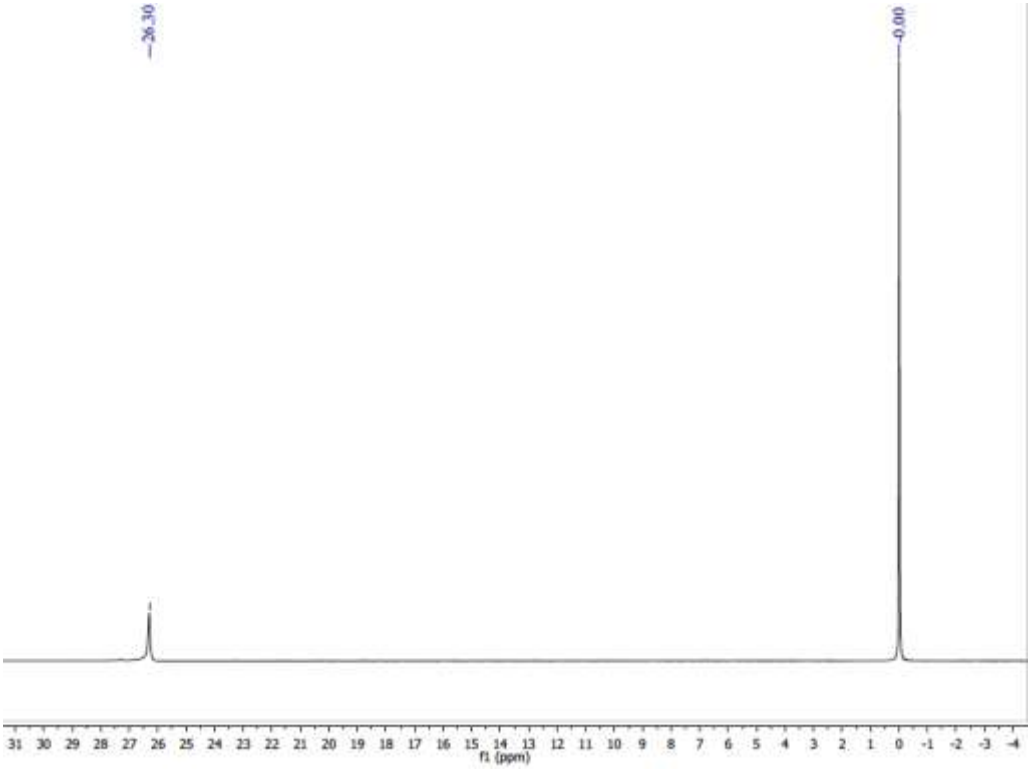
(RR/SS)-**4a** DEPT 135 (101 MHz, $CDCl_3$)



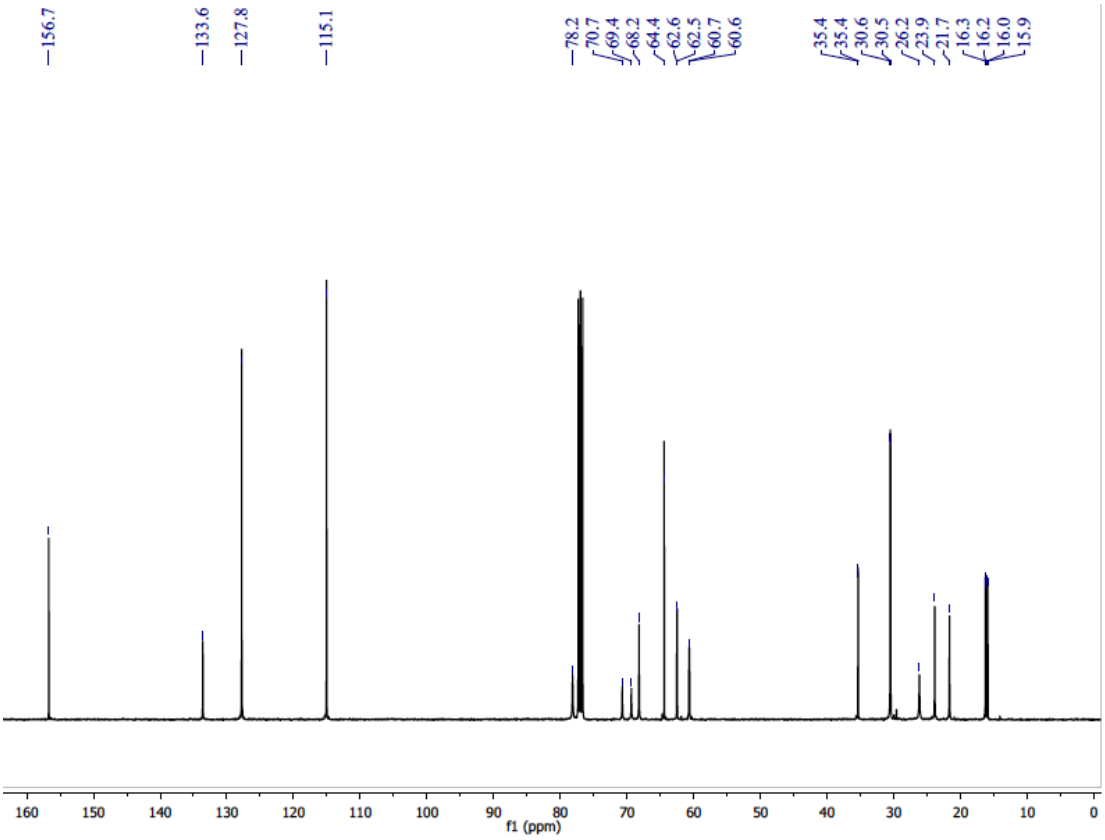
(RS/SR)-**4a** ^{1}H NMR (400 MHz, $CDCl_3$)



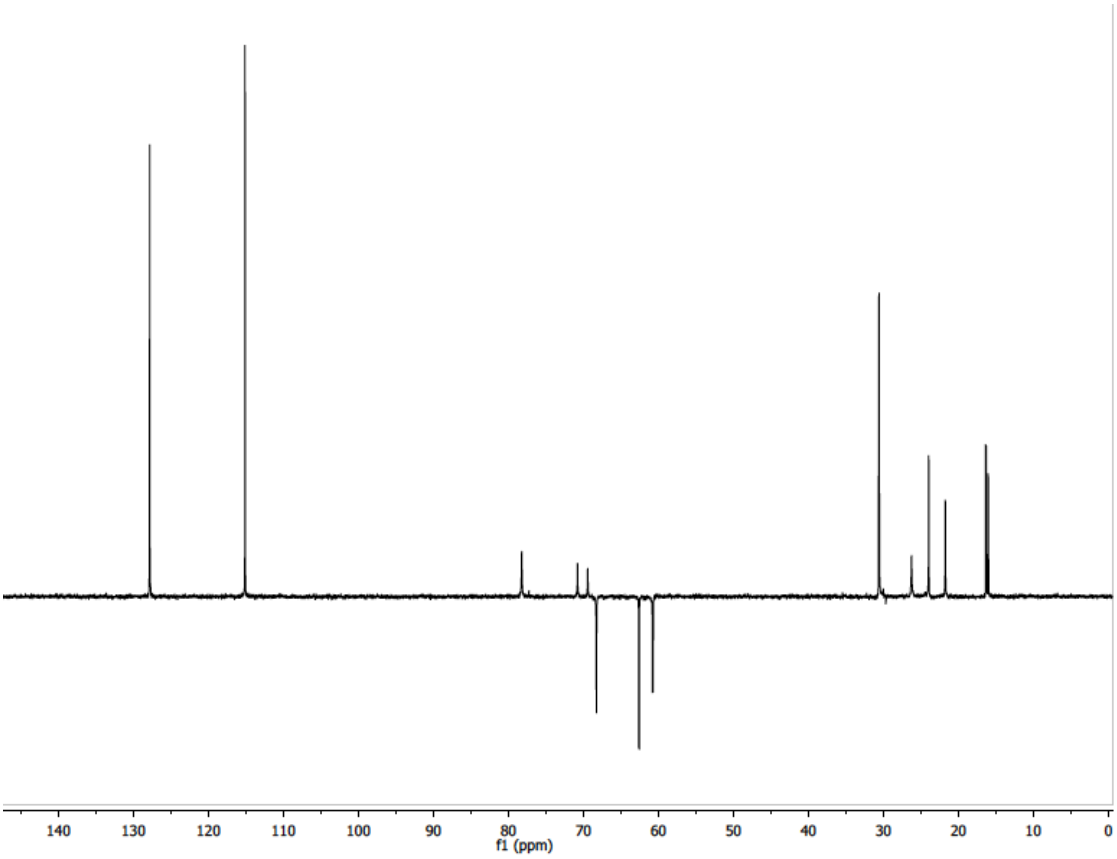
(RS/SR)-**4a** ^{31}P NMR (121 MHz, $CDCl_3$)



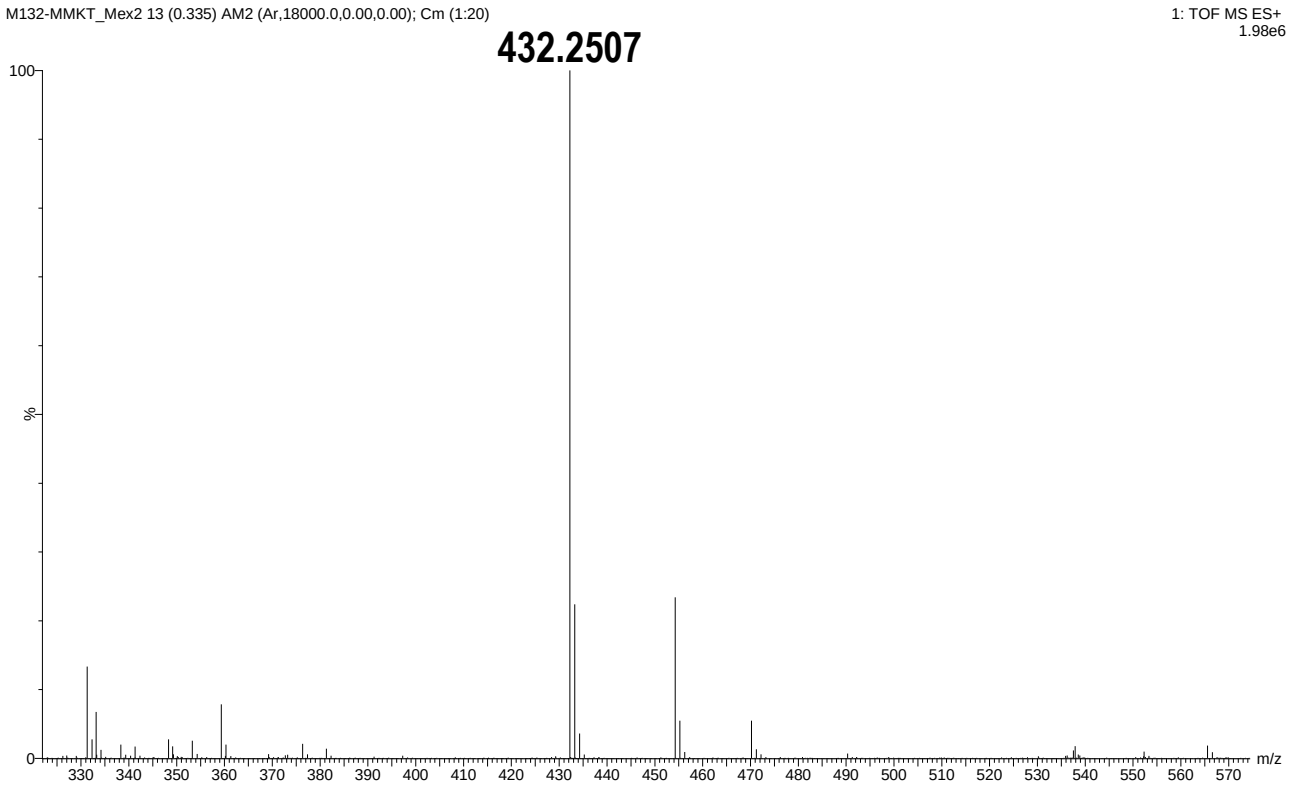
(RS/SR)-**4a** ^{13}C NMR (101 MHz, $CDCl_3$)



(RS/SR)-**4a** DEPT 135 (101 MHz, $CDCl_3$)

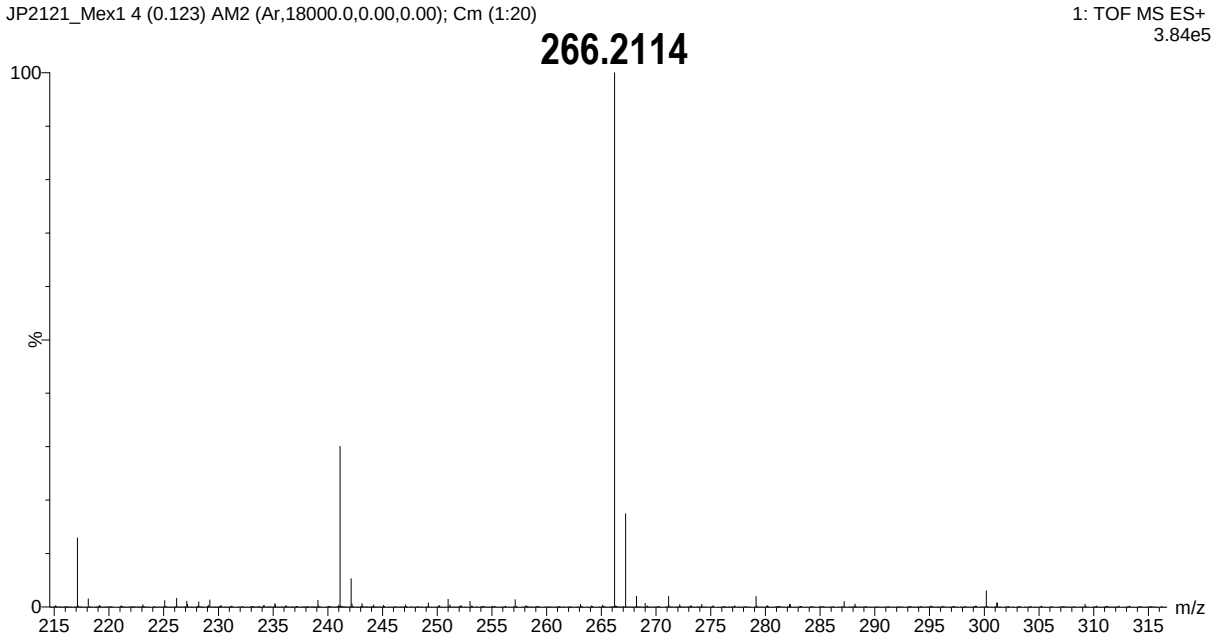


HRMS (mixture of diastereoisomers)



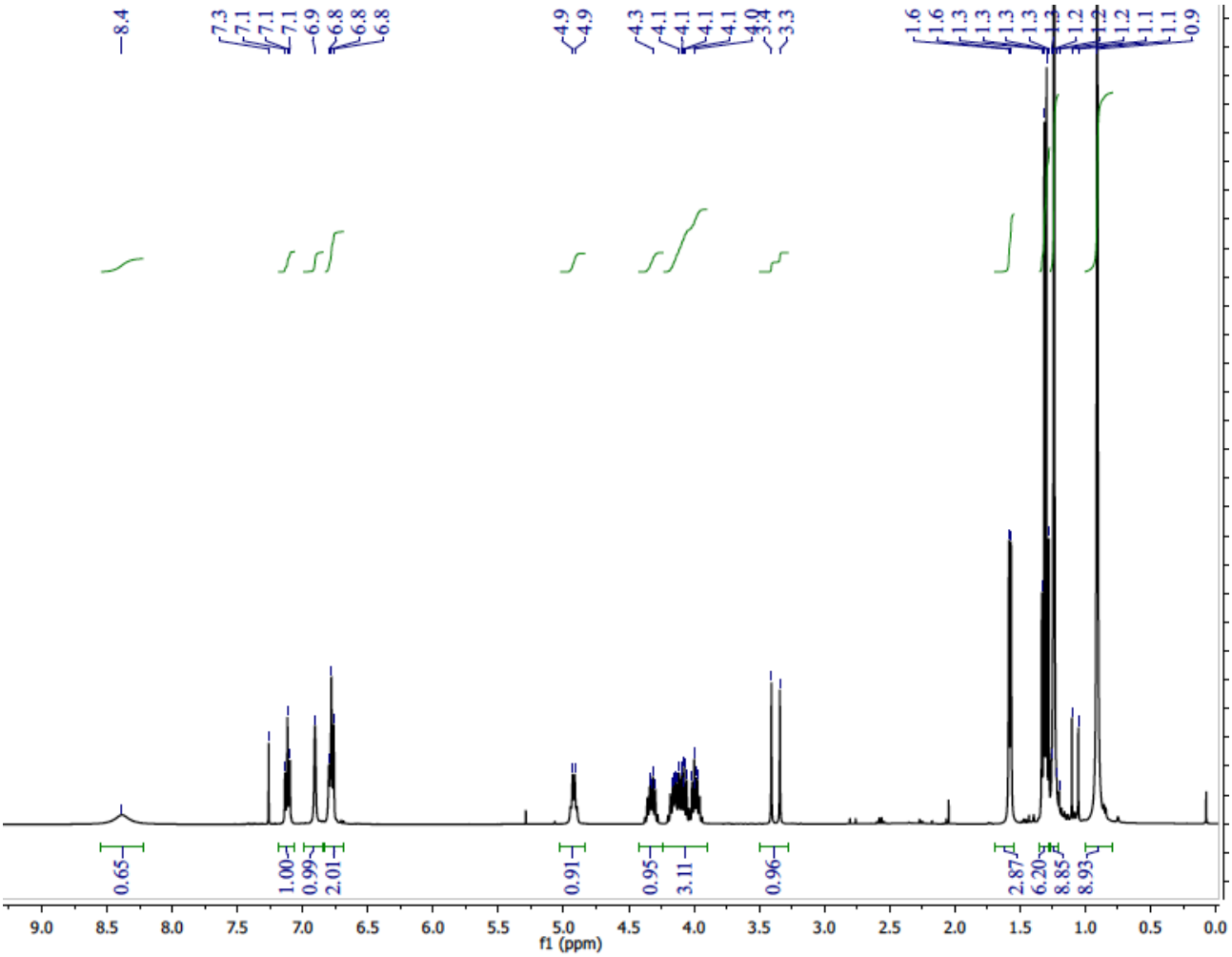
***4-(1-((di-tert-butylamino)oxy)ethyl)phenol* (5a).**

HRMS

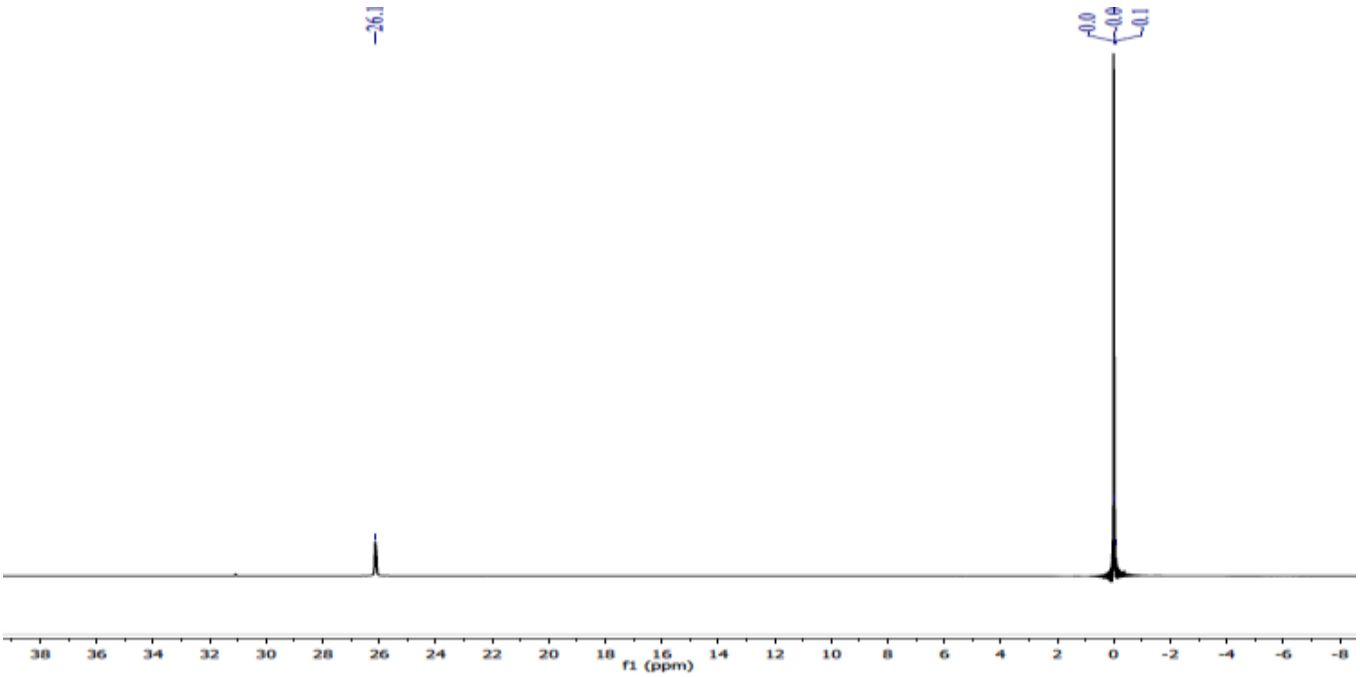


***diethyl (1-(tert-butyl(1-(3-hydroxyphenyl)ethoxy)amino)-2,2-dimethylpropyl)phosphonate* (3e).**

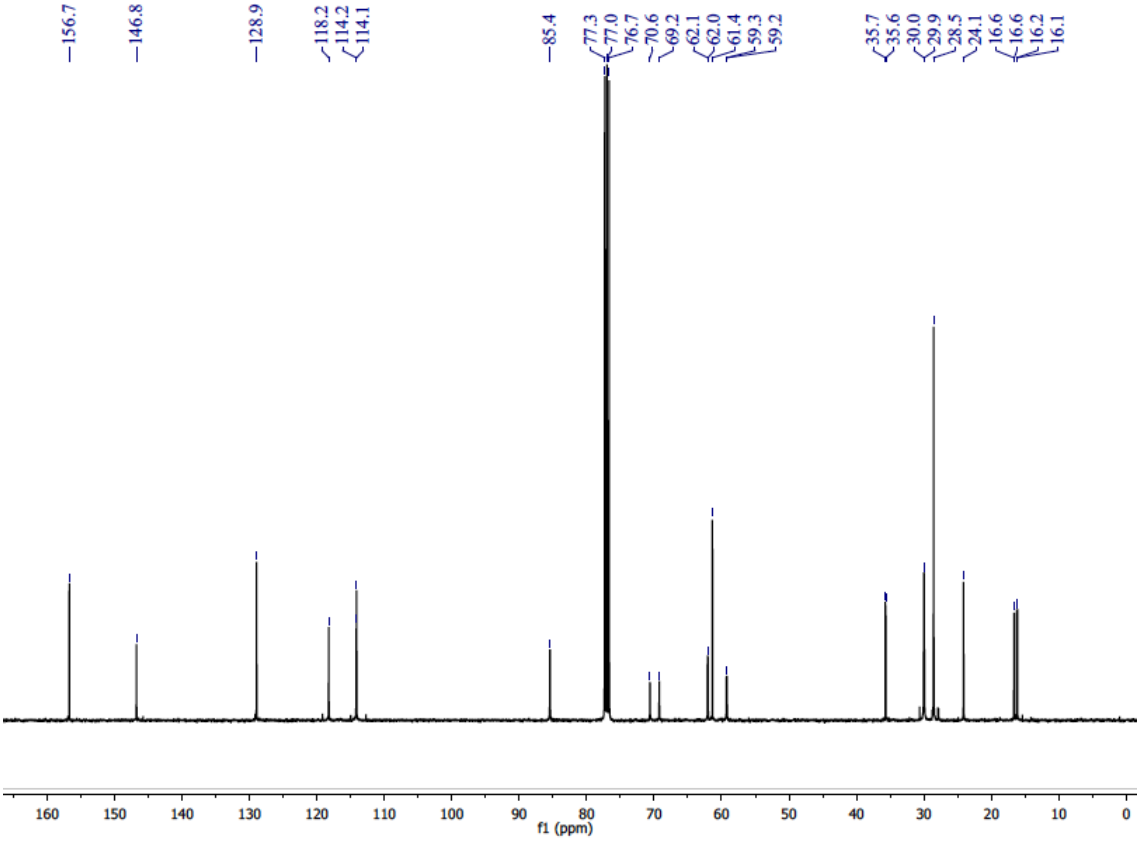
(RR/SS)-**3e** ^{1}H NMR (400 MHz, $CDCl_3$)



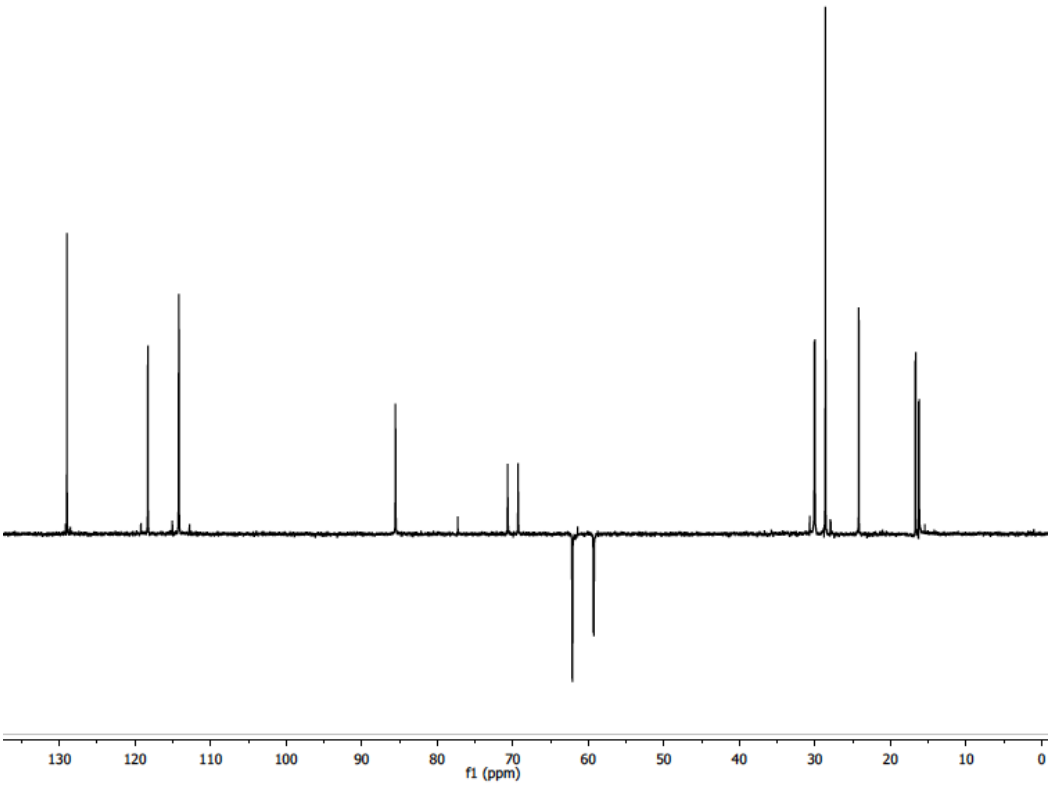
(RR/SS)-**3e** ^{31}P NMR (121 MHz, $CDCl_3$)



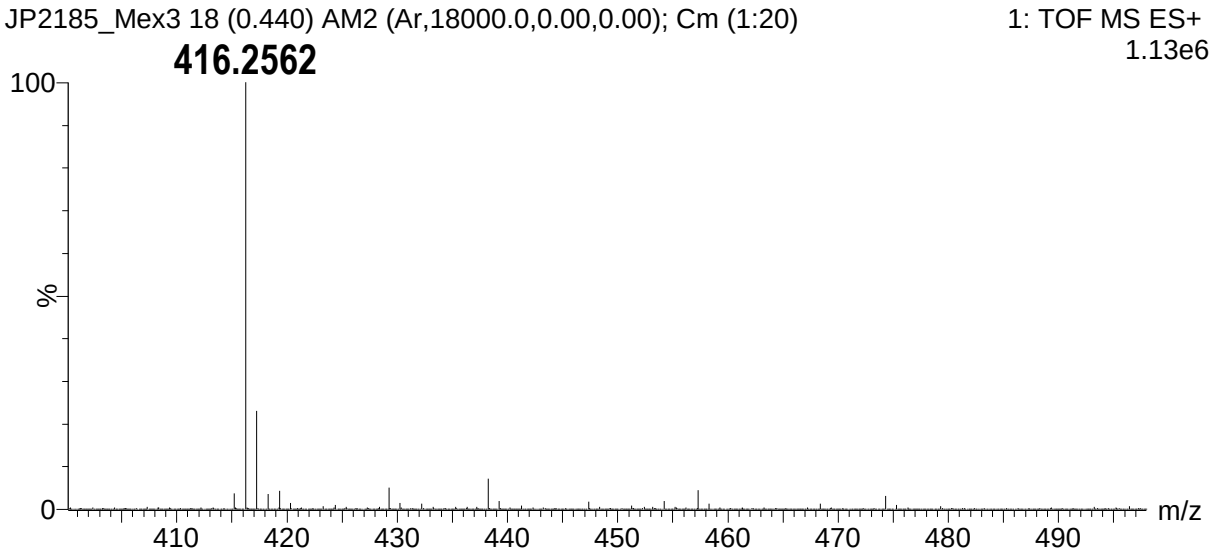
(RR/SS)-**3e** ^{13}C NMR (101 MHz, $CDCl_3$)



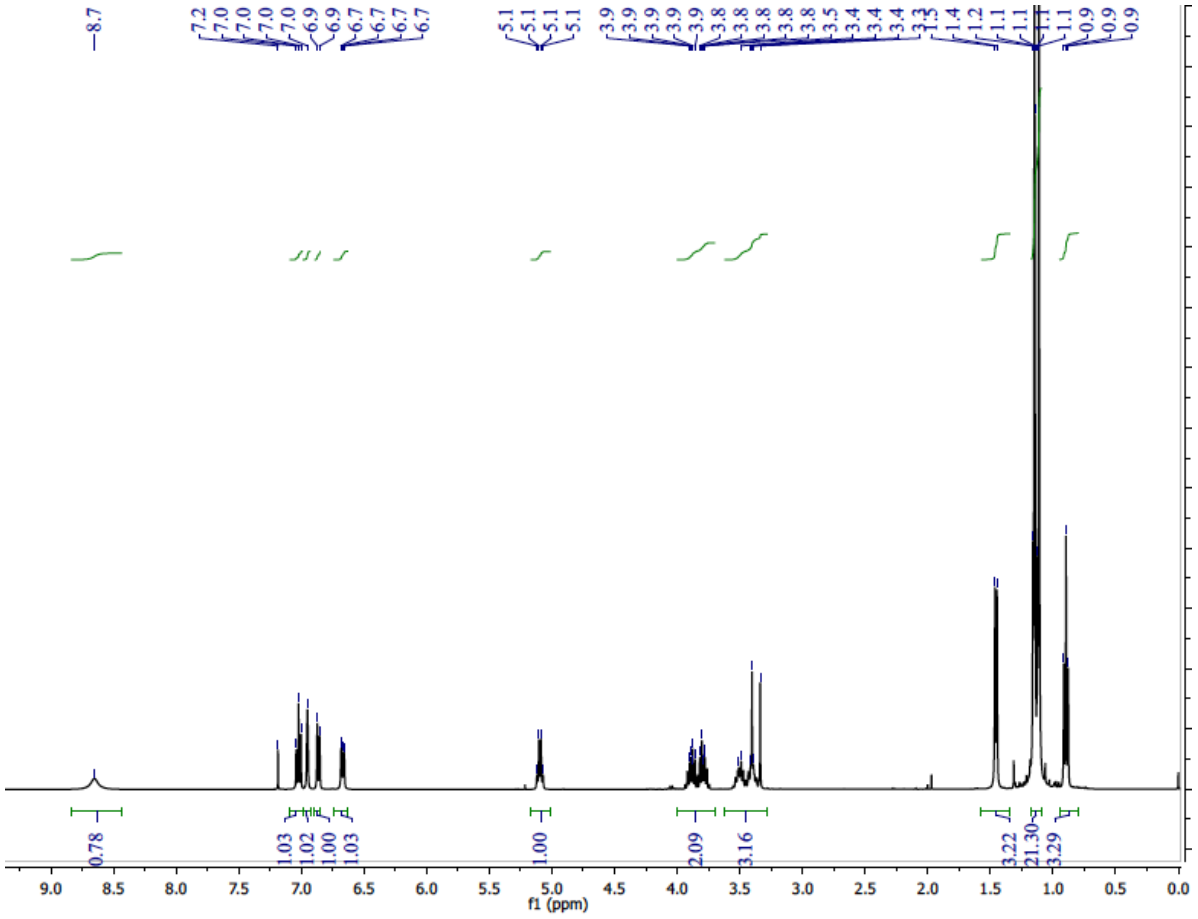
(RR/SS)-**3e** DEPT 135 (101 MHz, $CDCl_3$)



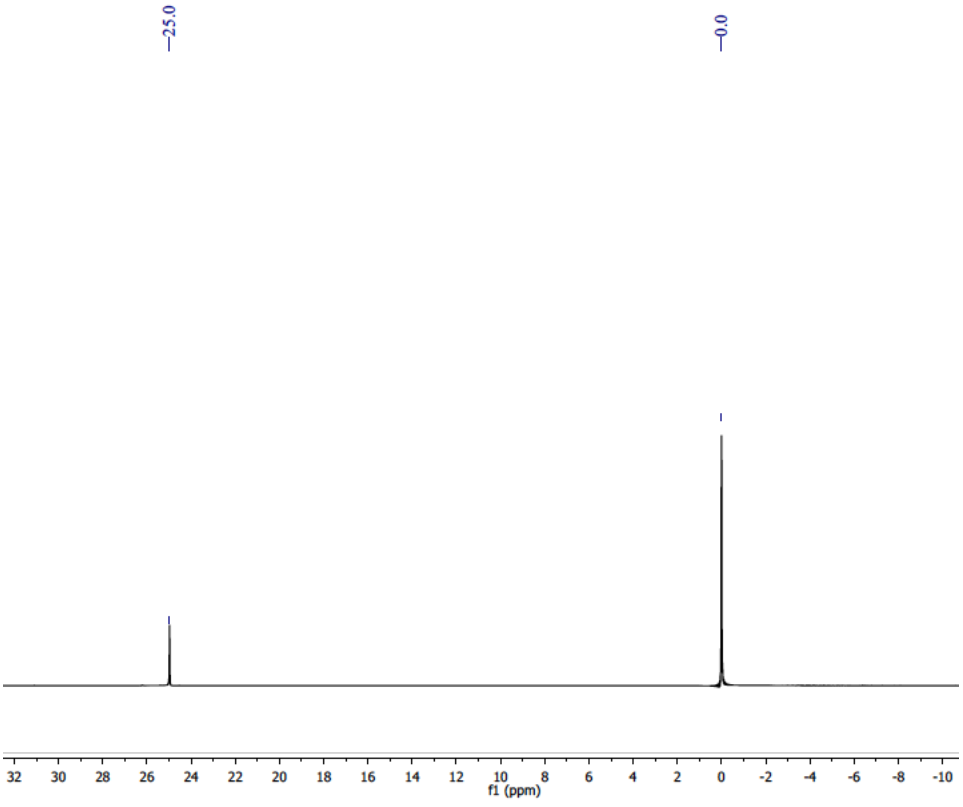
HRMS


JP2185_Mex3 18 (0.440) AM2 (Ar,18000.0,0.00,0.00); Cm (1:20)
1: TOF MS ES+
1.13e6
416.2562
100
%
0
410
420
430
440
450
460
470
480
490
m/z

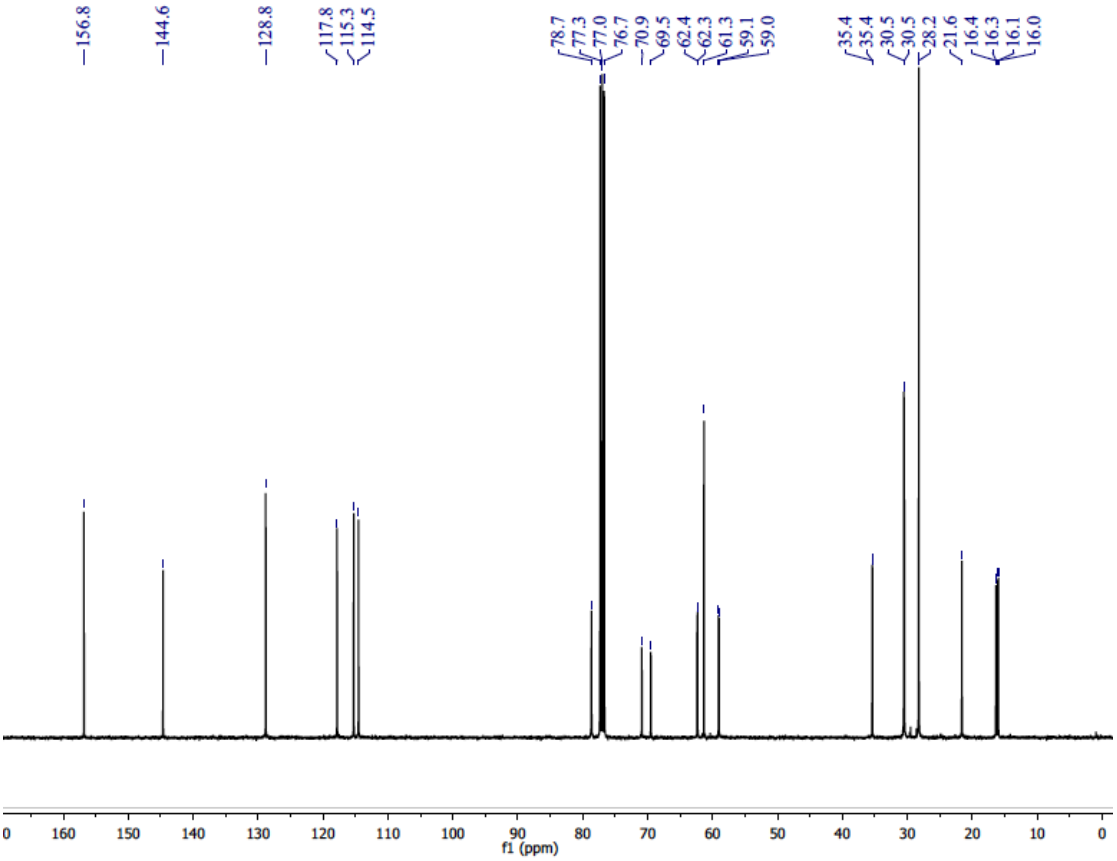
(RS/SR)-**3e** ^{1}H NMR (400 MHz, $CDCl_3$)



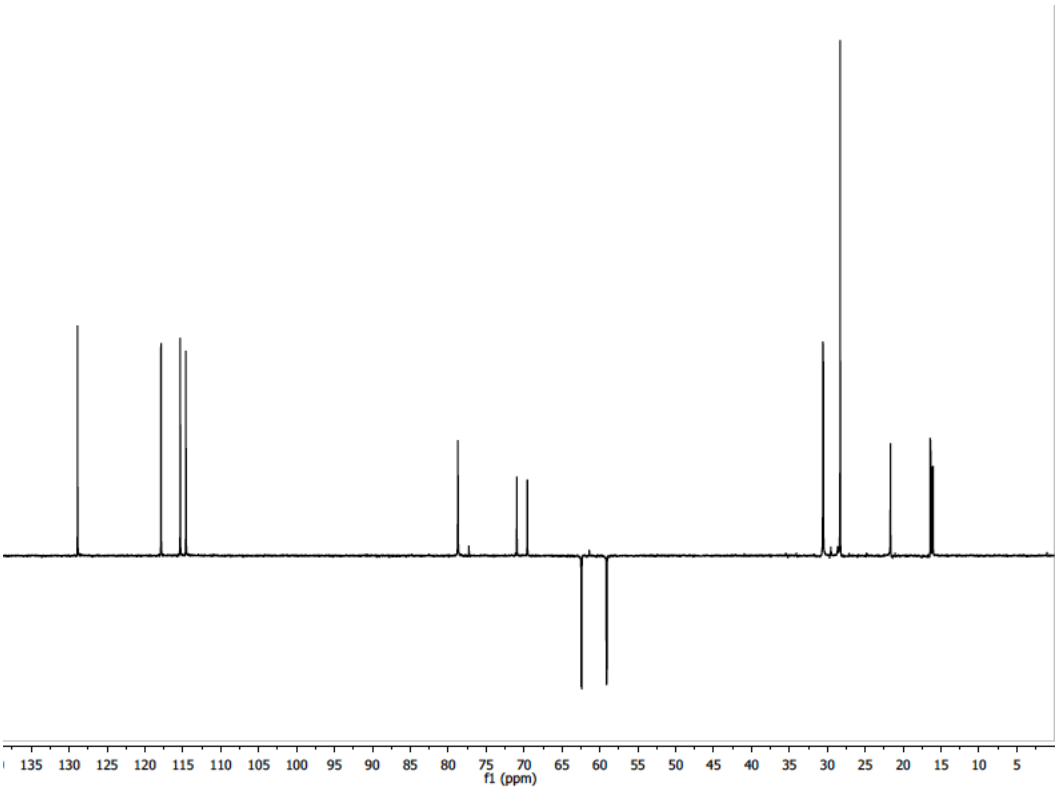
(RS/SR)-**3e** ^{31}P NMR (121 MHz, $CDCl_3$)



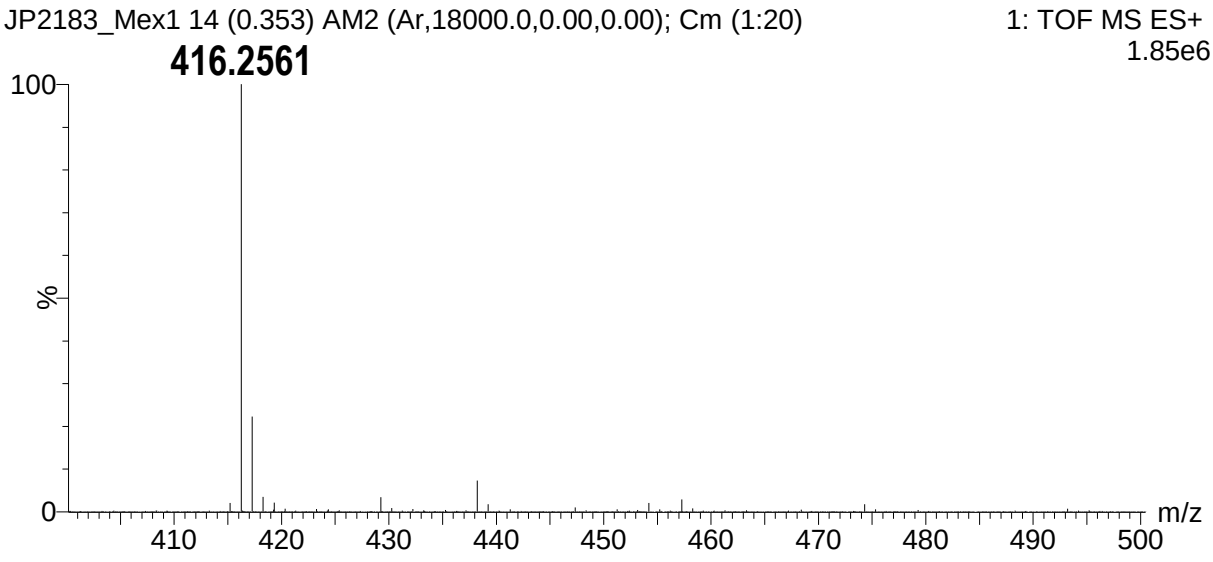
(RS/SR)-**3e** ^{13}C NMR (101 MHz, $CDCl_3$)



(RS/SR)-**3e** DEPT 135 (101 MHz, $CDCl_3$)



HRMS


JP2183_Mex1 14 (0.353) AM2 (Ar,18000.0,0.00,0.00); Cm (1:20)
1: TOF MS ES+
1.85e6
416.2561
100
%
0
m/z
410
420
430
440
450
460
470
480
490
500

2) pKa measurement of 4-vinylphenol.

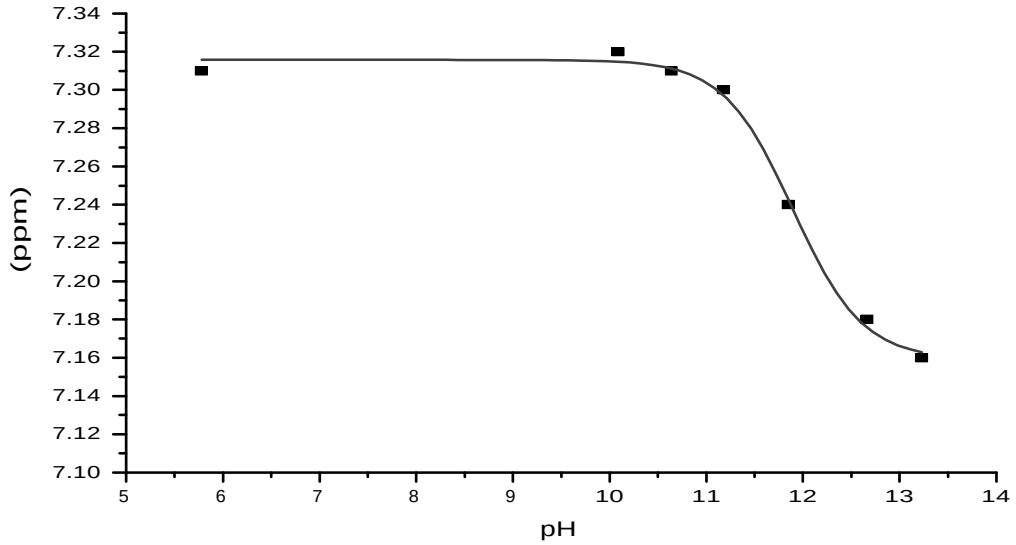


Figure 1SI. pH curve for 4-vinylphenol by one peak in the aromatic zone. Data were fitted with eq.1.

Eq. 1SI $$\delta_{\mathrm{p}H} = \delta + \frac{\delta_{\mathrm{H}^+} - \delta}{1 + 10^{\mathrm{p}K_a - \mathrm{p}H}}$$

3) HPLC – ESI analysis in THF for chemical oxidation of 3a and 3e with PbO_2.

Table 1SI. Retention times in HPLC using UV detection (λ = 280 nm), mass analysis (ESI-MS), and mass balances for pure **A-C** , **3a**, and **3e**, and for **3a** and **3e** in the presence of 500 eq. of PbO_2 in THF

	t^a	M_E/Z^b	M_O/Z^b	$n_a{}^c$	$n_{3\bullet}{}^c$	$n_o{}^c$
A	11.9	153.2	121.2	n.a.[d]	n.a.[d]	1.0
B	5.0	138.2	121.2	n.a.[d]	n.a.[d]	1.0
C	13.2	121.2	121.2	n.a.[d]	n.a.[d]	1.0
3•	14.7	296.4	296.4	n.a.[d]	0.8[e]	n.a.[d]
3a[f]	16.1 16.7	416.2	438.2	0.6 0.4	n.a.[d]	n.a.[d]
3e[g]	16.26	416.2	416.2	1.0	n.a.[d]	n.a.[d]
3a + PbO_2	5.0 14.7 16.1 16.7	n.a.[d]	121.2 296.2 438.2 438.2	n.a.[d] 0.05 0.10	n.a.[d] 0.7 n.a.[d] n.a.[d]	0.13[h] n.a.[d] n.a.[d] n.a.[d]
3e + PbO_2	13.8 14.7 16.26	n.a.[d]	121.2 296.2 416.2	n.a.[d] n.a.[d] 0.37	n.a.[d] 0.12 n.a.d	n.a.[d] n.a.[d] n.a.[d]

[a] Retention time in min. [b] Me/Z and Mo/Z are for the expected an observed masses by ESI-MS, respectively, in THF. [c] In 10^{-8} moles. n_a, $n_{3\bullet}$, and n_o number of moles for alkoxyamines, **3•**, and other molecules, respectively. [d] n.a.: not applicable. [e] As displayed in **Error! Reference source not found.**, 20% of impurities are detected. [f] Mixture of 2 diastereoisomers. [g] Only one diastereoisomers was available. [h] Amount of **B**.

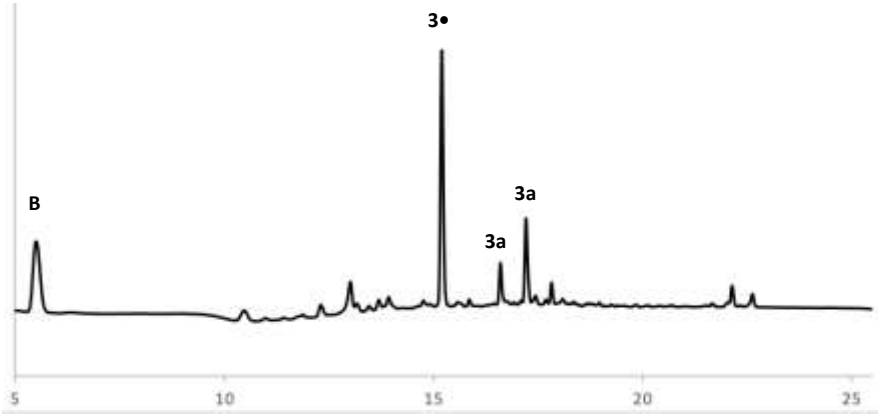
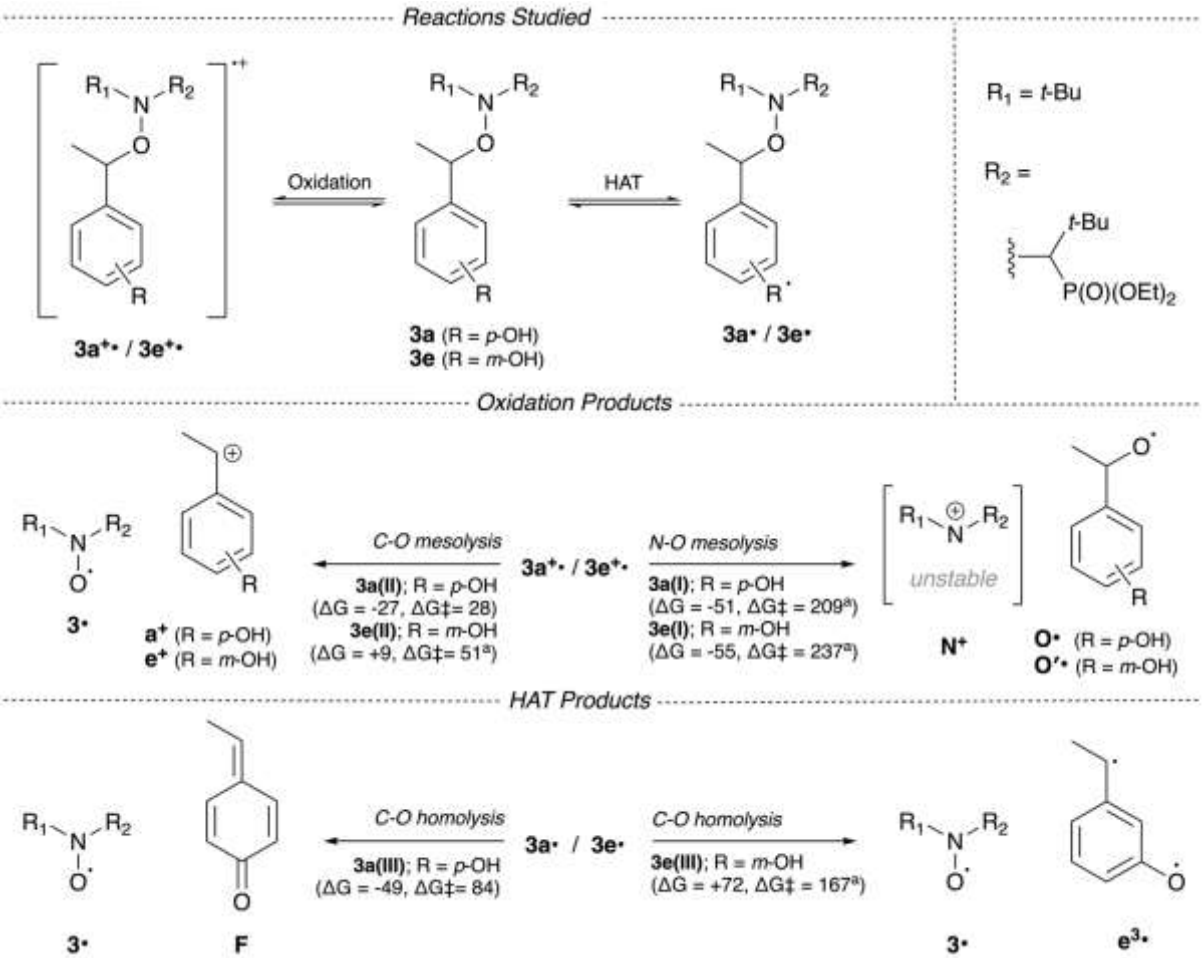


Figure 2SI. HPLC signal for decomposition of **3a** in the presence of PbO_2 (500 eq.)

4) DFT calculations



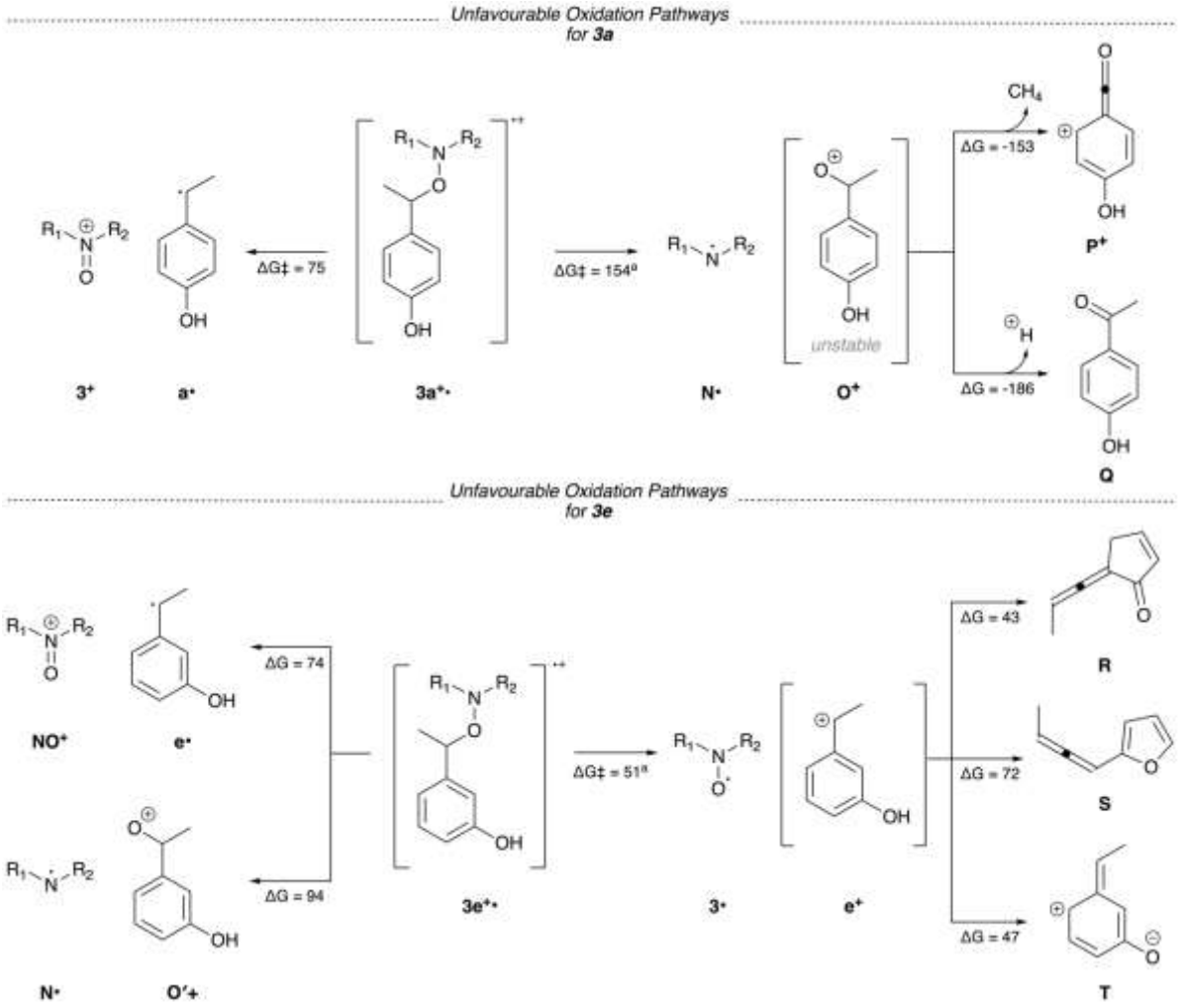
Scheme 1SI. Selected (preferred) pathways of decomposition radicals based on **3a** and **3e** according to M06-2X/6-31+G(d,p) calculations. [a] No transition state could be located; an approximate barrier was obtained via a relaxed scan.

Table 2SI. Species in Scheme 1SI. Boltzmann-weighted Gibbs free energy in SMD Methanol, and energy components in gas-phase and SMD Methanol. Energies are in Hartree.

Species	E(Gas)	ZPVE	TC	TS	H	G	E (Methanol)	G (Methanol)	Boltzmann Weight	Weighted G(Methanol)
3a+•_cd	-1594.59256	0.58116	0.03259	0.09039	-1593.97881	-1594.06920	-1594.68368	-1594.15730	0.00950	
3a+•_dn	-1594.59182	0.58107	0.03262	0.09047	-1593.97813	-1594.06860	-1594.68381	-1594.15758	0.01272	
3a+•_cu	-1594.59262	0.58115	0.03252	0.09010	-1593.97895	-1594.06905	-1594.68428	-1594.15769	0.01437	
3a+•_bf	-1594.59395	0.58141	0.03247	0.09000	-1593.98007	-1594.07007	-1594.68496	-1594.15806	0.02117	
3a+•_ap	-1594.59266	0.58147	0.03251	0.09011	-1593.97868	-1594.06879	-1594.68501	-1594.15812	0.02268	
3a+•_ao	-1594.59261	0.58105	0.03266	0.09057	-1593.97890	-1594.06947	-1594.68493	-1594.15876	0.04477	
3a+•_an	-1594.59365	0.58105	0.03270	0.09069	-1593.97990	-1594.07059	-1594.68575	-1594.15967	0.11709	
3a+•_df	-1594.59460	0.58114	0.03262	0.09049	-1593.98084	-1594.07133	-1594.68628	-1594.15999	0.16305	
3a+•_fd	-1594.59065	0.58068	0.03298	0.09121	-1593.97699	-1594.06820	-1594.68553	-1594.16006	0.17739	
3a+•_fl	-1594.59264	0.58111	0.03279	0.09066	-1593.97875	-1594.06941	-1594.68713	-1594.16087	0.41728	-1594.16011
3a•_ae	-1594.20266	0.56725	0.03201	0.08916	-1593.60340	-1593.69256	-1594.23859	-1593.72547	0.17202	
3a•_ac	-1594.20344	0.56735	0.03194	0.08896	-1593.60414	-1593.69311	-1594.23891	-1593.72556	0.19053	
3a•_as	-1594.20341	0.56695	0.03211	0.08945	-1593.60435	-1593.69380	-1594.23934	-1593.72670	0.63744	-1593.72627
3•_at	-1209.48128	0.42514	0.02445	0.07397	-1209.03168	-1209.10566	-1209.50788	-1209.12923	0.02106	
3•_ce	-1209.48160	0.42531	0.02442	0.07404	-1209.03187	-1209.10591	-1209.50804	-1209.12933	0.02341	
3•_ab	-1209.48353	0.42532	0.02439	0.07394	-1209.03382	-1209.10776	-1209.50829	-1209.12951	0.02820	
3•_cu	-1209.48370	0.42539	0.02443	0.07395	-1209.03388	-1209.10783	-1209.50845	-1209.12957	0.03000	
3•_al	-1209.48178	0.42531	0.02439	0.07397	-1209.03208	-1209.10605	-1209.50842	-1209.12968	0.03389	
3•_au	-1209.48184	0.42525	0.02437	0.07389	-1209.03221	-1209.10610	-1209.50903	-1209.13028	0.06356	
3•_ak	-1209.48153	0.42521	0.02441	0.07383	-1209.03191	-1209.10574	-1209.50915	-1209.13033	0.06755	
3•_ao	-1209.48382	0.42524	0.02449	0.07418	-1209.03409	-1209.10827	-1209.50897	-1209.13040	0.07218	
3•_ag	-1209.48189	0.42524	0.02446	0.07419	-1209.03219	-1209.10639	-1209.50899	-1209.13047	0.07807	

Species	E(Gas)	ZPVE	TC	TS	H	G	E (Methanol)	G (Methanol)	Boltzmann Weight	Weighted G(Methanol)
3•_aw	-1209.48067	0.42505	0.02449	0.07416	-1209.03114	-1209.10530	-1209.50907	-1209.13067	0.09617	
3•_as	-1209.48414	0.42528	0.02450	0.07418	-1209.03436	-1209.10854	-1209.50945	-1209.13083	0.11467	
3•_br	-1209.48287	0.42519	0.02449	0.07412	-1209.03319	-1209.10731	-1209.51052	-1209.13194	0.37125	-1209.13092
3a(II) TS_dn	-1594.58227	0.57886	0.03265	0.09071	-1593.97076	-1594.06147	-1594.67005	-1594.14623	0.01086	
3a(II) TS_bh	-1594.58195	0.57881	0.03258	0.09046	-1593.97057	-1594.06103	-1594.67112	-1594.14718	0.02962	
3a(II) TS_ap	-1594.58379	0.57872	0.03278	0.09102	-1593.97230	-1594.06332	-1594.67231	-1594.14882	0.16863	
3a(II) TS_an	-1594.58481	0.57883	0.03275	0.09093	-1593.97323	-1594.06416	-1594.67319	-1594.14952	0.35620	
3a(II) TS_df	-1594.58568	0.57902	0.03266	0.09073	-1593.97400	-1594.06473	-1594.67367	-1594.14971	0.43468	-1594.14938
3a(III) TS	-1594.16706	0.56514	0.03220	0.08951	-1593.56973	-1593.65924	-1594.20494	-1593.69410	1.00000	-1593.69410
a+	-385.06733	0.15108	0.00911	0.04174	-384.90714	-384.94888	-385.16100	-385.03953	1.00000	-385.03953
e+	-385.06733	0.15108	0.00911	0.04174	-384.90714	-384.94888	-385.16100	-385.03953	1.00000	-385.03953
e•	-384.65486	0.13490	0.00919	0.04305	-384.51076	-384.55381	-384.66970	-384.56563	1.00000	-384.56563
F	-384.70374	0.13827	0.00903	0.04177	-384.55645	-384.59822	-384.72244	-384.61389	1.00000	-384.61389
N+_av	-1134.10657	0.42273	0.02366	0.07193	-1133.66018	-1133.73211	-1134.18782	-1133.81035	0.00346	
N+_ad	-1134.10922	0.42292	0.02354	0.07162	-1133.66275	-1133.73437	-1134.18948	-1133.81161	0.01323	
N+_am	-1134.10802	0.42274	0.02368	0.07199	-1133.66161	-1133.73360	-1134.18929	-1133.81185	0.01695	
N+_ae	-1134.10809	0.42284	0.02359	0.07175	-1133.66166	-1133.73340	-1134.18958	-1133.81187	0.01733	
N+_be	-1134.10787	0.42299	0.02349	0.07149	-1133.66139	-1133.73288	-1134.19004	-1133.81203	0.02055	
N+_bf	-1134.10854	0.42267	0.02365	0.07194	-1133.66222	-1133.73416	-1134.18980	-1133.81241	0.03080	
N+_cc	-1134.10760	0.42290	0.02353	0.07162	-1133.66118	-1133.73279	-1134.19112	-1133.81330	0.07864	
N+_ca	-1134.10809	0.42302	0.02355	0.07167	-1133.66152	-1133.73319	-1134.19122	-1133.81331	0.07973	
N+_ao	-1134.10658	0.42264	0.02368	0.07206	-1133.66026	-1133.73232	-1134.19062	-1133.81335	0.08283	
N+_ay	-1134.10606	0.42273	0.02360	0.07183	-1133.65973	-1133.73155	-1134.19099	-1133.81346	0.09396	

Species	E(Gas)	ZPVE	TC	TS	H	G	E (Methanol)	G (Methanol)	Boltzmann Weight	Weighted G(Methanol)
N+_bz	-1134.10732	0.42283	0.02360	0.07183	-1133.66088	-1133.73271	-1134.19137	-1133.81374	0.12613	
N+_ar	-1134.10893	0.42270	0.02366	0.07197	-1133.66257	-1133.73454	-1134.19121	-1133.81380	0.13455	
N+_bw	-1134.10765	0.42281	0.02359	0.07178	-1133.66126	-1133.73304	-1134.19148	-1133.81385	0.14142	
N+_ax	-1134.10824	0.42265	0.02364	0.07187	-1133.66195	-1133.73382	-1134.19141	-1133.81397	0.16041	-1133.81349
O•	-460.46952	0.15353	0.01018	0.04488	-460.30582	-460.35070	-460.48794	-460.36609	1.00000	-460.36609
O• •	-460.47125	0.15362	0.01003	0.04452	-460.30760	-460.35211	-460.48975	-460.36760	1.00000	-460.36760



Scheme 2SI. Selected (highly endergonic) pathways of decomposition radicals based on **3a** and **3e** according to M06-2X/6-31+G(d,p) calculations. [a] No transition state could be located; an approximate barrier was obtained via a relaxed scan. A reference value for $G(H^+)$; Methanol) = -1100.7 kJ/mol was taken from Malloum, A.; Fifen, J. J.; Conradie, J.; *Phys. Chem. Chem. Phys.* (2018), 20, 29184-19206.

Table 3SI. SG1-OH-RADCAT C-O Cleavage Pathway 2. Boltzmann-weighted Gibbs free energy in SMD Methanol, and energy components in gas-phase and SMD Methanol. Energies are in Hartree, frequencies are in wavenumbers.

Species	E(Gas)	ZPVE	TC	TS	H	G	E (Methanol)	G (Methanol)	Boltzmann Weight	Weighted G(Methanol)
3•_at	-1209.48128	0.42514	0.02445	0.07397	-1209.03168	-1209.10566	-1209.50788	-1209.12923	0.02106	
3•_ce	-1209.48160	0.42531	0.02442	0.07404	-1209.03187	-1209.10591	-1209.50804	-1209.12933	0.02341	
3•_ab	-1209.48353	0.42532	0.02439	0.07394	-1209.03382	-1209.10776	-1209.50829	-1209.12951	0.02820	
3•_cu	-1209.48370	0.42539	0.02443	0.07395	-1209.03388	-1209.10783	-1209.50845	-1209.12957	0.03000	
3•_al	-1209.48178	0.42531	0.02439	0.07397	-1209.03208	-1209.10605	-1209.50842	-1209.12968	0.03389	
3•_au	-1209.48184	0.42525	0.02437	0.07389	-1209.03221	-1209.10610	-1209.50903	-1209.13028	0.06356	
3•_ak	-1209.48153	0.42521	0.02441	0.07383	-1209.03191	-1209.10574	-1209.50915	-1209.13033	0.06755	
3•_ao	-1209.48382	0.42524	0.02449	0.07418	-1209.03409	-1209.10827	-1209.50897	-1209.13040	0.07218	
3•_ag	-1209.48189	0.42524	0.02446	0.07419	-1209.03219	-1209.10639	-1209.50899	-1209.13047	0.07807	
3•_aw	-1209.48067	0.42505	0.02449	0.07416	-1209.03114	-1209.10530	-1209.50907	-1209.13067	0.09617	
3•_as	-1209.48414	0.42528	0.02450	0.07418	-1209.03436	-1209.10854	-1209.50945	-1209.13083	0.11467	
3•_br	-1209.48287	0.42519	0.02449	0.07412	-1209.03319	-1209.10731	-1209.51052	-1209.13194	0.37125	-1209.13092
3a+•_cd	-1594.59256	0.58116	0.03259	0.09039	-1593.97881	-1594.06920	-1594.68368	-1594.15730	0.00950	
3a+•_dn	-1594.59182	0.58107	0.03262	0.09047	-1593.97813	-1594.06860	-1594.68381	-1594.15758	0.01272	
3a+•_cu	-1594.59262	0.58115	0.03252	0.09010	-1593.97895	-1594.06905	-1594.68428	-1594.15769	0.01437	
3a+•_bf	-1594.59395	0.58141	0.03247	0.09000	-1593.98007	-1594.07007	-1594.68496	-1594.15806	0.02117	
3a+•_ap	-1594.59266	0.58147	0.03251	0.09011	-1593.97868	-1594.06879	-1594.68501	-1594.15812	0.02268	
3a+•_ao	-1594.59261	0.58105	0.03266	0.09057	-1593.97890	-1594.06947	-1594.68493	-1594.15876	0.04477	
3a+•_an	-1594.59365	0.58105	0.03270	0.09069	-1593.97990	-1594.07059	-1594.68575	-1594.15967	0.11709	
3a+•_df	-1594.59460	0.58114	0.03262	0.09049	-1593.98084	-1594.07133	-1594.68628	-1594.15999	0.16305	
3a+•_fd	-1594.59065	0.58068	0.03298	0.09121	-1593.97699	-1594.06820	-1594.68553	-1594.16006	0.17739	

Species	E(Gas)	ZPVE	TC	TS	H	G	E (Methanol)	G (Methanol)	Boltzmann Weight	Weighted G(Methanol)
3a+•_fl	-1594.59264	0.58111	0.03279	0.09066	-1593.97875	-1594.06941	-1594.68713	-1594.16087	0.41728	-1594.16011
a•	-385.29919	0.14797	0.00951	0.04311	-385.14172	-385.18483	-385.31501	-385.19763	1.00000	-385.19763
e•	-385.29916	0.14800	0.00951	0.04314	-385.14165	-385.18479	-385.31523	-385.19783	1.00000	-385.19783
N•_bk	-1134.29248	0.41938	0.02352	0.07209	-1133.84958	-1133.92167	-1134.31389	-1133.94005	0.00774	
N•_ba	-1134.29117	0.41915	0.02358	0.07215	-1133.84844	-1133.92059	-1134.31384	-1133.94024	0.00941	
N•_bu	-1134.29261	0.41936	0.02355	0.07217	-1133.84970	-1133.92186	-1134.31440	-1133.94064	0.01437	
N•_bv	-1134.29059	0.41910	0.02368	0.07263	-1133.84780	-1133.92044	-1134.31400	-1133.94083	0.01757	
N•_bh	-1134.29149	0.41914	0.02367	0.07253	-1133.84868	-1133.92121	-1134.31445	-1133.94115	0.02477	
N•_ax	-1134.29137	0.41905	0.02366	0.07241	-1133.84867	-1133.92107	-1134.31453	-1133.94122	0.02650	
N•_ap	-1134.29072	0.41911	0.02370	0.07258	-1133.84791	-1133.92049	-1134.31454	-1133.94129	0.02851	
N•_bw	-1134.29302	0.41936	0.02363	0.07252	-1133.85003	-1133.92255	-1134.31483	-1133.94134	0.03029	
N•_bq	-1134.29368	0.41916	0.02371	0.07263	-1133.85080	-1133.92343	-1134.31478	-1133.94151	0.03621	
N•_al	-1134.29105	0.41900	0.02368	0.07245	-1133.84837	-1133.92082	-1134.31498	-1133.94174	0.04595	
N•_bb	-1134.29390	0.41913	0.02369	0.07243	-1133.85108	-1133.92351	-1134.31572	-1133.94231	0.08453	
N•_av	-1134.29403	0.41907	0.02374	0.07259	-1133.85121	-1133.92380	-1134.31565	-1133.94241	0.09425	
N•_as	-1134.29363	0.41912	0.02368	0.07250	-1133.85083	-1133.92333	-1134.31590	-1133.94258	0.11185	
N•_ad	-1134.29135	0.41906	0.02373	0.07261	-1133.84856	-1133.92117	-1134.31596	-1133.94276	0.13624	
N•_aq	-1134.29351	0.41908	0.02373	0.07268	-1133.85070	-1133.92338	-1134.31600	-1133.94285	0.14973	
N•_at	-1134.29401	0.41898	0.02380	0.07280	-1133.85123	-1133.92402	-1134.31604	-1133.94304	0.18206	-1133.94237
NO+_au	-1209.22629	0.42636	0.02454	0.07366	-1208.77539	-1208.84904	-1209.31171	-1208.93145	0.00680	
NO+_ak	-1209.22690	0.42631	0.02454	0.07365	-1208.77606	-1208.84971	-1209.31185	-1208.93164	0.00830	
NO+_aq	-1209.22518	0.42623	0.02459	0.07378	-1208.77437	-1208.84815	-1209.31176	-1208.93171	0.00899	

Species	E(Gas)	ZPVE	TC	TS	H	G	E (Methanol)	G (Methanol)	Boltzmann Weight	Weighted G(Methanol)
NO+_ae	-1209.22758	0.42636	0.02454	0.07375	-1208.77669	-1208.85043	-1209.31193	-1208.93176	0.00944	
NO+_bq	-1209.22781	0.42645	0.02445	0.07338	-1208.77691	-1208.85028	-1209.31236	-1208.93182	0.01005	
NO+_aa	-1209.22704	0.42624	0.02461	0.07390	-1208.77618	-1208.85008	-1209.31217	-1208.93219	0.01501	
NO+_am	-1209.22776	0.42644	0.02446	0.07348	-1208.77686	-1208.85034	-1209.31271	-1208.93227	0.01628	
NO+_af	-1209.22597	0.42599	0.02465	0.07401	-1208.77533	-1208.84934	-1209.31207	-1208.93242	0.01896	
NO+_bd	-1209.22857	0.42651	0.02450	0.07359	-1208.77757	-1208.85116	-1209.31337	-1208.93293	0.03283	
NO+_ac	-1209.22711	0.42629	0.02454	0.07370	-1208.77627	-1208.84998	-1209.31326	-1208.93311	0.03943	
NO+_bs	-1209.22709	0.42649	0.02442	0.07336	-1208.77618	-1208.84954	-1209.31373	-1208.93316	0.04170	
NO+_av	-1209.22827	0.42644	0.02458	0.07385	-1208.77725	-1208.85111	-1209.31369	-1208.93350	0.06004	
NO+_br	-1209.22631	0.42646	0.02445	0.07344	-1208.77540	-1208.84884	-1209.31419	-1208.93371	0.07444	
NO+_bn	-1209.22703	0.42655	0.02444	0.07342	-1208.77604	-1208.84946	-1209.31449	-1208.93390	0.09181	
NO+_bt	-1209.22526	0.42621	0.02467	0.07405	-1208.77439	-1208.84843	-1209.31379	-1208.93394	0.09578	
NO+_az	-1209.22765	0.42617	0.02462	0.07385	-1208.77686	-1208.85071	-1209.31449	-1208.93452	0.17704	
NO+_bj	-1209.22846	0.42625	0.02457	0.07380	-1208.77765	-1208.85144	-1209.31504	-1208.93500	0.29311	-1208.93403
P+	-460.25258	0.15147	0.01235	0.04987	-460.08876	-460.13863	-460.34684	-460.22987	1.00000	-460.22987
Q	-459.94759	0.14338	0.00985	0.04362	-459.79436	-459.83796	-459.96898	-459.85635	1.00000	-459.85635
R	-384.66637	0.13674	0.00951	0.04310	-384.52012	-384.56322	-384.68279	-384.57663	1.00000	-384.57663
S_ab	-384.66094	0.13728	0.00932	0.04282	-384.51434	-384.55716	-384.66857	-384.56178	0.19947	
S_ad	-384.66130	0.13738	0.00930	0.04275	-384.51462	-384.55738	-384.67003	-384.56309	0.80053	-384.56283
T	-384.63908	0.13635	0.00924	0.04230	-384.49349	-384.53579	-384.68143	-384.57512	1.00000	-384.57512

Transition state for β-fragmentation

Geometric parameters of the calculated TS of **3a•** (**Figure 3SI**) support lengthening of the C—O bond up to 1.88 Å, with no concurrent changes in the N—O bond length. We also observe increased sp^2 hybridized character on the methine of **F**, <MeCC> = 123°, increased pyramidalization on nitrogen, <CNO> = 113°, and an orthogonal relationship between **F** and the cleaving C—O bond, <OCCC> = -86°.

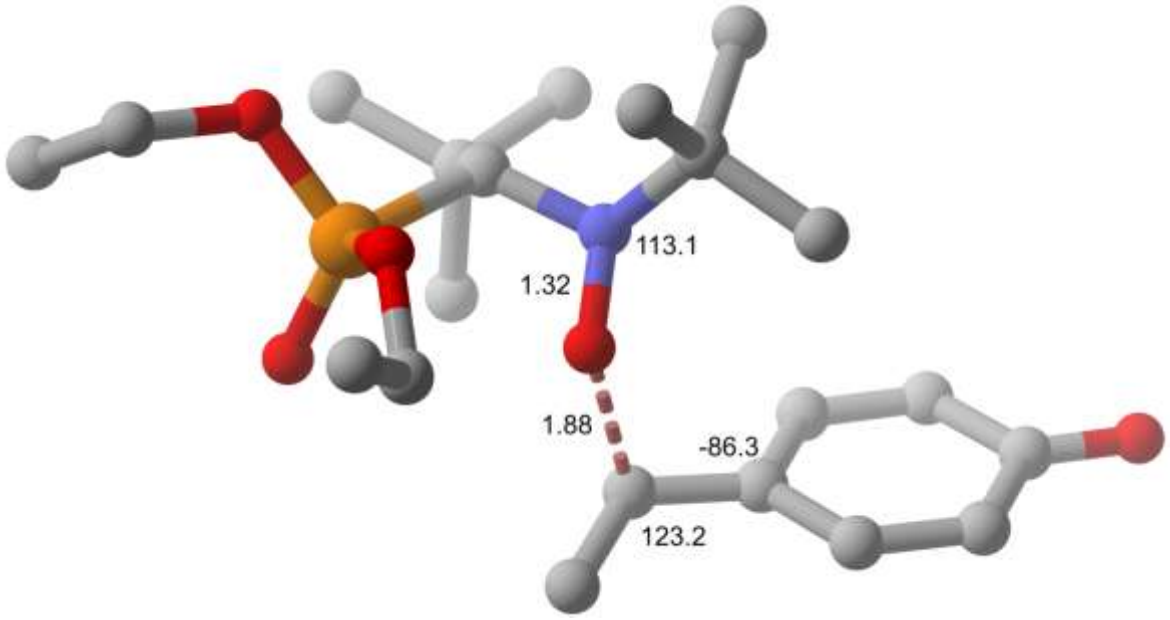


Figure 3SI. Calculated β-fragmentation transition state of **3a•** at the M06-2X/6-31+G(d,p) level of theory in the gas-phase. Hydrogen atoms are omitted for clarity.

Transition state for mesolysis.

Geometric parameters of the calculated TS of **3a•**+ (**Figure 4SI**) support lengthening of the C—O bond up to 2.00 Å, with no significant concurrent changes in the N—O bond length. We also observe increased sp^2 hybridized character on the methine of **F**, <MeCC> = 123.7°, increased pyramidalization on nitrogen, <CNO> = 115°, and an orthogonal relationship between **F** and the cleaving C—O bond, <OCCC> = -99°.

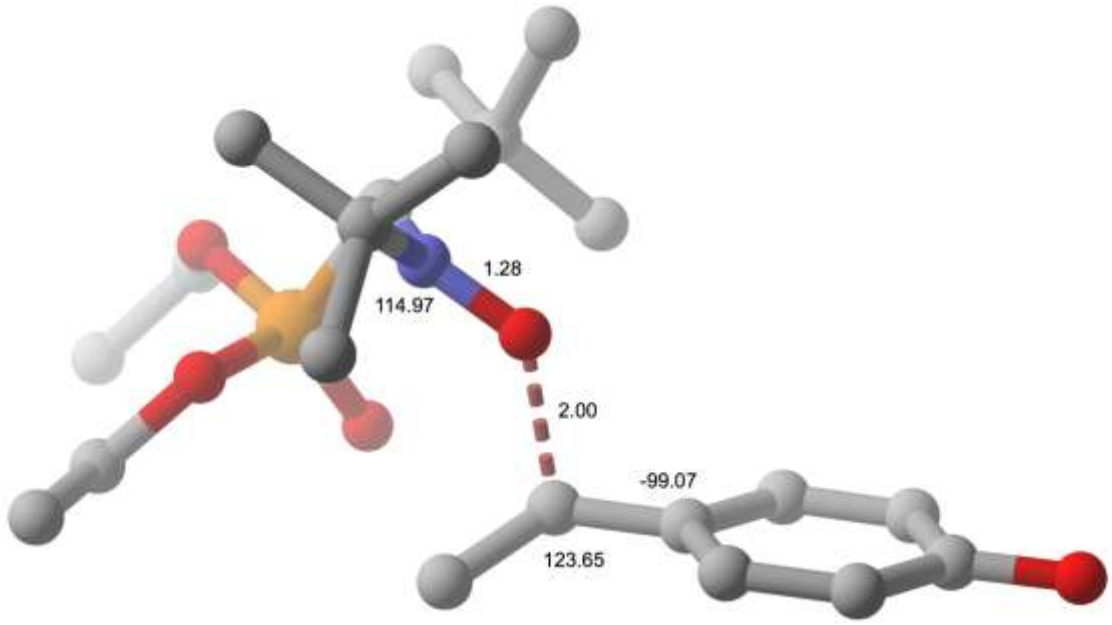


Figure 4SI. Calculated mesolysis transition state of **3a•** at the M06-2X/6-31+G(d,p) level of theory in the gas-phase. Hydrogen atoms are omitted for clarity.

Computational Geometries

3a•_ae

N	0.36603	-1.09667	0.13658
O	0.73176	0.18059	-0.39454
C	2.12803	0.48096	-0.24652
C	2.26692	1.82905	0.46427
C	2.81092	0.56024	-1.59187
C	2.16748	1.21089	-2.67278
C	2.79367	1.34607	-3.88361
C	4.13793	0.83341	-4.08899
C	4.77219	0.17912	-2.95931
C	4.11682	0.05599	-1.75743
O	4.72048	0.94794	-5.18832
C	-0.63118	-0.87505	1.20572
P	-1.46944	0.77714	1.13500
O	-0.80680	1.90978	1.83115
O	-1.88930	1.13646	-0.37704
C	-1.30637	2.26502	-1.04694
C	-2.14937	3.50496	-0.82102
O	-2.90016	0.32761	1.72348
C	-3.93121	1.32464	1.85331
C	-5.00708	1.08309	0.81289
C	-0.05671	-1.18105	2.63448
C	0.40604	-2.64335	2.66529
C	-1.14839	-1.00220	3.70162
C	1.13642	-0.29322	3.00131
C	-0.06944	-1.97699	-0.99758
C	1.12199	-2.12854	-1.94708
C	-0.39527	-3.37099	-0.44786
C	-1.27145	-1.42995	-1.77381
H	2.57882	-0.32354	0.34235
H	1.92514	2.63726	-0.18995
H	3.31753	2.01602	0.70536
H	1.66303	1.84804	1.37225
H	1.15609	1.58114	-2.52556
H	2.31866	1.83390	-4.72878
H	5.77430	-0.20801	-3.11277
H	4.59794	-0.44352	-0.91965
H	-1.46235	-1.57350	1.05734
H	-1.27452	1.98739	-2.10531
H	-0.28576	2.41467	-0.68708
H	-3.18575	3.32663	-1.12186
H	-1.75663	4.33961	-1.40935
H	-2.12188	3.78440	0.23565
H	-3.49310	2.32448	1.75751
H	-4.32308	1.22606	2.86895
H	-5.43418	0.08430	0.93352
H	-4.58393	1.16237	-0.19138
H	-5.80860	1.81985	0.92091
H	1.19455	-2.81858	1.92881
H	-0.42109	-3.33428	2.46838
H	0.80657	-2.87478	3.65763
H	-1.42179	0.04825	3.83450
H	-0.76984	-1.37369	4.65938
H	-2.05540	-1.56167	3.44996
H	1.50406	-0.58454	3.99130
H	0.85409	0.76087	3.03473
H	1.95941	-0.42916	2.29454
H	1.29523	-1.21934	-2.52347
H	2.03162	-2.37485	-1.38850
H	0.92269	-2.93798	-2.65529
H	0.46550	-3.80239	0.06837
H	-1.25166	-3.38022	0.23074
H	-0.64745	-4.01888	-1.29192
H	-1.05128	-0.43609	-2.16989
H	-1.49345	-2.09895	-2.61134
H	-2.16819	-1.35610	-1.15058

3a•_ac

N	0.37199	-0.80918	-0.77430
O	0.10228	-0.60245	0.61559
C	-0.74640	-1.60884	1.18875
C	-1.93528	-0.92031	1.86273
C	-0.00048	-2.42443	2.21892
C	0.86540	-1.78008	3.13590
C	1.50694	-2.49228	4.11444
C	1.30956	-3.92633	4.24352
C	0.41000	-4.55471	3.29348
C	-0.21704	-3.81354	2.32048
O	1.88936	-4.58897	5.12992
C	-0.13984	0.36385	-1.51501
P	-0.40823	1.87108	-0.46915
O	-1.72596	2.01248	0.20423
O	0.83125	2.08538	0.53246
C	0.64314	2.00736	1.95388
C	0.34601	3.38067	2.52281
O	-0.06468	2.98213	-1.58399
C	-0.26215	4.36933	-1.25114
C	-1.67379	4.80989	-1.58986
C	-1.40204	0.01738	-2.38242
C	-1.01548	-1.08248	-3.37942
C	-1.86233	1.24747	-3.18079
C	-2.58065	-0.48825	-1.54476
C	1.83370	-1.10632	-0.93747
C	2.13311	-2.38823	-0.15576
C	2.12053	-1.39612	-2.41583
C	2.74849	0.01720	-0.44063
H	-1.07749	-2.26413	0.37756
H	-1.60002	-0.37025	2.74763
H	-2.66241	-1.66914	2.19042
H	-2.40607	-0.21188	1.18012
H	1.02589	-0.71006	3.03136
H	2.18072	-2.02253	4.82383
H	0.26515	-5.62617	3.38617
H	-0.88257	-4.29565	1.60812
H	0.63114	0.69531	-2.21966
H	1.58124	1.60361	2.34776
H	-0.16661	1.30846	2.17621
H	1.13358	4.08896	2.25055
H	0.28683	3.33045	3.61415
H	-0.61366	3.74092	2.14146
H	0.48122	4.91376	-1.83773
H	-0.03682	4.52476	-0.18946
H	-1.79338	5.87578	-1.37408
H	-2.39796	4.24454	-0.99809
H	-1.87672	4.64650	-2.65177
H	-0.21292	-0.75737	-4.05060
H	-1.88531	-1.33463	-3.99470
H	-0.69297	-1.98649	-2.85641
H	-2.29796	2.01315	-2.53275
H	-2.63159	0.93693	-3.89528
H	-1.03698	1.70182	-3.73879
H	-2.31597	-1.40037	-1.00339
H	-3.41174	-0.73505	-2.21447
H	-2.92156	0.27041	-0.83752
H	2.13730	-2.21150	0.92016
H	1.39367	-3.16279	-0.38683
H	3.12252	-2.76213	-0.43459
H	1.51606	-2.23053	-2.77898
H	1.95562	-0.53429	-3.06702
H	3.17454	-1.67198	-2.50950
H	2.55248	0.23299	0.61203
H	2.61306	0.94322	-1.00774
H	3.79215	-0.29626	-0.54473

3a•_as

N	0.85957	-0.08830	-0.74090
O	0.40202	-0.67247	0.48280
C	0.48062	-2.10604	0.49627
C	-0.89649	-2.66848	0.85431
C	1.48814	-2.58297	1.51605
C	1.54974	-1.96535	2.78900
C	2.41659	-2.41908	3.74776
C	3.28931	-3.55182	3.48782
C	3.19565	-4.16715	2.17665
C	2.31809	-3.68696	1.23413
O	4.08588	-3.97526	4.35218
C	-0.26840	0.66375	-1.33203
P	-1.62357	1.06391	-0.13451
O	-2.68854	0.04707	0.06462
O	-0.99942	1.60838	1.24331
C	-1.21082	0.89324	2.47021
C	-2.44906	1.41431	3.17274
O	-2.11098	2.44985	-0.79686
C	-3.32055	3.04325	-0.29382
C	-3.67449	4.20347	-1.19930
C	-0.82013	-0.01489	-2.63661
C	0.32226	-0.10013	-3.65687
C	-1.94801	0.82920	-3.25216
C	-1.34875	-1.43182	-2.39159
C	2.10275	0.70208	-0.45535
C	3.15759	-0.27371	0.07311
C	2.63694	1.28274	-1.77031
C	1.89512	1.82686	0.56342
H	0.79226	-2.43032	-0.50119
H	-1.14121	-2.43006	1.89416
H	-0.89138	-3.75774	0.75271
H	-1.66655	-2.23357	0.21634
H	0.90808	-1.10886	2.97976
H	2.48759	-1.95809	4.72771
H	3.85021	-5.01002	1.97983
H	2.26218	-4.14974	0.25151

H	0.08944	1.65566	-1.63170
H	-0.30819	1.06452	3.06525
H	-1.30062	-0.17497	2.25771
H	-2.36988	2.49177	3.34189
H	-2.57042	0.91859	4.14048
H	-3.33435	1.20847	2.56454
H	-3.14322	3.37774	0.73536
H	-4.10942	2.28326	-0.28550
H	-4.59088	4.68627	-0.84937
H	-3.83345	3.85100	-2.22161
H	-2.87000	4.94286	-1.20634
H	0.70593	0.89176	-3.91981
H	-0.04656	-0.57072	-4.57406
H	1.14569	-0.70561	-3.26939
H	-2.85531	0.80610	-2.64155
H	-2.19687	0.41989	-4.23665
H	-1.64852	1.87476	-3.37926
H	-1.68423	-1.85512	-3.34467
H	-2.19281	-1.42896	-1.69912
H	-0.56081	-2.08330	-2.00430
H	2.94229	-0.58386	1.09599
H	3.21451	-1.16274	-0.56446
H	4.13692	0.21354	0.07333
H	2.84595	0.49245	-2.49509
H	1.96241	2.00953	-2.22928
H	3.57332	1.80490	-1.55511
H	1.51208	1.42495	1.50407
H	1.19081	2.58432	0.20639
H	2.85415	2.31768	0.75744

3a(III) TS

N	0.73139	0.21861	-0.10213
O	0.03646	-0.36234	0.85582
C	-0.25016	-2.22175	0.90665
C	-1.22761	-2.14600	2.04179
C	1.01987	-2.82766	1.02026
C	1.63114	-3.10740	2.28884
C	2.88986	-3.61191	2.37519
C	3.68825	-3.88509	1.17691
C	3.04295	-3.60452	-0.10716
C	1.77796	-3.10513	-0.16394
O	4.84111	-4.32610	1.24627
C	-0.12071	0.90715	-1.09513
P	-1.71968	1.41621	-0.29679
O	-2.83158	0.43211	-0.27810
O	-1.38510	2.04107	1.14368
C	-1.78378	1.41050	2.37346
C	-2.17292	2.50193	3.34854
O	-1.98822	2.76492	-1.13107
C	-3.23364	3.45899	-0.91612
C	-4.28936	2.97496	-1.89129
C	-0.32511	0.16729	-2.46178
C	1.04037	-0.05005	-3.12364
C	-1.17811	1.04856	-3.39033
C	-1.01283	-1.19729	-2.33196
C	1.97400	0.90690	0.40402
C	2.69991	-0.04186	1.35605
C	2.90845	1.23782	-0.76023
C	1.60294	2.19067	1.16029
H	-0.70860	-2.27236	-0.07336
H	-0.77809	-1.68643	2.92637
H	-1.56869	-3.15121	2.30998
H	-2.09082	-1.55134	1.73596
H	1.06843	-2.90886	3.19687
H	3.35693	-3.83134	3.33009
H	3.61923	-3.81913	-1.00160
H	1.31870	-2.90626	-1.12877
H	0.36854	1.85843	-1.33663
H	-0.93392	0.82492	2.73753
H	-2.61595	0.73047	2.16963
H	-1.33874	3.19083	3.50576
H	-2.44709	2.06125	4.31114
H	-3.02659	3.07125	2.97141
H	-3.00259	4.51645	-1.06146
H	-3.55433	3.31968	0.12301
H	-5.21632	3.53788	-1.74769
H	-4.49165	1.91318	-1.73036
H	-3.95045	3.12270	-2.92025
H	1.54281	0.89744	-3.34541
H	0.90028	-0.58487	-4.06876
H	1.69356	-0.65413	-2.48744
H	-2.22286	1.08293	-3.06890
H	-1.15114	0.62325	-4.39848
H	-0.80360	2.07609	-3.43821
H	-1.29958	-1.54264	-3.33104
H	-1.91147	-1.14940	-1.71156
H	-0.32345	-1.94008	-1.92742
H	2.07180	-0.30879	2.20758
H	3.00741	-0.95713	0.84460
H	3.59665	0.46075	1.72924
H	3.22101	0.33210	-1.28478
H	2.46491	1.93069	-1.48020
H	3.80227	1.71986	-0.35470
H	0.96780	1.95946	2.01848
H	1.07140	2.90863	0.52871
H	2.51973	2.66699	1.52060

3•_at

N	-0.07311	0.76097	0.98316
O	0.05753	1.91679	0.46201
C	-1.03864	-0.15334	0.36856
P	-0.31026	-0.88919	-1.15677
O	-1.20256	-1.82104	-1.88104
O	0.23777	0.27739	-2.09808
C	1.49245	0.97538	-1.97294
C	2.04823	1.18679	-3.36590
O	1.00740	-1.58863	-0.52464
C	1.50068	-2.80027	-1.13528
C	2.16767	-2.52074	-2.46886
C	-2.46094	0.46340	0.18391
C	-2.79629	1.29109	1.43141
C	-3.46388	-0.69692	0.07705
C	-2.57217	1.34168	-1.06992
C	0.78136	0.47089	2.17689
C	2.24358	0.55922	1.72527
C	0.47903	1.55058	3.22168
C	0.49374	-0.91348	2.75229
H	-1.14464	-1.01235	1.03541
H	2.17412	0.38311	-1.35363
H	1.29118	1.92018	-1.46458
H	1.33671	1.74784	-3.97621
H	2.98212	1.75373	-3.30943
H	2.24702	0.23107	-3.85761
H	0.66433	-3.49501	-1.25415
H	2.20861	-3.20799	-0.41022
H	2.58213	-3.44633	-2.87839
H	1.44020	-2.12618	-3.18464
H	2.98204	-1.79953	-2.35138
H	-2.16157	2.17780	1.50770
H	-2.67641	0.69329	2.34413
H	-3.84061	1.61535	1.38053
H	-4.47216	-0.29208	-0.05861
H	-3.46571	-1.29902	0.99384
H	-3.23377	-1.34938	-0.76878
H	-1.82757	2.14009	-1.05969
H	-3.57180	1.78828	-1.10432
H	-2.44082	0.74927	-1.98154
H	2.46446	-0.23502	1.00631
H	2.43083	1.53021	1.25964
H	2.90523	0.44949	2.58976
H	1.12720	1.41071	4.09175
H	-0.56294	1.49044	3.55079
H	0.65632	2.54240	2.80092
H	-0.53631	-0.99910	3.11392
H	0.69313	-1.70211	2.02126
H	1.15647	-1.06930	3.60811

3•_ce

N	0.26466	0.95604	1.07966
O	-0.51260	1.85151	0.60492
C	0.15539	-0.36885	0.45641
P	0.43339	-0.07543	-1.34464
O	1.57418	0.83710	-1.59940
O	0.63103	-1.57617	-1.87692
C	1.00309	-1.75714	-3.25786
C	1.17188	-3.24221	-3.49443
O	-0.93595	0.36208	-2.05492
C	-1.15833	1.74636	-2.42187
C	-2.52533	2.17435	-1.93480
C	-1.10440	-1.15128	0.94479
C	-0.90463	-1.43929	2.44022
C	-1.21520	-2.49052	0.20270
C	-2.41090	-0.37130	0.75911
C	1.39805	1.45038	1.92480
C	2.17242	2.49448	1.11180
C	0.77423	2.09661	3.16592
C	2.32495	0.30743	2.32978
H	1.02904	-0.96225	0.74340
H	1.93096	-1.20774	-3.44508
H	0.21043	-1.34031	-3.88921
H	0.23939	-3.77127	-3.28262
H	1.44970	-3.42533	-4.53586
H	1.95585	-3.64419	-2.84814
H	-1.08606	1.79044	-3.51269
H	-0.36673	2.36292	-1.98967
H	-2.73898	3.18620	-2.29193
H	-3.30034	1.50313	-2.31592
H	-2.55027	2.17446	-0.84321
H	-0.78241	-0.51267	3.01023
H	-0.02740	-2.07468	2.61027
H	-1.77989	-1.96358	2.83691
H	-1.98551	-3.09959	0.68695
H	-0.27219	-3.04692	0.22316
H	-1.49816	-2.34979	-0.84327

H	-2.41025	0.56017	1.33016
H	-3.24129	-0.99459	1.10942
H	-2.58036	-0.12980	-0.29245
H	2.54285	2.05684	0.18169
H	1.51776	3.33231	0.86182
H	3.01227	2.86491	1.70788
H	1.55529	2.58424	3.75656
H	0.28078	1.34987	3.79605
H	0.03975	2.84673	2.86474
H	1.78909	-0.49064	2.85305
H	2.85323	-0.11022	1.46724
H	3.07755	0.70691	3.01507

3•_ab

N	0.44558	0.17686	1.40823
O	0.93915	1.35267	1.40841
C	-0.69801	-0.06739	0.51854
P	0.04418	-0.19545	-1.16077
O	1.03085	-1.30512	-1.23518
O	-1.22699	-0.30478	-2.12780
C	-0.99443	-0.52536	-3.53788
C	-0.94053	-2.00921	-3.84328
O	0.65128	1.22771	-1.57185
C	2.06344	1.49110	-1.42196
C	2.77068	1.23975	-2.73769
C	-1.89188	0.90487	0.76805
C	-2.02854	1.11279	2.28352
C	-3.17378	0.22860	0.25629
C	-1.72395	2.26313	0.07556
C	1.17090	-0.85678	2.21233
C	0.51111	-2.22694	2.08124
C	2.61166	-0.92273	1.69271
C	1.14369	-0.38319	3.66910
H	-1.05518	-1.08013	0.72042
H	-0.06947	-0.01683	-3.83312
H	-1.82927	-0.03577	-4.04358
H	-1.87072	-2.49308	-3.53481
H	-0.80936	-2.16176	-4.91864
H	-0.10619	-2.47377	-3.31290
H	2.47222	0.86674	-0.62359
H	2.12695	2.53459	-1.10704
H	3.83003	1.49898	-2.65093
H	2.69255	0.18255	-3.00650
H	2.32916	1.84726	-3.53277
H	-1.18023	1.67016	2.68879
H	-2.09837	0.15171	2.80865
H	-2.94480	1.67481	2.49084
H	-4.02774	0.89119	0.43099
H	-3.36408	-0.71003	0.79035
H	-3.11821	0.01503	-0.81308
H	-0.78666	2.73979	0.36931
H	-2.55975	2.91217	0.35921
H	-1.73192	2.15688	-1.01340
H	-0.51656	-2.22511	2.46067
H	0.52672	-2.57747	1.04470
H	1.08206	-2.93638	2.68671
H	3.18732	-1.62586	2.30229
H	3.07844	0.06321	1.76106
H	2.61956	-1.26246	0.65268
H	1.57357	0.61808	3.74586
H	0.11798	-0.35585	4.05042
H	1.72742	-1.06927	4.28984

3•_cu

N	0.48643	0.84825	0.82384
O	1.41030	1.45951	0.19475
C	-0.73039	0.53270	0.07684
P	-0.39369	-0.87413	-1.08712
O	-1.13058	-0.88001	-2.37352
O	1.19665	-1.01564	-1.23507
C	1.89081	-0.28660	-2.27023
C	3.35947	-0.28758	-1.91051
O	-0.69600	-2.09583	-0.08417
C	-0.56622	-3.44450	-0.58542
C	-1.88235	-3.92498	-1.16481
C	-1.42001	1.78847	-0.53951
C	-1.44250	2.88317	0.53619
C	-2.86459	1.39571	-0.88733
C	-0.72998	2.32735	-1.79973
C	0.84971	0.28063	2.15894
C	1.91983	-0.79569	1.94235
C	1.41032	1.44039	2.98720
C	-0.36952	-0.31849	2.85710
H	-1.44623	0.10827	0.78457
H	1.50827	0.73699	-2.31123
H	1.69203	-0.78202	-3.22525
H	3.72933	-1.31115	-1.80662
H	3.93552	0.21508	-2.69234
H	3.50484	0.24477	-0.96745
H	-0.26044	-4.04196	0.27671
H	0.23869	-3.47754	-1.32754
H	-1.78435	-4.96163	-1.50031
H	-2.66927	-3.87748	-0.40776
H	-2.16982	-3.30144	-2.01440
H	-0.43345	3.24164	0.75791
H	-1.89461	2.51690	1.46654
H	-2.04039	3.72973	0.18372
H	-3.39027	2.26567	-1.29408
H	-3.40917	1.06330	0.00466
H	-2.89078	0.59974	-1.63623
H	-0.74515	1.58365	-2.60248
H	0.30022	2.62115	-1.58809
H	-1.27618	3.20917	-2.15253
H	1.51657	-1.63298	1.36598
H	2.76630	-0.37357	1.39527
H	2.26929	-1.16536	2.91140
H	1.73255	1.06992	3.96456
H	0.64458	2.20811	3.13906
H	2.26303	1.89302	2.47821
H	-1.16454	0.42362	2.98795
H	-0.76247	-1.18551	2.31834
H	-0.06149	-0.65271	3.85173

3•_al

N	0.86254	-0.08058	1.21980
O	1.70735	0.76710	0.77371
C	-0.45056	-0.05800	0.56783
P	-0.10952	-0.26013	-1.23568
O	0.96546	-1.24134	-1.52071
O	-1.56407	-0.66128	-1.77891
C	-1.68909	-1.05632	-3.16208
C	-1.51951	-2.55612	-3.30468
O	0.10739	1.17348	-1.92307
C	1.44132	1.70059	-2.11123
C	1.47768	2.40029	-3.45279
C	-1.32764	1.14010	1.05081
C	-1.67236	0.88327	2.52523
C	-2.63248	1.19414	0.24465
C	-0.61526	2.49379	0.93924
C	1.41972	-1.18942	2.05670
C	2.51874	-1.88641	1.24652
C	2.01090	-0.53870	3.31126
C	0.33336	-2.19056	2.44114
H	-0.98922	-0.97491	0.82565
H	-0.95398	-0.50973	-3.76341
H	-2.68701	-0.73038	-3.46377
H	-2.25728	-3.08001	-2.69143
H	-1.66458	-2.84930	-4.34873
H	-0.51726	-2.85222	-2.98716
H	2.15714	0.87591	-2.05978
H	1.64221	2.38435	-1.28182
H	2.46357	2.84615	-3.61185
H	1.28307	1.69093	-4.26163
H	0.72661	3.19338	-3.49560
H	-0.76693	0.79846	3.13524
H	-2.26186	-0.03367	2.64278
H	-2.26459	1.71554	2.91889
H	-3.30366	1.92583	0.70612
H	-3.13968	0.22399	0.22671
H	-2.45350	1.49940	-0.78950
H	0.28067	2.53208	1.56240
H	-1.30547	3.27738	1.27118
H	-0.32773	2.70692	-0.09296
H	2.11527	-2.27662	0.30902
H	3.31161	-1.17482	1.00602
H	2.94034	-2.70479	1.83856
H	2.53295	-1.29438	3.90547
H	1.22662	-0.09232	3.93105
H	2.72182	0.23980	3.02630
H	-0.50409	-1.71035	2.95686
H	-0.04021	-2.73889	1.57091
H	0.77129	-2.92136	3.12653

3•_au

N	0.53862	0.62341	1.39314
O	0.97372	1.63031	0.73885
C	-0.33940	-0.27827	0.64136
P	0.61133	-0.75210	-0.86817
O	2.05219	-0.97891	-0.60773
O	-0.21475	-2.03916	-1.35005
C	0.18013	-2.69181	-2.57523
C	-0.78915	-2.33287	-3.68451
O	0.31468	0.28493	-2.05919
C	1.21487	1.38883	-2.30927
C	1.28055	1.59554	-3.80732
C	-1.78071	0.30276	0.48224
C	-2.41895	0.31581	1.87913
C	-2.61873	-0.60298	-0.43086
C	-1.79831	1.72949	-0.08084
C	1.25325	0.30673	2.66948
C	1.02996	1.49868	3.60545
C	0.71165	-0.97243	3.30252
C	2.74400	0.14848	2.34924
H	-0.43138	-1.22163	1.18835

H	0.16621	-3.76220	-2.35811
H	1.20857	-2.40948	-2.82572
H	-0.76360	-1.25725	-3.87588
H	-0.52073	-2.86297	-4.60311
H	-1.80718	-2.61670	-3.40466
H	2.19312	1.14839	-1.88449
H	0.81665	2.26310	-1.78681
H	1.92722	2.44673	-4.03800
H	1.68619	0.70748	-4.29982
H	0.28537	1.79636	-4.21343
H	-1.83231	0.92263	2.57682
H	-2.50841	-0.69837	2.28599
H	-3.42428	0.74573	1.82510
H	-3.66318	-0.27695	-0.38970
H	-2.57123	-1.65139	-0.11916
H	-2.28387	-0.54510	-1.47008
H	-1.28601	2.43213	0.57964
H	-2.84159	2.04730	-0.18671
H	-1.32621	1.77388	-1.06516
H	1.33603	2.42262	3.11017
H	-0.02316	1.58288	3.89262
H	1.62656	1.36938	4.51321
H	1.19695	-1.10329	4.27359
H	0.94327	-1.85477	2.69812
H	-0.36809	-0.92075	3.47426
H	2.89626	-0.64463	1.61323
H	3.13582	1.07895	1.93268
H	3.28808	-0.08875	3.26885

3•_ak

N	0.06350	0.73910	0.80904
O	1.06155	1.49044	0.55501
C	-0.81517	0.38190	-0.30676
P	-0.00331	-0.89418	-1.35797
O	-0.80866	-1.34482	-2.51382
O	1.44513	-0.38570	-1.80292
C	2.63872	-0.47863	-1.00016
C	3.51511	0.70935	-1.32842
O	0.28056	-2.01670	-0.22809
C	0.67468	-3.33320	-0.67321
C	-0.54166	-4.22498	-0.82094
C	-1.37016	1.61318	-1.09157
C	-1.72713	2.71004	-0.08034
C	-2.65268	1.17060	-1.81448
C	-0.37426	2.16196	-2.12236
C	-0.09326	0.29722	2.23054
C	-1.32663	-0.58379	2.41259
C	1.16905	-0.48505	2.61120
C	-0.21218	1.56208	3.08772
H	-1.67472	-0.14805	0.11033
H	3.13027	-1.42393	-1.25816
H	2.37681	-0.49159	0.05993
H	3.00215	1.63054	-1.04516
H	4.45508	0.64181	-0.77297
H	3.74000	0.73417	-2.39751
H	1.36289	-3.70395	0.09133
H	1.22058	-3.25259	-1.62055
H	-0.23340	-5.23410	-1.10939
H	-1.08387	-4.28482	0.12661
H	-1.20558	-3.82286	-1.58947
H	-0.83476	3.11517	0.40446
H	-2.40410	2.32642	0.69371
H	-2.24125	3.52616	-0.59787
H	-3.06088	2.01665	-2.37704
H	-3.41559	0.84714	-1.09596
H	-2.45879	0.35032	-2.50990
H	-0.18390	1.43451	-2.91835
H	0.57665	2.42178	-1.65263
H	-0.79900	3.05931	-2.58517
H	-2.25186	-0.04477	2.18359
H	-1.26790	-1.48893	1.80104
H	-1.37486	-0.88641	3.46234
H	1.12550	-0.76236	3.66862
H	2.05520	0.13360	2.44779
H	1.24562	-1.39547	2.00929
H	0.64985	2.21137	2.92025
H	-1.12270	2.11588	2.83986
H	-0.25045	1.28636	4.14571

3•_ao

N	0.46233	-0.22251	1.34735
O	1.00271	0.92084	1.51156
C	-0.58291	-0.32571	0.32005
P	0.33362	-0.35905	-1.27698
O	1.25880	-1.51847	-1.34679
O	-0.83661	-0.31500	-2.36966
C	-0.47472	-0.42399	-3.76287
C	-1.75705	-0.44696	-4.56563
O	1.04606	1.05702	-1.50060
C	2.43348	1.25467	-1.14576
C	2.59365	2.68982	-0.69702
C	-1.75146	0.68760	0.52561
C	-2.04422	0.77916	2.03063
C	-3.00068	0.12738	-0.17377
C	-1.44826	2.08651	-0.02549
C	1.04924	-1.36074	2.12297
C	0.35127	-2.67721	1.79187
C	2.53497	-1.45451	1.75700
C	0.87907	-1.01862	3.60663
H	-1.00746	-1.33003	0.39119
H	0.10747	-1.34037	-3.90081
H	0.14792	0.43766	-4.02614
H	-2.32929	0.46888	-4.39804
H	-1.52833	-0.52587	-5.63178
H	-2.37248	-1.30227	-4.27640
H	3.03275	1.03045	-2.03332
H	2.71252	0.55919	-0.35031
H	3.64454	2.89298	-0.47160
H	2.26620	3.37663	-1.48205
H	1.99927	2.86169	0.20286
H	-1.21994	1.25141	2.57102
H	-2.21820	-0.21598	2.45922
H	-2.94953	1.37416	2.18810
H	-3.83826	0.81676	-0.02528
H	-3.28725	-0.84280	0.24936
H	-2.84272	0.00531	-1.24731
H	-0.53162	2.48963	0.40955
H	-2.28247	2.75333	0.21897
H	-1.33508	2.06908	-1.11365
H	-0.71125	-2.65570	2.05766
H	0.46801	-2.93322	0.73433
H	0.82080	-3.46684	2.38506
H	3.00854	-2.23895	2.35508
H	3.03249	-0.50471	1.96937
H	2.64514	-1.69917	0.69633
H	1.34062	-0.05280	3.82444
H	-0.18082	-0.97089	3.87615
H	1.35915	-1.78790	4.21859

3•_ag

N	0.80118	0.96851	0.98328
O	1.30684	0.01135	1.66099
C	0.18754	0.57764	-0.28950
P	-1.04298	-0.73173	0.13516
O	-1.78636	-0.45117	1.38628
O	-1.93453	-0.75121	-1.19901
C	-3.09513	-1.60600	-1.22377
C	-3.79541	-1.38694	-2.54721
O	-0.35363	-2.17993	0.07960
C	0.15377	-2.79675	1.28559
C	-0.09394	-4.28609	1.18099
C	1.25371	0.29487	-1.39501
C	1.92659	1.63482	-1.72744
C	0.57032	-0.23781	-2.66200
C	2.33219	-0.70246	-0.95345
C	0.57673	2.25172	1.72050
C	1.95803	2.76601	2.13795
C	-0.12668	3.27987	0.83825
C	-0.27601	1.94347	2.95657
H	-0.43705	1.40113	-0.64890
H	-3.73816	-1.34776	-0.37653
H	-2.76389	-2.64466	-1.11429
H	-3.12811	-1.63172	-3.37737
H	-4.68155	-2.02418	-2.61073
H	-4.10735	-0.34440	-2.64551
H	-0.35489	-2.35576	2.14712
H	1.21871	-2.55803	1.35405
H	0.31012	-4.79177	2.06250
H	-1.16537	-4.49478	1.12137
H	0.39212	-4.69673	0.29206
H	2.39692	2.07273	-0.84081
H	1.20466	2.35363	-2.13274
H	2.70709	1.48256	-2.47980
H	1.30385	-0.26572	-3.47438
H	-0.26455	0.39909	-2.97227
H	0.18475	-1.25003	-2.51484
H	1.89451	-1.66569	-0.68073
H	2.90429	-0.32940	-0.10142
H	3.01931	-0.86378	-1.79160
H	2.49176	1.99032	2.69122
H	2.55335	3.05135	1.26460
H	1.84407	3.64405	2.78041
H	-0.17776	4.22286	1.38942
H	-1.15278	2.98027	0.60401
H	0.42032	3.46671	-0.09118
H	-1.22794	1.49400	2.66375
H	0.24891	1.23779	3.60410
H	-0.45748	2.86991	3.51045

3•_aw

N	0.78523	0.16675	1.15467
O	1.65378	1.05256	0.85822
C	-0.46691	0.21002	0.40333
P	-0.10054	0.22193	-1.40765

O	-0.02047	1.50197	-2.15172
O	1.20529	-0.70176	-1.55122
C	2.28373	-0.30887	-2.43253
C	3.19306	0.71679	-1.78925
O	-1.31085	-0.73542	-1.88514
C	-1.61645	-0.79679	-3.28946
C	-2.94315	-1.50931	-3.44165
C	-1.41402	1.36692	0.85491
C	-1.85000	1.07902	2.29706
C	-2.66155	1.37451	-0.04294
C	-0.73353	2.74026	0.79513
C	1.25890	-0.96320	2.01374
C	0.15319	-1.98883	2.25085
C	2.44921	-1.62628	1.31075
C	1.70900	-0.35283	3.34516
H	-1.00382	-0.72878	0.56037
H	1.85735	0.07702	-3.36335
H	2.81159	-1.24176	-2.64454
H	3.59392	0.34039	-0.84564
H	4.02343	0.93762	-2.46737
H	2.64316	1.63776	-1.58523
H	-0.81264	-1.34190	-3.79943
H	-1.65611	0.22252	-3.68634
H	-3.21029	-1.58226	-4.49934
H	-2.88821	-2.51766	-3.02426
H	-3.72959	-0.95777	-2.92017
H	-0.98595	1.01458	2.96630
H	-2.41899	0.14406	2.36478
H	-2.49183	1.88920	2.65778
H	-3.38886	2.08398	0.36455
H	-3.13280	0.38641	-0.08735
H	-2.42036	1.69044	-1.06257
H	0.09688	2.80436	1.50183
H	-1.47221	3.50672	1.05556
H	-0.34901	2.94876	-0.20631
H	-0.73613	-1.53460	2.69782
H	-0.12893	-2.50782	1.32960
H	0.53012	-2.74049	2.94990
H	2.82484	-2.44974	1.92579
H	3.25005	-0.89670	1.17004
H	2.15183	-2.01317	0.33259
H	2.43369	0.44345	3.16322
H	0.85867	0.06247	3.89466
H	2.17612	-1.12426	3.96447

3•_as

N	-0.71176	0.93229	-0.07857
O	0.00506	1.98000	-0.18626
C	-0.35554	-0.20653	-0.92418
P	1.17359	-1.01463	-0.24981
O	2.08408	-1.65675	-1.22608
O	1.88139	0.02611	0.74351
C	2.86128	0.95853	0.23976
C	3.03698	2.03287	1.28924
O	0.46767	-1.98568	0.82331
C	1.30048	-2.76347	1.70604
C	0.38678	-3.62620	2.54908
C	-0.34811	0.13092	-2.44639
C	-1.61101	0.94864	-2.75021
C	-0.41387	-1.19970	-3.21275
C	0.88849	0.91333	-2.90790
C	-1.65121	0.88254	1.08413
C	-0.81739	0.88559	2.37098
C	-2.51537	2.14414	0.99905
C	-2.53656	-0.36114	1.03033
H	-1.12527	-0.96926	-0.78402
H	2.49870	1.39408	-0.69526
H	3.78565	0.40689	0.04445
H	3.34227	1.59344	2.24268
H	3.80378	2.74437	0.97062
H	2.09385	2.56765	1.42530
H	1.88659	-2.07541	2.32456
H	1.98383	-3.36776	1.10078
H	0.97725	-4.23233	3.24118
H	-0.29758	-3.00183	3.13002
H	-0.20154	-4.29326	1.91446
H	-1.56724	1.93502	-2.28014
H	-2.51259	0.43320	-2.39585
H	-1.70652	1.08507	-3.83217
H	-0.43974	-0.99893	-4.28869
H	-1.32135	-1.75909	-2.95545
H	0.45880	-1.82343	-3.00188
H	1.80158	0.33128	-2.74822
H	0.96463	1.87016	-2.38721
H	0.80305	1.10946	-3.98240
H	-0.21637	-0.02519	2.44540
H	-0.14491	1.74683	2.37662
H	-1.48229	0.94561	3.23831
H	-3.19801	2.17863	1.85294
H	-3.10708	2.14140	0.07783
H	-1.88699	3.03635	1.00795
H	-3.11292	-0.40574	0.09991

H	-1.95561	-1.28073	1.14627
H	-3.24875	-0.30705	1.85852

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N	-0.40897	-1.34876	-0.17920
O	-0.03076	-1.99883	0.85224
C	-0.78682	0.04657	0.04301
P	0.56833	0.88500	0.98489
O	0.45911	1.00951	2.45700
O	1.93649	0.21037	0.47903
C	2.69308	-0.66361	1.34827
C	4.11403	-0.70110	0.82887
O	0.57765	2.28109	0.18149
C	1.37491	3.35660	0.71204
C	1.06678	4.59918	-0.09492
C	-2.19844	0.20520	0.68647
C	-3.23842	-0.30267	-0.32027
C	-2.45546	1.69719	0.95022
C	-2.33649	-0.58099	1.99606
C	-0.11691	-1.98312	-1.50263
C	1.39792	-2.20098	-1.59931
C	-0.84929	-3.32838	-1.51934
C	-0.59340	-1.10957	-2.66081
H	-0.80465	0.56239	-0.92050
H	2.22274	-1.65047	1.32737
H	2.63833	-0.27218	2.36759
H	4.55729	0.29809	0.84093
H	4.71997	-1.35928	1.45775
H	4.14087	-1.08120	-0.19610
H	2.43228	3.07928	0.63017
H	1.12667	3.48857	1.76986
H	1.65658	5.44163	0.27629
H	1.30704	4.44184	-1.14921
H	0.00678	4.85196	-0.01197
H	-3.06165	-1.35254	-0.57747
H	-3.22935	0.29238	-1.24129
H	-4.24009	-0.23071	0.11557
H	-3.49544	1.83144	1.26450
H	-2.28960	2.29938	0.04977
H	-1.81156	2.07899	1.74816
H	-1.56758	-0.29025	2.71574
H	-2.25675	-1.65701	1.82359
H	-3.32177	-0.37079	2.42722
H	1.92641	-1.24480	-1.55226
H	1.73804	-2.83239	-0.77426
H	1.63804	-2.69681	-2.54472

H	-0.58771	-3.87837	-2.42800
H	-1.93376	-3.18204	-1.50325
H	-0.56224	-3.92164	-0.64901
H	-0.02114	-0.18013	-2.73744
H	-0.44273	-1.66520	-3.59052
H	-1.65823	-0.87293	-2.58193

F

C	0.00000	0.50596	2.31592
C	0.00000	-0.48539	3.43258
C	0.00000	0.26484	0.98429
C	0.00000	1.39227	0.05107
C	0.00000	1.22214	-1.28218
C	0.00000	-0.12824	-1.87994
C	0.00000	-1.26431	-0.93258
C	0.00000	-1.07546	0.39896
O	0.00000	-0.30158	-3.09080
H	0.87846	-0.33181	4.06887
H	0.00000	-1.52105	3.09369
H	-0.87846	-0.33181	4.06887
H	0.00000	2.39220	0.47967
H	0.00000	2.05784	-1.97443
H	0.00000	-2.25579	-1.37426
H	0.00000	-1.93415	1.06267
H	0.00000	1.55189	2.62373

3a+•_cd

N	0.38883	-0.97495	0.72043
O	1.41021	-0.32776	0.21175
C	1.32473	0.37142	-1.12781
C	1.38236	-0.69046	-2.21001
C	2.48189	1.32364	-1.13803
C	3.78453	0.87845	-0.89910
C	4.85737	1.75904	-0.95952
C	4.63502	3.10160	-1.28341
C	3.33798	3.55642	-1.53544
C	2.27367	2.66990	-1.45344
O	5.63064	4.01138	-1.36831
C	-0.93712	-0.35627	0.85887
P	-1.94218	-0.70992	-0.66780
O	-1.49543	-1.99467	-1.25751
O	-3.46325	-0.68184	-0.20603
C	-4.21726	-1.90164	0.04120
C	-4.35157	-2.13633	1.53080
O	-1.79463	0.60897	-1.53919
C	-2.37714	0.66616	-2.87550

C	-1.77305	1.86219	-3.57395
C	-0.96959	1.02675	1.59783
C	-2.44954	1.33158	1.87972
C	-0.35643	2.21345	0.85064
C	-0.22546	0.84673	2.92894
C	0.81046	-2.30418	1.30613
C	1.39297	-3.12265	0.14563
C	1.87258	-2.03711	2.38083
C	-0.39144	-3.03664	1.89569
H	0.38000	0.91146	-1.15242
H	2.33887	-1.21793	-2.18930
H	1.31107	-0.17155	-3.17110
H	0.55696	-1.40202	-2.13284
H	3.96884	-0.16499	-0.65515
H	5.86598	1.40575	-0.76373
H	3.18976	4.60080	-1.78602
H	1.26524	3.03130	-1.64229
H	6.48939	3.60941	-1.19048
H	-1.44460	-1.03388	1.55031
H	-3.71962	-2.73027	-0.46925
H	-5.18892	-1.72850	-0.42320
H	-3.37762	-2.31927	1.99767
H	-4.97360	-3.01735	1.70887
H	-4.82133	-1.27861	2.01773
H	-3.46009	0.76079	-2.76028
H	-2.14437	-0.26992	-3.39199
H	-1.99055	2.78067	-3.02345
H	-2.19317	1.95402	-4.57829
H	-0.68892	1.74961	-3.66532
H	-2.94427	0.50493	2.40118
H	-3.00626	1.53766	0.96191
H	-2.50822	2.21656	2.51903
H	-0.82567	2.36862	-0.12459
H	0.72536	2.11369	0.73284
H	-0.52888	3.11362	1.44836
H	-0.32940	1.75442	3.52966
H	0.84436	0.67883	2.76960
H	-0.63419	0.01351	3.51331
H	0.64871	-3.24918	-0.64489
H	2.28881	-2.64798	-0.25864
H	1.67211	-4.10597	0.53142
H	2.70709	-1.45968	1.97786
H	1.44887	-1.51153	3.23958
H	2.25360	-3.00189	2.72455
H	-1.16414	-3.21070	1.13991
H	-0.81223	-2.52605	2.76767
H	-0.03796	-4.01184	2.23816

3a+•_dn

N	0.42690	-1.05537	-0.90873
O	1.03655	0.03842	-1.30315
C	0.44298	1.40405	-1.07763
C	-0.53391	1.67037	-2.20879
C	1.60499	2.35445	-1.06491
C	2.56538	2.33005	-2.07828
C	3.60349	3.25438	-2.09328
C	3.67576	4.23295	-1.09721
C	2.71231	4.27485	-0.08538
C	1.69207	3.33509	-0.07258
O	4.65139	5.16691	-1.05236
C	-0.05297	-1.22909	0.46587
P	-1.78932	-0.57689	0.61337
O	-2.41024	-0.38553	-0.71831
O	-2.36877	-1.72752	1.54148
C	-3.71808	-1.62761	2.07651
C	-4.00462	-2.90533	2.83016
O	-1.76693	0.73147	1.52986
C	-2.39482	1.97173	1.09815
C	-3.83845	2.02291	1.54567
C	1.00756	-0.98939	1.59688
C	0.37269	-1.50054	2.90080
C	1.45631	0.45852	1.79919
C	2.23642	-1.84438	1.25681
C	0.46656	-2.13069	-1.97048
C	-0.30057	-1.57150	-3.17687
C	1.93475	-2.40051	-2.32454
C	-0.21420	-3.40220	-1.47134
H	-0.04539	1.38776	-0.10030
H	-0.01112	1.65767	-3.16842
H	-0.92873	2.68113	-2.06490
H	-1.36219	0.96056	-2.20738
H	2.51272	1.57971	-2.86316
H	4.35178	3.22147	-2.88027
H	2.78775	5.04217	0.67688
H	0.95305	3.36544	0.72504
H	5.26448	5.06993	-1.79085
H	-0.26268	-2.29859	0.51750
H	-4.40886	-1.48487	1.23973
H	-3.75384	-0.75275	2.73327
H	-3.95052	-3.76727	2.16189
H	-5.00928	-2.86009	3.25729
H	-3.28763	-3.04012	3.64321
H	-2.31874	2.04459	0.00910
H	-1.79654	2.75868	1.56281
H	-4.42343	1.24519	1.04638
H	-4.27007	2.99179	1.28124
H	-3.91316	1.89692	2.62848
H	0.00460	-2.52678	2.80391
H	-0.45812	-0.86558	3.22108
H	1.13216	-1.48313	3.68719
H	0.61261	1.12224	2.00737
H	2.02803	0.83748	0.94958
H	2.12018	0.49032	2.66850
H	1.97059	-2.89765	1.10832
H	2.95259	-1.79681	2.08170
H	2.74387	-1.47486	0.35985
H	0.20562	-0.69948	-3.59449
H	-0.33566	-2.34743	-3.94519
H	-1.32229	-1.30528	-2.89282
H	2.44463	-1.48480	-2.62991
H	2.47042	-2.85194	-1.48633
H	1.95511	-3.10262	-3.16159
H	-0.21052	-4.11425	-2.29962
H	-1.25820	-3.22686	-1.19348
H	0.32365	-3.87180	-0.64267

3a+•_cu

N	0.56183	-0.73687	0.81168
O	1.44673	-0.17326	0.02482
C	1.11395	0.22394	-1.39737
C	1.20350	-1.02794	-2.25020
C	2.12132	1.27440	-1.75822
C	3.49000	1.04719	-1.59616
C	4.41870	2.00533	-1.98431
C	3.98104	3.20067	-2.56359
C	2.61470	3.43395	-2.74199
C	1.69771	2.47658	-2.33282
O	4.82674	4.17266	-2.97155
C	-0.76631	-0.15196	1.03666
P	-1.96164	-0.79843	-0.23456
O	-1.47383	-2.09954	-0.75146
O	-3.37000	-0.85827	0.50356
C	-3.88735	-2.08506	1.08705
C	-3.87636	-1.97513	2.59719
O	-2.14921	0.40559	-1.25171
C	-2.99185	0.22241	-2.43131
C	-2.14763	-0.23852	-3.59902
C	-0.78111	1.34204	1.51126
C	-2.22643	1.64269	1.93952
C	-0.33972	2.37839	0.47629
C	0.14398	1.44210	2.73234
C	1.15427	-1.90356	1.56991
C	1.59991	-2.92447	0.51409
C	2.35131	-1.39142	2.38161
C	0.10831	-2.53699	2.48292
H	0.10655	0.64182	-1.39290
H	2.21609	-1.43788	-2.22658
H	0.99092	-0.72976	-3.28129
H	0.47542	-1.78170	-1.94371
H	3.84099	0.11724	-1.15556
H	5.48092	1.82390	-1.84581
H	2.29835	4.36722	-3.19416
H	0.63512	2.66785	-2.46457
H	5.74646	3.92276	-2.82242
H	-1.12796	-0.70747	1.90520
H	-3.29523	-2.92846	0.72057
H	-4.90482	-2.17787	0.70403
H	-2.85618	-1.89540	2.98783
H	-4.33087	-2.86772	3.03481
H	-4.44556	-1.10188	2.92403
H	-3.44062	1.20111	-2.60340
H	-3.78814	-0.48842	-2.19065
H	-1.35334	0.48528	-3.80508
H	-2.77019	-0.32352	-4.49344
H	-1.70222	-1.21473	-3.39042
H	-2.59446	0.91631	2.67252
H	-2.91191	1.64593	1.08795
H	-2.25535	2.63305	2.40185
H	-0.95014	2.33646	-0.42884
H	0.71670	2.27800	0.21654
H	-0.46631	3.37227	0.91630
H	0.06517	2.44191	3.16793
H	1.19106	1.28747	2.45323
H	-0.12875	0.71891	3.51044
H	0.75390	-3.22473	-0.10972
H	2.39663	-2.51931	-0.11196
H	1.98787	-3.80313	1.03476
H	3.07134	-0.87656	1.74239
H	2.03336	-0.72117	3.18327
H	2.84602	-2.25468	2.83350
H	-0.75875	-2.89268	1.91636
H	-0.20894	-1.87020	3.29064
H	0.57393	-3.40681	2.95177

3a+•_bf

N	0.86745	-0.86762	-0.33795
O	1.14855	0.23350	-0.99498
C	0.11910	1.33111	-1.18553
C	-0.84919	0.85929	-2.25249
C	0.91538	2.54140	-1.56605
C	1.81793	2.50641	-2.63215
C	2.51910	3.64615	-3.00587
C	2.30399	4.84699	-2.32154
C	1.39434	4.89729	-1.26188
C	0.71445	3.74736	-0.88705
O	2.94433	5.99534	-2.63481
C	0.31333	-0.83871	1.01815
P	-1.54368	-0.68276	1.01249
O	-2.09639	0.68912	0.97109
O	-1.82396	-1.65431	-0.22833
C	-3.16044	-2.18001	-0.47250
C	-4.06513	-1.13612	-1.09524
O	-1.98201	-1.54945	2.27344
C	-2.85805	-1.00651	3.30281
C	-4.29638	-1.36667	3.00487
C	1.11473	0.03331	2.04951
C	0.55994	-0.31018	3.44238
C	1.02295	1.54897	1.85302
C	2.58661	-0.39242	1.97165
C	1.42291	-2.08691	-1.04120
C	0.70403	-2.17035	-2.39480
C	2.93109	-1.88595	-1.24489
C	1.15270	-3.34962	-0.22855
H	-0.39239	1.47690	-0.23539
H	-0.35139	0.75507	-3.21952
H	-1.62447	1.62528	-2.34489
H	-1.32678	-0.08166	-1.97235
H	1.98593	1.57965	-3.17565
H	3.22563	3.60784	-3.83039
H	1.24088	5.84008	-0.74894
H	0.01011	3.79036	-0.05978
H	3.53871	5.87198	-3.38449
H	0.42754	-1.86868	1.36073
H	-3.55362	-2.55729	0.47656
H	-2.99859	-3.02825	-1.13975
H	-4.16830	-0.26184	-0.44701
H	-5.05540	-1.56905	-1.25991
H	-3.67309	-0.80712	-2.06076
H	-2.72270	0.07744	3.34451
H	-2.50503	-1.45705	4.23186
H	-4.63035	-0.88776	2.07911
H	-4.93829	-1.01289	3.81582
H	-4.41715	-2.44953	2.91900
H	0.50558	-1.38981	3.61667
H	-0.43405	0.11930	3.59681
H	1.22125	0.12347	4.19723
H	-0.01457	1.89645	1.84162
H	1.53622	1.87988	0.94699
H	1.52625	2.03076	2.69694
H	2.70772	-1.47246	2.11739
H	3.15179	0.11336	2.75923
H	3.03324	-0.10756	1.01429
H	0.92000	-1.29469	-3.00962
H	1.06777	-3.05637	-2.92027
H	-0.37586	-2.26217	-2.25468
H	3.14140	-0.94965	-1.76526
H	3.46803	-1.90181	-0.29442
H	3.29906	-2.71271	-1.85742
H	1.51311	-4.19583	-0.81793
H	0.08439	-3.49867	-0.04837
H	1.69963	-3.36352	0.71852

3a+•_ap

N	-0.20088	1.10122	-0.90676
O	1.03997	1.00052	-0.48792
C	1.36825	0.39557	0.85930
C	1.11218	1.46824	1.90119
C	2.80439	-0.02420	0.77024
C	3.79026	0.85999	0.32597
C	5.12576	0.47643	0.29778
C	5.48942	-0.79955	0.73991
C	4.51275	-1.68746	1.19951
C	3.18094	-1.29903	1.20475
O	6.76817	-1.23739	0.74815
C	-1.09499	-0.05741	-0.95735
P	-1.95258	-0.37652	0.66737
O	-1.29143	-1.28523	1.63049
O	-2.12072	1.14566	1.13384
C	-2.46909	1.45363	2.51385
C	-3.82269	0.89723	2.90257
O	-3.39048	-0.83291	0.15931
C	-4.06416	-2.00958	0.69061
C	-5.05186	-2.48933	-0.34776
C	-0.52318	-1.30798	-1.71898
C	-1.70114	-2.27370	-1.92663
C	0.60107	-2.06078	-1.00321
C	-0.01569	-0.83005	-3.08530
C	-0.46345	2.44560	-1.54903
C	-1.89297	2.51908	-2.07798
C	-0.25918	3.49961	-0.45257
C	0.54868	2.64883	-2.68511
H	0.71632	-0.46564	1.00840
H	1.80385	2.30519	1.77821
H	1.29120	1.01930	2.88240
H	0.08342	1.82951	1.86040
H	3.51858	1.85751	-0.01114
H	5.88527	1.16680	-0.05861
H	4.81839	-2.67028	1.54031
H	2.42342	-1.99498	1.55742
H	7.37351	-0.55827	0.42738
H	-1.93078	0.29282	-1.56517
H	-2.45498	2.54437	2.55175
H	-1.67766	1.05890	3.15793
H	-4.58665	1.18314	2.17542
H	-4.10715	1.29068	3.88159
H	-3.78658	-0.19268	2.98439
H	-4.57188	-1.71051	1.61113
H	-3.31129	-2.76311	0.93810
H	-5.76166	-1.69786	-0.59800
H	-5.60974	-3.34051	0.05047
H	-4.54249	-2.80821	-1.25978
H	-1.38363	-3.06940	-2.60595
H	-2.57187	-1.77598	-2.36561
H	-2.00413	-2.74796	-0.98787
H	0.30774	-2.37001	0.00440
H	1.52452	-1.47932	-0.95980
H	0.82287	-2.96527	-1.57798
H	-0.79005	-0.28873	-3.64189
H	0.27907	-1.69577	-3.68465
H	0.86518	-0.18942	-2.98117
H	-2.06692	1.83551	-2.91386
H	-2.63051	2.34468	-1.28913
H	-2.04491	3.53228	-2.45702
H	-0.95222	3.33361	0.37590
H	0.76721	3.49035	-0.08165
H	-0.45886	4.48306	-0.88417
H	0.42876	3.66759	-3.06175
H	0.36748	1.95755	-3.51032
H	1.57433	2.53007	-2.33035

3a+•_ao

N	0.30593	-1.01069	0.45365
O	1.08486	-0.98384	-0.60239
C	0.72346	-0.18629	-1.84087
C	-0.31518	-0.98530	-2.60468
C	2.01612	-0.00687	-2.57717
C	2.83442	-1.09829	-2.87848
C	4.00752	-0.92628	-3.60329
C	4.36182	0.34907	-4.05503
C	3.54377	1.44604	-3.77138
C	2.38489	1.26359	-3.03062
O	5.48309	0.58928	-4.77073
C	-0.15994	0.21635	1.10423
P	-1.69293	0.89335	0.29831
O	-1.51494	1.85553	-0.81097
O	-2.38055	-0.50802	-0.05642
C	-3.72901	-0.51197	-0.61040
C	-4.72854	-0.85966	0.47183
O	-2.51588	1.44509	1.54539
C	-3.16240	2.75093	1.50657
C	-3.39272	3.19162	2.93301
C	0.96206	1.24561	1.48753
C	0.29988	2.29625	2.39485
C	1.62820	1.96802	0.31385
C	2.03300	0.48904	2.28352
C	0.18664	-2.40889	1.01906
C	-0.68967	-2.41159	2.26843
C	-0.46192	-3.26708	-0.07560
C	1.59663	-2.92276	1.34180
H	0.31932	0.77182	-1.51533
H	0.09935	-1.93287	-2.95698
H	-0.59897	-0.39080	-3.47762
H	-1.20713	-1.16587	-2.00203
H	2.56312	-2.09512	-2.53903
H	4.64322	-1.77907	-3.82491
H	3.83644	2.42449	-4.13534
H	1.75359	2.12059	-2.80841
H	5.97736	-0.22347	-4.93089
H	-0.56474	-0.13663	2.05432
H	-3.71117	-1.26156	-1.40483
H	-3.92893	0.46203	-1.06943
H	-4.50159	-1.83825	0.90235
H	-5.73456	-0.89732	0.04620
H	-4.71369	-0.11394	1.27050
H	-4.10381	2.63613	0.96092
H	-2.52344	3.44172	0.95002
H	-4.00844	2.46523	3.46815
H	-3.90998	4.15419	2.93746

H	-2.44401	3.30722	3.46264
H	1.08151	2.92862	2.82429
H	-0.26138	1.84024	3.21699
H	-0.37453	2.94856	1.83072
H	0.89635	2.48278	-0.31571
H	2.23479	1.29388	-0.29530
H	2.30636	2.72367	0.72213
H	1.60465	-0.04206	3.14197
H	2.76957	1.20018	2.66732
H	2.56753	-0.22582	1.65049
H	-0.23239	-1.87283	3.10325
H	-1.68919	-2.01516	2.06649
H	-0.80040	-3.45204	2.58239
H	-1.44704	-2.87508	-0.34066
H	0.16715	-3.31161	-0.96631
H	-0.57973	-4.28165	0.31194
H	1.51243	-3.97215	1.63478
H	2.04194	-2.37216	2.17280
H	2.25183	-2.85832	0.47084

3a+•_an

N	0.42367	-1.01619	-0.22829
O	1.24468	-0.15907	-0.78885
C	0.80161	1.23993	-1.16985
C	-0.00960	1.12600	-2.44658
C	2.07292	2.01838	-1.32077
C	3.10623	1.56236	-2.14303
C	4.26256	2.31413	-2.31195
C	4.38477	3.55042	-1.66936
C	3.35203	4.02288	-0.85497
C	2.21060	3.25379	-0.67999
O	5.47641	4.33767	-1.79355
C	-0.33367	-0.68511	0.98151
P	-1.91987	0.20659	0.59271
O	-1.86824	1.68224	0.50303
O	-2.29260	-0.59001	-0.74672
C	-3.55291	-0.27080	-1.40307
C	-3.62545	-1.07514	-2.68055
O	-2.91674	-0.37482	1.68896
C	-3.78998	0.50364	2.45841
C	-4.21174	-0.24305	3.70183
C	0.52084	-0.13562	2.17975
C	-0.40039	-0.13369	3.41128
C	1.09027	1.27348	1.99635
C	1.67698	-1.11608	2.41380
C	0.58038	-2.39930	-0.82187
C	0.21584	-2.27593	-2.30734
C	2.04323	-2.83580	-0.66137
C	-0.35883	-3.38776	-0.13692
H	0.19372	1.63192	-0.35531
H	0.60577	0.76200	-3.27287
H	-0.35780	2.13223	-2.69616
H	-0.87953	0.47963	-2.31368
H	3.01736	0.60614	-2.65321
H	5.06525	1.94776	-2.94592
H	3.46732	4.98575	-0.37011
H	1.41131	3.62321	-0.04199
H	6.13030	3.94009	-2.38072
H	-0.71522	-1.65134	1.31631
H	-3.57465	0.80624	-1.59618
H	-4.36501	-0.53331	-0.71747
H	-2.82202	-0.79248	-3.36624
H	-4.57888	-0.88586	-3.17930
H	-3.55458	-2.14495	-2.46780
H	-4.64545	0.75450	1.82516
H	-3.24778	1.42562	2.68495
H	-4.72165	-1.17280	3.44049
H	-4.89855	0.37746	4.28271
H	-3.34721	-0.47885	4.32704
H	0.20509	0.06860	4.29883
H	-0.90535	-1.09469	3.55371
H	-1.15823	0.65356	3.34775
H	0.30687	2.00402	1.77371
H	1.86274	1.30887	1.22458
H	1.56621	1.57108	2.93577
H	1.31914	-2.14305	2.55414
H	2.21929	-0.82733	3.31825
H	2.39013	-1.09548	1.58420
H	0.90343	-1.60704	-2.82803
H	0.29193	-3.26690	-2.76082
H	-0.80855	-1.91385	-2.42339
H	2.72699	-2.09531	-1.08129
H	2.29607	-3.01147	0.38593
H	2.17371	-3.77468	-1.20515
H	-0.25854	-4.34246	-0.65830
H	-1.40429	-3.07447	-0.21099
H	-0.09187	-3.56538	0.90876

3a+•_df

N	0.67516	-0.95814	0.10220
O	1.46991	0.07348	-0.06209
C	0.96125	1.39490	-0.60483
C	0.77352	1.22906	-2.10068
C	2.01081	2.39381	-0.22430
C	3.35365	2.19241	-0.55351
C	4.31279	3.14572	-0.23453
C	3.92761	4.32922	0.40386
C	2.58550	4.54728	0.72658
C	1.64051	3.57907	0.41899
O	4.80441	5.30238	0.73721
C	-0.56784	-0.86268	0.87241
P	-1.98875	-0.25017	-0.16361
O	-2.17862	1.21390	-0.26272
O	-1.61529	-1.03274	-1.50991
C	-2.51774	-0.92777	-2.64759
C	-1.85898	-1.60843	-3.82531
O	-3.22707	-1.05499	0.42747
C	-4.45360	-0.37660	0.82511
C	-5.41371	-0.30246	-0.34100
C	-0.41588	-0.26392	2.31688
C	-1.74380	-0.52771	3.04682
C	-0.11555	1.23591	2.38355
C	0.70979	-1.03109	3.02193
C	1.33451	-2.24053	-0.35735
C	2.65080	-2.41593	0.41268
C	0.40971	-3.43257	-0.12890
C	1.60871	-2.07099	-1.85759
H	0.01289	1.61378	-0.11638
H	1.72686	1.03929	-2.59963
H	0.36950	2.17193	-2.47971
H	0.06481	0.43070	-2.33073
H	3.66204	1.27899	-1.05658
H	5.35630	2.97697	-0.48580
H	2.30984	5.47375	1.21768
H	0.59791	3.75134	0.67514
H	5.70106	5.07496	0.46356
H	-0.85656	-1.90500	1.01975
H	-2.70288	0.13375	-2.84179
H	-3.45829	-1.41570	-2.37407
H	-0.93191	-1.09974	-4.10336
H	-2.53134	-1.58225	-4.68606
H	-1.63835	-2.65360	-3.59327
H	-4.20074	0.62177	1.19166
H	-4.84580	-0.98015	1.64502
H	-5.00737	0.33284	-1.13363
H	-6.35880	0.13602	-0.01029
H	-5.61791	-1.29933	-0.73972
H	-2.07113	-1.56862	2.95688
H	-2.54254	0.12244	2.67874
H	-1.60742	-0.30425	4.10825
H	0.88445	1.47376	2.01289
H	-0.14585	1.54111	3.43404
H	-0.86268	1.82574	1.84387
H	0.76057	-0.71820	4.06834
H	1.68223	-0.81644	2.56880
H	0.53739	-2.11389	3.00675
H	3.28597	-1.53264	0.32004
H	2.47227	-2.62617	1.46885
H	3.17965	-3.26909	-0.01936
H	0.24381	-3.63757	0.93260
H	-0.54786	-3.30969	-0.64324
H	0.90519	-4.31058	-0.54955
H	2.30629	-1.25178	-2.04104
H	2.05873	-2.99459	-2.22892
H	0.67821	-1.89029	-2.40091

3a+•_fd

N	0.73678	-0.11328	1.14919
O	0.44721	1.13708	1.43156
C	1.26091	2.32509	1.02258
C	0.76924	3.39143	1.98308
C	0.99823	2.62483	-0.42521
C	-0.31295	2.71049	-0.89982
C	-0.56677	3.05772	-2.22037
C	0.49865	3.35375	-3.07611
C	1.81543	3.28070	-2.61065
C	2.05660	2.90837	-1.29451
O	0.32497	3.69617	-4.37344
C	-0.48203	-0.91145	1.02197
P	-1.13908	-0.75276	-0.71556
O	-2.19969	0.24277	-0.98160
O	0.25711	-0.53456	-1.45866
C	0.29645	-0.24245	-2.88342
C	0.59211	-1.50673	-3.66223
O	-1.55943	-2.26599	-1.00659
C	-2.81532	-2.58571	-1.66783
C	-3.19456	-3.99601	-1.28001
C	-1.54479	-0.71980	2.15833
C	-2.60899	-1.80699	1.92417
C	-2.25046	0.64516	2.19596
C	-0.84281	-0.97379	3.49822
C	2.15150	-0.64734	1.23136
C	3.01827	-0.09384	0.08115
C	2.70550	-0.26653	2.61206

C	2.10762	-2.17318	1.10400
H	2.31208	2.10720	1.20117
H	-0.29871	3.57245	1.83874
H	1.30445	4.31946	1.77068
H	0.95330	3.10275	3.02134
H	-1.15130	2.47589	-0.24967
H	-1.59127	3.09341	-2.58135
H	2.62590	3.52071	-3.29001
H	3.08352	2.86042	-0.94008
H	-0.61089	3.80188	-4.58386
H	-0.16845	-1.95283	1.06754
H	1.08469	0.50649	-2.99600
H	-0.65310	0.21882	-3.17279
H	1.54289	-1.94139	-3.34358
H	0.65876	-1.27581	-4.72852
H	-0.19447	-2.25203	-3.51743
H	-2.65534	-2.49233	-2.74641
H	-3.56693	-1.85167	-1.36521
H	-2.41118	-4.70093	-1.56703
H	-4.11916	-4.27898	-1.78920
H	-3.35795	-4.07006	-0.20204
H	-2.16557	-2.80240	1.81447
H	-3.21295	-1.59184	1.03621
H	-3.28647	-1.82879	2.78186
H	-1.59680	1.43588	2.56686
H	-3.09699	0.56780	2.88530
H	-2.63859	0.92604	1.21420
H	-1.57866	-0.94625	4.30676
H	-0.09723	-0.19999	3.70941
H	-0.35586	-1.95604	3.52470
H	2.43482	0.01212	-0.83419
H	3.48689	0.85894	0.32574
H	3.82486	-0.80738	-0.10196
H	2.66772	0.80846	2.80094
H	2.16137	-0.78006	3.40815
H	3.75209	-0.57943	2.65206
H	1.72196	-2.48925	0.13000
H	1.53657	-2.64481	1.90764
H	3.13620	-2.52981	1.18782

3a+•_fl

N	0.61476	-0.16055	1.23249
O	0.29474	1.11504	1.23701
C	1.15805	2.24676	0.79487
C	0.56094	3.41614	1.55749
C	1.07832	2.39281	-0.69995
C	-0.14845	2.31475	-1.36257
C	-0.22758	2.56175	-2.72903
C	0.92208	2.91722	-3.44080
C	2.15312	3.00876	-2.78338
C	2.22433	2.73934	-1.42340
O	0.91601	3.17216	-4.76926
C	-0.60169	-0.97570	1.24703
P	-1.31870	-1.01997	-0.47053
O	-2.31778	0.01058	-0.82942
O	0.05602	-1.00962	-1.28786
C	-0.00275	-1.02133	-2.74098
C	1.37833	-0.70643	-3.26483
O	-1.84471	-2.52291	-0.56382
C	-3.18660	-2.82477	-1.03750
C	-3.20246	-2.94953	-2.54510
C	-1.61737	-0.64062	2.39441
C	-2.70646	-1.72561	2.33179
C	-2.29785	0.73442	2.30213
C	-0.86660	-0.74845	3.72715
C	2.03408	-0.65865	1.40193
C	2.89376	-0.24705	0.19056
C	2.57942	-0.10694	2.72828
C	2.00774	-2.18906	1.46557
H	2.17932	2.06120	1.12196
H	-0.48483	3.55817	1.27321
H	1.11419	4.31954	1.29161
H	0.62928	3.26014	2.63762
H	-1.05325	2.04149	-0.82580
H	-1.18746	2.49093	-3.23478
H	3.03191	3.28995	-3.35300
H	3.18538	2.82019	-0.92015
H	0.01832	3.16116	-5.12283
H	-0.27740	-2.00210	1.40902
H	-0.73237	-0.26950	-3.05804
H	-0.34098	-2.01448	-3.05351
H	1.70422	0.27717	-2.91413
H	1.36162	-0.69028	-4.35768
H	2.09877	-1.46388	-2.94413
H	-3.86480	-2.03613	-0.70120
H	-3.44455	-3.76333	-0.54494
H	-2.97467	-1.98667	-3.01214
H	-4.19705	-3.25788	-2.87787
H	-2.47972	-3.69787	-2.88003
H	-2.28722	-2.73652	2.29110
H	-3.36179	-1.58303	1.46722
H	-3.32980	-1.65154	3.22674
H	-1.62075	1.54605	2.57302
H	-3.12794	0.74785	3.01532
H	-2.70158	0.92229	1.30464
H	-1.56997	-0.61336	4.55357
H	-0.10536	0.03360	3.81772
H	-0.38977	-1.72794	3.85256
H	2.30820	-0.27723	-0.72903
H	3.34251	0.73935	0.29953
H	3.71345	-0.96395	0.10371
H	2.47326	0.97626	2.81729
H	2.08317	-0.57472	3.58111
H	3.64499	-0.34645	2.77708
H	1.63292	-2.62646	0.53544
H	1.43714	-2.56529	2.31805
H	3.03996	-2.51912	1.59947

3a(II) TS_dn

N	0.44026	-1.03274	-0.68407
O	1.07375	0.05396	-0.91120
C	0.36267	1.94662	-1.09080
C	-0.68770	1.76079	-2.11889
C	1.60865	2.59543	-1.33108
C	2.17951	2.68543	-2.62027
C	3.38200	3.33085	-2.81623
C	4.04422	3.91175	-1.71882
C	3.49735	3.83472	-0.42644
C	2.30333	3.17459	-0.24188
O	5.20797	4.55702	-1.83926
C	-0.20555	-1.22466	0.62230
P	-1.91428	-0.52285	0.52155
O	-2.46874	-0.69715	-0.84480
O	-2.78194	-1.21841	1.66596
C	-3.73161	-2.27548	1.36253
C	-3.08498	-3.63394	1.53487
O	-1.75904	0.97618	1.04926
C	-2.95573	1.76712	1.30783
C	-3.18142	1.86656	2.80047
C	0.71162	-0.94601	1.85433
C	-0.07433	-1.34289	3.11333
C	1.19184	0.50189	2.01001
C	1.94107	-1.85543	1.71426
C	0.53221	-2.07598	-1.77179
C	0.04729	-1.41765	-3.06624
C	2.00440	-2.48632	-1.88741
C	-0.34594	-3.28382	-1.45416
H	0.00989	1.96089	-0.06164
H	-0.29485	1.61070	-3.12392
H	-1.26579	2.69726	-2.12071
H	-1.37989	0.95672	-1.85817
H	1.68087	2.23377	-3.47112
H	3.81968	3.39350	-3.80823
H	4.03263	4.29878	0.39388
H	1.87276	3.11218	0.75364
H	5.52008	4.57612	-2.75355
H	-0.43615	-2.29287	0.67674
H	-4.10885	-2.12530	0.34795
H	-4.54449	-2.12823	2.07508
H	-2.28641	-3.79000	0.80215
H	-3.83027	-4.41896	1.38246
H	-2.67193	-3.74147	2.54082
H	-3.80728	1.31452	0.78981
H	-2.76088	2.74259	0.85660
H	-3.36452	0.87715	3.22561
H	-4.04807	2.50137	3.00281
H	-2.30943	2.30701	3.29057
H	-0.47197	-2.36107	3.04064
H	-0.91186	-0.66482	3.30096
H	0.59466	-1.30231	3.97745
H	0.35345	1.20014	2.07502
H	1.85221	0.78937	1.18984
H	1.76167	0.57549	2.94196
H	1.65376	-2.90845	1.60828
H	2.56671	-1.76942	2.60730
H	2.55008	-1.56756	0.85177
H	0.67916	-0.56408	-3.32177
H	0.11274	-2.14719	-3.87719
H	-0.99279	-1.09647	-2.96267
H	2.63615	-1.60875	-2.04448
H	2.34060	-3.01523	-0.99159
H	2.11866	-3.15778	-2.74245
H	-0.29108	-3.96542	-2.30654
H	-1.39260	-2.99063	-1.32655
H	0.00571	-3.84003	-0.57918

3a(II) TS_bh

N	0.68287	-0.57357	1.14570
O	1.40101	0.01603	0.26801
C	1.07155	0.26028	-1.72902
C	0.98779	-1.15725	-2.15127
C	2.18080	1.10901	-2.01031
C	3.47756	0.60212	-2.25146
C	4.52477	1.45086	-2.54045

C	4.29583	2.83804	-2.60380
C	3.01514	3.36675	-2.36790
C	1.98145	2.50989	-2.06372
O	5.26317	3.71522	-2.88574
C	-0.63526	-0.02026	1.48043
P	-1.87138	-0.71027	0.28975
O	-1.45049	-2.04943	-0.19766
O	-3.26100	-0.71167	1.07441
C	-3.89953	-1.96156	1.45568
C	-4.76974	-2.47708	0.33041
O	-2.06363	0.43318	-0.81039
C	-3.08576	0.27144	-1.83394
C	-2.53383	-0.48318	-3.02573
C	-0.63974	1.49616	1.84938
C	-2.06211	1.85345	2.30750
C	-0.22548	2.44671	0.72036
C	0.33391	1.67940	3.02238
C	1.33296	-1.74638	1.83985
C	1.79744	-2.71523	0.74947
C	2.52874	-1.20586	2.63157
C	0.34541	-2.45616	2.76347
H	0.11804	0.76262	-1.57109
H	1.94372	-1.67885	-2.11354
H	0.66100	-1.13394	-3.20197
H	0.22746	-1.70114	-1.58640
H	3.66504	-0.46484	-2.19642
H	5.52123	1.05745	-2.71889
H	2.87504	4.43968	-2.43098
H	0.98844	2.91055	-1.88081
H	6.11277	3.28211	-3.04170
H	-0.94264	-0.53580	2.39472
H	-4.48384	-1.71029	2.34180
H	-3.12885	-2.68984	1.72392
H	-5.51737	-1.73034	0.04999
H	-5.29385	-3.38063	0.65311
H	-4.15744	-2.73046	-0.53992
H	-3.38225	1.28856	-2.09393
H	-3.94809	-0.23586	-1.39022
H	-1.68517	0.05392	-3.45991
H	-3.30535	-0.57100	-3.79523
H	-2.21349	-1.48713	-2.73454
H	-2.41464	1.18538	3.10035
H	-2.77896	1.80890	1.48283
H	-2.06279	2.87396	2.70053
H	-0.86294	2.32817	-0.15958
H	0.82003	2.29974	0.44292
H	-0.33729	3.47535	1.07834
H	0.28815	2.71176	3.38086
H	1.36509	1.47887	2.71560
H	0.08128	1.02298	3.86368
H	0.94399	-3.06559	0.16254
H	2.52852	-2.23530	0.09564
H	2.27589	-3.57490	1.22507
H	3.19310	-0.63403	1.97909
H	2.20296	-0.56988	3.45879
H	3.08760	-2.04773	3.04869
H	-0.53554	-2.80175	2.21364
H	0.04463	-1.83769	3.61439
H	0.84852	-3.33613	3.17151

3a(II) TS_ap

N	-0.16267	1.00589	-0.99149
O	1.01039	0.73681	-0.55052
C	1.57484	0.09554	1.25648
C	1.04743	1.20333	2.08929
C	2.96493	-0.09724	0.98906
C	3.89236	0.96681	0.98818
C	5.23052	0.73684	0.74434
C	5.67567	-0.57602	0.50523
C	4.77187	-1.65113	0.50199
C	3.43521	-1.40571	0.72831
O	6.95923	-0.87006	0.27123
C	-1.15327	-0.07214	-1.10680
P	-1.93326	-0.36942	0.53994
O	-1.18311	-1.20783	1.50765
O	-2.16229	1.15833	0.97494
C	-2.95105	1.43590	2.16452
C	-4.34722	1.86908	1.77028
O	-3.39539	-0.90174	0.18975
C	-3.96042	-2.06413	0.85592
C	-5.08926	-2.58105	-0.00552
C	-0.64780	-1.33334	-1.87837
C	-1.84751	-2.27559	-2.07021
C	0.47297	-2.10987	-1.17667
C	-0.14758	-0.86418	-3.25066
C	-0.34135	2.41235	-1.51432
C	-1.76969	2.64376	-2.00129
C	-0.02206	3.36397	-0.35752
C	0.65692	2.61380	-2.66037
H	0.94818	-0.79372	1.24123
H	1.61849	2.12785	2.00819
H	1.11462	0.84554	3.12672
H	-0.00739	1.38585	1.88111
H	3.55656	1.98361	1.16283
H	5.93987	1.55926	0.73729
H	5.15139	-2.65023	0.32145
H	2.72988	-2.23196	0.73191
H	7.52143	-0.08486	0.29804
H	-1.97803	0.33745	-1.69402
H	-2.41448	2.22936	2.69049
H	-2.95678	0.54899	2.80796
H	-4.30564	2.75587	1.13298
H	-4.92464	2.11580	2.66507
H	-4.86138	1.07183	1.22820
H	-4.31703	-1.74456	1.83998
H	-3.17018	-2.80584	1.00179
H	-5.84938	-1.80984	-0.14959
H	-5.55582	-3.44163	0.48019
H	-4.71804	-2.89416	-0.98439
H	-1.56681	-3.06905	-2.76833
H	-2.72135	-1.75562	-2.47652
H	-2.13786	-2.75599	-1.13033
H	0.18378	-2.40475	-0.16302
H	1.39604	-1.52796	-1.14252
H	0.67268	-3.02155	-1.74911
H	-0.91813	-0.30272	-3.79252
H	0.12185	-1.73217	-3.85916
H	0.74429	-0.23832	-3.15243
H	-2.01027	2.04242	-2.88304
H	-2.50351	2.45826	-1.21190
H	-1.85158	3.69236	-2.29778
H	-0.70970	3.20161	0.47685
H	1.00663	3.22388	-0.01873
H	-0.13104	4.39355	-0.70697
H	0.62957	3.66172	-2.97022
H	0.39859	1.99736	-3.52484
H	1.67123	2.37103	-2.33559

3a(II) TS_an

N	0.49828	-1.04764	-0.11408
O	1.22759	-0.09097	-0.55649
C	0.68528	1.67843	-1.31379
C	-0.16612	1.21832	-2.43760
C	1.98679	2.24050	-1.48791
C	2.80502	1.93319	-2.59636
C	4.05015	2.51019	-2.73619
C	4.50350	3.42361	-1.76707
C	3.70686	3.74616	-0.65615
C	2.47287	3.14924	-0.51867
O	5.69543	4.02494	-1.84595
C	-0.31613	-0.83329	1.08930
P	-1.87842	0.03774	0.63028
O	-1.80635	1.50831	0.44431
O	-2.25223	-0.80930	-0.68236
C	-3.54640	-0.57853	-1.29896
C	-3.57326	-1.32875	-2.61138
O	-2.93584	-0.45227	1.71764
C	-3.80438	0.48815	2.40832
C	-4.31088	-0.19091	3.65950
C	0.47321	-0.25173	2.30645
C	-0.46715	-0.26435	3.52271
C	0.99558	1.17670	2.10984
C	1.66039	-1.18530	2.57534
C	0.70596	-2.37780	-0.80083
C	0.40389	-2.16367	-2.28675
C	2.17274	-2.78037	-0.60844
C	-0.22301	-3.44591	-0.22930
H	0.13329	1.99240	-0.43026
H	0.39325	0.79511	-3.27156
H	-0.69087	2.11667	-2.79321
H	-0.92751	0.51671	-2.09428
H	2.46752	1.22328	-3.34420
H	4.67962	2.26584	-3.58687
H	4.08526	4.45965	0.06674
H	1.84828	3.39583	0.33532
H	6.18262	3.76112	-2.63740
H	-0.67006	-1.82049	1.39428
H	-3.67485	0.49934	-1.44624
H	-4.31615	-0.94279	-0.61123
H	-2.81390	-0.94235	-3.29687
H	-4.55124	-1.21149	-3.08414
H	-3.39389	-2.39458	-2.44847
H	-4.62115	0.74879	1.72894
H	-3.23702	1.39738	2.62611
H	-4.85063	-1.10705	3.41009
H	-4.99162	0.48000	4.18933
H	-3.48281	-0.44242	4.32666
H	0.11447	-0.04611	4.42263
H	-0.95566	-1.23497	3.65801
H	-1.24254	0.50411	3.44177
H	0.18842	1.86762	1.84686
H	1.77395	1.21115	1.34512
H	1.43669	1.51623	3.05266
H	1.33510	-2.22234	2.72135

H	2.17806	-0.86728	3.48481
H	2.38233	-1.15227	1.75416
H	1.08196	-1.42124	-2.71314
H	0.55091	-3.10786	-2.81685
H	-0.63121	-1.84054	-2.42570
H	2.83883	-1.97966	-0.93790
H	2.38608	-3.01958	0.43611
H	2.37354	-3.67180	-1.20845
H	-0.07627	-4.35780	-0.81333
H	-1.27444	-3.15726	-0.31334
H	0.01471	-3.69078	0.81013

3a(II) TS_df

N	0.68763	-0.98471	0.23969
O	1.33451	0.11736	0.14373
C	0.83226	1.81013	-0.80014
C	0.62300	1.28168	-2.16989
C	1.95830	2.60230	-0.42133
C	3.20118	2.52337	-1.08602
C	4.26039	3.31772	-0.69911
C	4.09489	4.22379	0.36433
C	2.86769	4.32058	1.04089
C	1.82300	3.50918	0.65619
O	5.07686	5.02843	0.78440
C	-0.58126	-1.01019	0.97946
P	-1.94455	-0.40233	-0.11044
O	-2.07377	1.06703	-0.27825
O	-1.56984	-1.22522	-1.43674
C	-2.48322	-1.17903	-2.56403
C	-1.79707	-1.83177	-3.74262
O	-3.25274	-1.13024	0.43424
C	-4.45262	-0.38608	0.77949
C	-5.38610	-0.31521	-0.40885
C	-0.50118	-0.39103	2.41225
C	-1.83492	-0.67629	3.12204
C	-0.24511	1.12081	2.44364
C	0.63095	-1.10505	3.16195
C	1.41948	-2.20117	-0.27899
C	2.71806	-2.34468	0.52325
C	0.56488	-3.45905	-0.14600
C	1.73368	-1.93628	-1.75407
H	-0.08296	1.96030	-0.23152
H	1.54519	1.02934	-2.69265
H	0.12137	2.08959	-2.72165
H	-0.05671	0.42850	-2.16369
H	3.34079	1.82139	-1.90140
H	5.21705	3.24942	-1.20877
H	2.77429	5.03457	1.85102
H	0.86893	3.58007	1.17101
H	5.88571	4.91278	0.26888
H	-0.83147	-2.06501	1.11239
H	-2.72999	-0.13147	-2.76957
H	-3.39500	-1.71318	-2.27973
H	-0.90357	-1.27247	-4.03358
H	-2.47702	-1.85690	-4.59749
H	-1.50939	-2.85800	-3.50012
H	-4.16496	0.61441	1.11421
H	-4.89052	-0.93832	1.61274
H	-4.93522	0.26806	-1.21703
H	-6.31745	0.17674	-0.11631
H	-5.62588	-1.31722	-0.77343
H	-2.13342	-1.72646	3.03833
H	-2.64427	-0.05470	2.72841
H	-1.72934	-0.43609	4.18355
H	0.75632	1.35905	2.07978
H	-0.31477	1.46208	3.48163
H	-0.99000	1.66839	1.85757
H	0.64896	-0.76972	4.20284
H	1.60493	-0.87255	2.72173
H	0.49184	-2.19285	3.16401
H	3.29055	-1.41457	0.49996
H	2.51627	-2.61757	1.56173
H	3.32134	-3.13843	0.07496
H	0.38830	-3.73294	0.89838
H	-0.38877	-3.35944	-0.67170
H	1.11745	-4.28367	-0.60304
H	2.36718	-1.05278	-1.85880
H	2.27246	-2.79564	-2.16067
H	0.81151	-1.79873	-2.32469

a+

C	-0.83396	3.29972	0.11256
C	0.24084	2.29376	0.18824
C	0.14228	0.92436	0.09694
C	-1.10781	0.23996	-0.09794
C	-1.15321	-1.12054	-0.18145
C	0.05430	-1.86546	-0.07358
C	1.30591	-1.22579	0.11858
C	1.34248	0.13419	0.20093
O	0.07886	-3.17579	-0.14531
H	-0.60113	4.00188	-0.69848
H	-0.81580	3.90272	1.02963
H	-1.83292	2.89510	-0.03480
H	1.24437	2.69537	0.33631
H	-2.02831	0.80696	-0.18022
H	-2.09481	-1.64088	-0.32857
H	2.19506	-1.84107	0.19393
H	2.29111	0.64291	0.34800
H	-0.79500	-3.57464	-0.27685

NO+_au

N	1.06310	-1.19967	0.52208
O	0.58229	-2.28495	0.53855
C	0.69225	-0.28967	-0.56692
P	-0.97623	0.39409	0.01918
O	-1.74601	-0.64698	0.72647
O	-0.39797	1.62281	0.85078
C	-1.29085	2.66988	1.34448
C	-2.08228	2.19906	2.54637
O	-1.66338	1.05591	-1.24161
C	-3.01524	0.67999	-1.66155
C	-4.01712	1.64386	-1.06906
C	0.73004	-0.98214	-1.97433
C	0.83721	0.15997	-2.99823
C	-0.49804	-1.84694	-2.27916
C	2.00771	-1.83482	-2.06081
C	1.98658	-0.82788	1.69671
C	2.98599	-1.98387	1.80560
C	2.68629	0.50012	1.44416
C	1.05379	-0.76332	2.91589
H	1.39863	0.53893	-0.54448
H	-1.93329	2.97995	0.51476
H	-0.62113	3.49391	1.59088
H	-2.71212	1.33941	2.30227
H	-2.72357	3.01247	2.89588
H	-1.41452	1.91850	3.36458
H	-3.20704	-0.34685	-1.34067
H	-2.98619	0.72997	-2.75124
H	-3.78532	2.67276	-1.35469
H	-4.03426	1.56203	0.02223
H	-5.01693	1.40134	-1.43835
H	1.76196	0.73112	-2.86379
H	-0.01144	0.84462	-2.93852
H	0.85668	-0.27092	-4.00301
H	-0.66898	-2.61637	-1.52467
H	-0.34066	-2.34304	-3.24123
H	-1.40301	-1.24252	-2.37282
H	1.94984	-2.74674	-1.45933
H	2.89390	-1.26197	-1.76022
H	2.15541	-2.14506	-3.09835
H	3.66138	-1.75964	2.63396
H	2.48369	-2.92952	2.01339
H	3.58402	-2.07906	0.89444
H	3.33160	0.68781	2.30573
H	3.33007	0.46571	0.55989
H	1.98249	1.33220	1.37002
H	0.32863	0.04773	2.81797
H	0.52477	-1.70838	3.05396
H	1.67742	-0.57381	3.79292

NO+_ak

N	1.26916	-0.45562	1.10628
O	1.33274	-1.64140	1.07507
C	0.72970	0.25192	-0.06016
P	-1.12702	0.34522	0.30202
O	-1.37293	1.29451	1.40615
O	-1.83168	0.69014	-1.07274
C	-2.27560	2.05617	-1.35937
C	-3.14680	1.99060	-2.59075
O	-1.40540	-1.18823	0.53972
C	-2.77399	-1.69429	0.67707
C	-3.21008	-2.33248	-0.62183
C	1.20942	-0.33677	-1.43024
C	1.02019	0.79002	-2.46050
C	0.43775	-1.58030	-1.88631
C	2.71371	-0.64571	-1.33052
C	1.74363	0.23613	2.40347
C	3.15616	-0.31148	2.63957
C	1.74070	1.75074	2.25491
C	0.75828	-0.23166	3.48470
H	1.06391	1.28694	0.03530
H	-1.38459	2.67161	-1.52292
H	-2.80835	2.42995	-0.48310
H	-2.59086	1.59174	-3.44262
H	-3.49317	2.99571	-2.84294
H	-4.01974	1.35906	-2.41157
H	-3.42695	-0.86981	0.97943
H	-2.72062	-2.41316	1.49492
H	-2.52677	-3.13808	-0.90053
H	-3.24112	-1.59509	-1.42766
H	-4.21025	-2.75644	-0.50016
H	1.58540	1.68840	-2.18896
H	-0.03243	1.05058	-2.58790
H	1.39310	0.44491	-3.42851

H	0.49635	-2.39316	-1.16036
H	0.87394	-1.92924	-2.82679
H	-0.61502	-1.35016	-2.07043
H	2.92807	-1.52598	-0.71838
H	3.27405	0.21076	-0.93470
H	3.09792	-0.85318	-2.33234
H	3.54200	0.15803	3.54699
H	3.14813	-1.39295	2.78328
H	3.82666	-0.05606	1.81354
H	2.07642	2.15954	3.21118
H	2.44970	2.09276	1.49444
H	0.73945	2.14315	2.06202
H	-0.24369	0.16114	3.29603
H	0.73648	-1.32177	3.54730
H	1.11425	0.16350	4.43912

NO+_aq

N	1.15138	-1.25760	0.20928
O	0.69018	-2.35326	0.19350
C	0.49798	-0.21994	-0.59211
P	-1.03632	0.20301	0.42356
O	-1.83950	-0.97871	0.78400
O	-0.27974	0.93631	1.61988
C	-0.96716	1.10731	2.89953
C	-2.22493	1.93828	2.76163
O	-1.73219	1.34873	-0.41281
C	-3.09604	1.24107	-0.93232
C	-3.77680	2.57635	-0.74036
C	0.24397	-0.67183	-2.07662
C	0.10573	0.62318	-2.89436
C	-1.00509	-1.54324	-2.24529
C	1.48297	-1.42822	-2.58258
C	2.39742	-1.04054	1.09253
C	3.43371	-2.03601	0.55394
C	2.89549	0.39408	1.00090
C	1.95340	-1.40573	2.51411
H	1.14313	0.65804	-0.57094
H	-0.22450	1.59820	3.52953
H	-1.18451	0.11069	3.29461
H	-2.01011	2.88958	2.26900
H	-2.63151	2.14217	3.75524
H	-2.99193	1.40012	2.19540
H	-3.60258	0.42648	-0.40784
H	-3.00860	0.98635	-1.99237
H	-3.21936	3.36974	-1.24275
H	-3.86624	2.82364	0.31931
H	-4.78051	2.53186	-1.17070
H	1.02893	1.21169	-2.86801
H	-0.71277	1.25224	-2.54008
H	-0.09080	0.35909	-3.93703
H	-0.96967	-2.44561	-1.63233
H	-1.07905	-1.84176	-3.29493
H	-1.92077	-1.00419	-1.98863
H	1.59266	-2.41624	-2.12511
H	2.40051	-0.85004	-2.41740
H	1.38501	-1.58479	-3.65982
H	4.33266	-1.93731	1.16655
H	3.07231	-3.06333	0.62778
H	3.70263	-1.81494	-0.48244
H	3.75888	0.47335	1.66605
H	3.24161	0.64931	-0.00511
H	2.14617	1.11318	1.33935
H	1.19446	-0.70919	2.87685
H	2.83003	-1.33493	3.16199
H	1.56939	-2.42654	2.55755

NO+_ae

N	1.31318	-0.72394	0.50290
O	1.09598	-1.88665	0.39634
C	0.75726	0.19266	-0.49928
P	-0.92532	0.67392	0.22222
O	-0.74285	1.59664	1.36185
O	-1.77308	1.22861	-0.99118
C	-2.19584	2.63115	-1.03582
C	-3.48603	2.80574	-0.26821
O	-1.48420	-0.77630	0.50741
C	-2.86308	-0.95758	0.95988
C	-3.05736	-2.42887	1.23601
C	0.82612	-0.35912	-1.96343
C	0.74141	0.87616	-2.87699
C	-0.29452	-1.34437	-2.31544
C	2.20105	-1.01666	-2.17800
C	2.14570	-0.27661	1.72437
C	3.39839	-1.15902	1.68798
C	2.49152	1.20345	1.64415
C	1.25912	-0.58799	2.93982
H	1.34134	1.11185	-0.42291
H	-2.31384	2.83810	-2.10012
H	-1.39418	3.25148	-0.62738
H	-4.26200	2.14585	-0.66375
H	-3.83156	3.83816	-0.36606
H	-3.33156	2.59797	0.79405
H	-3.52037	-0.59897	0.16259
H	-3.00656	-0.34726	1.85642
H	-2.37835	-2.76800	2.02148
H	-2.88012	-3.01637	0.33248
H	-4.08361	-2.60382	1.56763
H	1.57467	1.56491	-2.70037
H	-0.20025	1.41364	-2.75099
H	0.79907	0.54634	-3.91770
H	-0.30205	-2.21288	-1.65445
H	-0.13380	-1.69623	-3.33855
H	-1.27570	-0.86450	-2.27726
H	2.29443	-1.98361	-1.67640
H	3.01644	-0.36097	-1.84704
H	2.34046	-1.19711	-3.24685
H	4.02859	-0.86885	2.53134
H	3.14831	-2.21616	1.78773
H	3.96925	-1.00277	0.76773
H	3.07276	1.43815	2.53936
H	3.12511	1.43324	0.78173
H	1.60034	1.83556	1.65482
H	0.37126	0.04888	2.95018
H	0.97415	-1.64236	2.95431
H	1.85053	-0.37564	3.83372

NO+_bq

N	1.21288	-0.47203	-0.21942
O	1.16499	-1.48755	-0.83306
C	0.31184	0.62522	-0.58305
P	-1.38097	0.25428	0.19924
O	-2.53466	0.24742	-0.71680
O	-1.10485	-1.12531	0.95336
C	-1.98317	-2.28100	0.75984
C	-1.39497	-3.20409	-0.28224
O	-1.34551	1.39975	1.29711
C	-2.60100	1.86576	1.88793
C	-3.27561	0.77280	2.68895
C	0.26824	0.93227	-2.12373
C	-0.52338	2.24553	-2.25040
C	-0.39074	-0.15655	-2.98107
C	1.70676	1.16700	-2.60616
C	2.22376	-0.34902	0.92440
C	2.76333	-1.74431	1.20107
C	3.32085	0.59178	0.39994
C	1.51901	0.23877	2.15049
H	0.68322	1.50579	-0.05574
H	-2.97098	-1.91980	0.46616
H	-2.04137	-2.74732	1.74412
H	-1.33772	-2.70427	-1.25424
H	-2.03153	-4.08579	-0.39240
H	-0.39613	-3.54019	0.00993
H	-3.23498	2.22908	1.07578
H	-2.29576	2.70376	2.51386
H	-2.59424	0.35960	3.43683
H	-3.63169	-0.03288	2.03928
H	-4.14563	1.18685	3.20455
H	-0.08502	3.04270	-1.63995
H	-1.57249	2.11404	-1.97539
H	-0.49010	2.57172	-3.29341
H	0.19471	-1.07797	-3.00506
H	-0.44831	0.21845	-4.00723
H	-1.40793	-0.37502	-2.65109
H	2.32048	0.26156	-2.54195
H	2.19754	1.97379	-2.05187
H	1.68180	1.45856	-3.65940
H	3.46316	-1.66805	2.03557
H	1.95883	-2.42732	1.48670
H	3.29468	-2.15878	0.34274
H	4.08484	0.65007	1.17926
H	3.78685	0.20085	-0.50778
H	2.95146	1.60337	0.21695
H	1.14110	1.24991	1.98937
H	0.69991	-0.40135	2.48337
H	2.26833	0.28795	2.94443

NO+_aa

N	1.19570	-0.80559	0.68835
O	0.92158	-1.95477	0.56373
C	0.69277	0.15024	-0.30403
P	-0.98478	0.67376	0.40294
O	-0.78276	1.49433	1.61429
O	-1.76425	1.36587	-0.78639
C	-1.83428	2.82596	-0.88007
C	-2.84298	3.15596	-1.95372
O	-1.63999	-0.75286	0.55349
C	-3.01891	-0.89676	1.02371
C	-3.29171	-2.37436	1.16688
C	0.76953	-0.37500	-1.77814
C	0.73146	0.87594	-2.67287
C	-0.37224	-1.31947	-2.17076
C	2.12963	-1.06620	-1.97993
C	2.04802	-0.42019	1.91772
C	3.27732	-1.33316	1.83618

C	2.43236	1.05191	1.88494
C	1.16655	-0.75106	3.13095
H	1.30852	1.04570	-0.19814
H	-0.83461	3.19490	-1.13357
H	-2.11721	3.21438	0.09997
H	-2.54150	2.73664	-2.91654
H	-2.91871	4.24109	-2.05668
H	-3.82748	2.76345	-1.69082
H	-3.66955	-0.42928	0.27981
H	-3.10666	-0.36589	1.97567
H	-2.61627	-2.82348	1.89847
H	-3.16912	-2.88331	0.20830
H	-4.31882	-2.52207	1.50903
H	1.55312	1.56397	-2.44512
H	-0.21864	1.40683	-2.58700
H	0.84116	0.56361	-3.71480
H	-0.41947	-2.20039	-1.52822
H	-0.20245	-1.65392	-3.19828
H	-1.33915	-0.81070	-2.13932
H	2.19219	-2.03691	-1.48046
H	2.95711	-0.43262	-1.63640
H	2.27770	-1.24743	-3.04740
H	3.92143	-1.09214	2.68456
H	2.99903	-2.38630	1.89794
H	3.84524	-1.15719	0.91770
H	3.01823	1.24245	2.78758
H	3.07337	1.29314	1.03122
H	1.55749	1.70559	1.91555
H	0.29271	-0.09609	3.16803
H	0.85951	-1.79909	3.11591
H	1.76980	-0.57963	4.02565

NO+_am

N	1.14030	-0.98566	0.57230
O	0.73310	-2.09768	0.65986
C	0.74665	-0.17907	-0.58898
P	-0.82563	0.70185	-0.00846
O	-0.47607	1.78613	0.93338
O	-1.58519	1.15021	-1.32064
C	-1.76897	2.56968	-1.63376
C	-3.01086	3.09205	-0.94871
O	-1.61588	-0.55513	0.53106
C	-2.99309	-0.42449	1.00791
C	-3.01532	0.05665	2.44247
C	0.71781	-0.98287	-1.93224
C	0.83784	0.06985	-3.04794
C	-0.55278	-1.81579	-2.13691
C	1.96322	-1.88522	-1.99294
C	2.03015	-0.47359	1.72610
C	3.10693	-1.55017	1.89911
C	2.63347	0.88429	1.39612
C	1.09228	-0.39975	2.94103
H	1.47972	0.62716	-0.65677
H	-1.85383	2.59278	-2.72084
H	-0.87510	3.11586	-1.32261
H	-3.88769	2.51018	-1.24339
H	-3.17749	4.13263	-1.23904
H	-2.89270	3.05804	0.13814
H	-3.40843	-1.42620	0.89933
H	-3.52596	0.25095	0.33105
H	-2.57293	1.05211	2.53264
H	-2.46792	-0.63612	3.08632
H	-4.04989	0.10284	2.79231
H	1.77535	0.63133	-2.97230
H	0.00001	0.76950	-3.04127
H	0.83517	-0.44199	-4.01396
H	-0.70291	-2.54202	-1.33618
H	-0.45658	-2.36358	-3.07877
H	-1.43981	-1.18167	-2.20854
H	1.89508	-2.75170	-1.32969
H	2.87745	-1.32532	-1.75826
H	2.06805	-2.27007	-3.01046
H	3.77292	-1.22234	2.70008
H	2.67372	-2.51156	2.17832
H	3.70235	-1.66739	0.98868
H	3.24343	1.17336	2.25561
H	3.30121	0.83920	0.53004
H	1.86904	1.65317	1.26102
H	0.33227	0.37355	2.80396
H	0.62245	-1.36784	3.12929
H	1.70520	-0.13616	3.80642

NO+_af

N	1.08367	-0.53580	0.77483
O	0.76469	-1.68227	0.81213
C	0.62897	0.27363	-0.35915
P	-1.10771	0.76066	0.20035
O	-1.02391	1.45807	1.50112
O	-1.58251	1.54535	-1.07855
C	-2.89839	2.19431	-1.08992
C	-3.04149	2.88859	-2.42251
O	-1.92173	-0.59887	0.22046
C	-2.49979	-1.15516	1.44109
C	-2.47358	-2.66011	1.31911
C	0.84339	-0.41980	-1.75271
C	0.89260	0.72034	-2.78458
C	-0.25747	-1.41459	-2.13228
C	2.21228	-1.12057	-1.74644
C	1.94491	-0.00946	1.94183
C	3.22997	-0.84735	1.86780
C	2.22493	1.47872	1.79352
C	1.14221	-0.30842	3.21427
H	1.19373	1.20609	-0.31814
H	-2.93144	2.89441	-0.25153
H	-3.65294	1.41430	-0.95199
H	-2.26123	3.64198	-2.54994
H	-4.01318	3.38620	-2.46804
H	-2.98272	2.16894	-3.24213
H	-3.51892	-0.76857	1.51193
H	-1.92934	-0.78979	2.29942
H	-1.44751	-3.03093	1.24868
H	-3.02573	-2.98514	0.43480
H	-2.94083	-3.10464	2.20142
H	1.72032	1.40866	-2.58231
H	-0.03976	1.28619	-2.81073
H	1.05729	0.28545	-3.77420
H	-0.37119	-2.21027	-1.39269
H	0.00972	-1.87246	-3.08896
H	-1.22289	-0.91709	-2.25449
H	2.23303	-2.01313	-1.11377
H	3.01048	-0.43728	-1.43125
H	2.44443	-1.44567	-2.76365
H	3.87718	-0.52213	2.68542
H	3.01735	-1.91107	1.99174
H	3.76409	-0.68606	0.92757
H	2.79407	1.78000	2.67649
H	2.84735	1.70178	0.92183
H	1.30319	2.06565	1.77682
H	0.22894	0.29108	3.23820
H	0.90792	-1.37222	3.29280
H	1.76724	-0.03165	4.06631

NO+_bd

N	1.44015	-0.65027	0.56263
O	1.31939	-1.76926	0.93218
C	0.62238	-0.18462	-0.57719
P	-1.05118	0.20560	0.21731
O	-0.99313	-0.09554	1.66504
O	-1.13634	1.70709	-0.28302
C	-2.34369	2.49694	-0.04732
C	-2.38008	3.01128	1.37609
O	-2.20740	-0.53223	-0.57435
C	-3.05310	-1.52456	0.09122
C	-4.22019	-0.83858	0.76368
C	0.67375	-1.12458	-1.82733
C	-0.07715	-0.36668	-2.93570
C	0.04950	-2.51074	-1.62327
C	2.14223	-1.29163	-2.24516
C	2.41548	0.27445	1.29602
C	3.57305	0.52026	0.31538
C	1.68650	1.57807	1.64468
C	2.87752	-0.45870	2.54578
H	1.03021	0.78835	-0.85854
H	-3.21058	1.87528	-0.29146
H	-2.27717	3.30467	-0.77590
H	-2.43120	2.19004	2.09572
H	-3.26028	3.64552	1.50942
H	-1.49107	3.61013	1.58877
H	-2.44368	-2.08043	0.80827
H	-3.37208	-2.18795	-0.71392
H	-4.79908	-0.26037	0.03919
H	-3.86920	-0.18124	1.56451
H	-4.87940	-1.58948	1.20692
H	0.34284	0.63173	-3.09662
H	-1.14240	-0.26968	-2.71489
H	0.02359	-0.92490	-3.87040
H	0.62175	-3.13029	-0.93067
H	0.04229	-3.02157	-2.59056
H	-0.98329	-2.45269	-1.27730
H	2.72926	-1.82471	-1.48891
H	2.61894	-0.32861	-2.45451
H	2.18606	-1.88788	-3.16045
H	4.30575	1.13570	0.84319
H	4.06002	-0.41305	0.02282
H	3.25948	1.06707	-0.57682
H	2.41538	2.20983	2.15846
H	1.33993	2.12640	0.76530
H	0.84351	1.39049	2.31190
H	2.03163	-0.70271	3.19319
H	3.42150	-1.37477	2.30778
H	3.54938	0.20892	3.08891

NO+_ac

N	1.53372	0.07296	0.36761

O	1.98049	-1.01405	0.54022
C	0.44443	0.24133	-0.60015
P	-1.11333	-0.02697	0.44263
O	-1.29377	1.10575	1.37444
O	-2.28958	-0.27008	-0.58621
C	-3.21785	0.81174	-0.92291
C	-4.34962	0.19846	-1.71172
O	-0.77543	-1.45030	1.03011
C	-1.67702	-2.09677	1.98752
C	-1.34974	-1.65418	3.39614
C	0.63863	-0.58790	-1.91540
C	-0.24192	0.09463	-2.97635
C	0.24190	-2.06331	-1.79404
C	2.10687	-0.46235	-2.35897
C	2.13475	1.21710	1.21342
C	3.64440	1.13497	0.95785
C	1.56338	2.56685	0.80409
C	1.77771	0.86495	2.66481
H	0.41477	1.30681	-0.83714
H	-2.66888	1.55578	-1.51014
H	-3.55211	1.27252	0.00845
H	-3.98008	-0.27052	-2.62670
H	-5.06310	0.97919	-1.98604
H	-4.87073	-0.55387	-1.11606
H	-1.50605	-3.16230	1.83547
H	-2.70781	-1.86346	1.70423
H	-1.51866	-0.58149	3.51812
H	-0.30927	-1.88692	3.63659
H	-1.99069	-2.18868	4.10210
H	0.03189	1.14609	-3.11730
H	-1.30261	0.02768	-2.72651
H	-0.09600	-0.41591	-3.93200
H	0.80561	-2.58067	-1.01599
H	0.44949	-2.55384	-2.74942
H	-0.82523	-2.17378	-1.58554
H	2.79255	-1.03410	-1.72753
H	2.43127	0.58571	-2.38272
H	2.20353	-0.85784	-3.37313
H	4.11802	1.93448	1.53162
H	4.05524	0.17927	1.28685
H	3.87934	1.29059	-0.09932
H	2.02813	3.31337	1.45295
H	1.82464	2.83139	-0.22531
H	0.48338	2.62026	0.96040
H	0.69776	0.91777	2.82382
H	2.15545	-0.12489	2.93039
H	2.26200	1.60483	3.30657

NO+_bs

N	1.33362	-0.66672	0.07112
O	1.24018	-1.84392	-0.05960
C	0.51524	0.20262	-0.77401
P	-1.16554	0.37163	0.07054
O	-2.18496	0.95983	-0.81414
O	-1.33061	-1.10923	0.59538
C	-2.61861	-1.55500	1.13471
C	-3.51902	-2.03495	0.01879
O	-0.82782	1.22714	1.37474
C	-1.42981	2.54712	1.57404
C	-2.82286	2.41404	2.14587
C	0.44916	-0.26376	-2.27350
C	0.04080	0.98492	-3.07390
C	-0.55843	-1.39230	-2.52319
C	1.85727	-0.69263	-2.71678
C	2.31493	-0.16800	1.15159
C	3.63844	-0.87641	0.84106
C	2.46771	1.34558	1.10457
C	1.70993	-0.64301	2.48026
H	0.95908	1.19789	-0.71953
H	-3.06136	-0.72889	1.70122
H	-2.35399	-2.35282	1.82869
H	-3.76206	-1.21835	-0.66522
H	-4.44906	-2.41924	0.44573
H	-3.03765	-2.84205	-0.53854
H	-1.43559	3.07632	0.61771
H	-0.74883	3.04736	2.26444
H	-3.22218	3.40717	2.36759
H	-2.80526	1.83661	3.07366
H	-3.49011	1.93562	1.42385
H	0.78758	1.78117	-2.97925
H	-0.93451	1.36527	-2.76354
H	-0.02049	0.71379	-4.13139
H	-0.34511	-2.27941	-1.92319
H	-0.50279	-1.67532	-3.57819
H	-1.58159	-1.06182	-2.32360
H	2.16746	-1.65029	-2.28872
H	2.60589	0.07091	-2.46946
H	1.86088	-0.81256	-3.80307
H	4.36998	-0.54953	1.58322
H	3.53640	-1.96044	0.90686
H	4.01297	-0.60372	-0.15000
H	3.17324	1.61754	1.89342
H	2.89445	1.69038	0.15794
H	1.52791	1.86180	1.31075
H	0.75210	-0.15470	2.67372
H	1.58297	-1.72757	2.48300
H	2.40985	-0.37206	3.27432

NO+_av

N	1.41405	-0.67907	0.75045
O	1.28074	-1.78574	1.15210
C	0.60337	-0.24054	-0.40499
P	-1.08458	0.14478	0.35945
O	-1.03454	-0.07680	1.82117
O	-1.20454	1.62033	-0.20773
C	-2.44792	2.36278	-0.00470
C	-2.22311	3.76984	-0.50433
O	-2.21387	-0.66019	-0.40479
C	-3.02893	-1.65456	0.29567
C	-4.20581	-0.98059	0.96321
C	0.67945	-1.20024	-1.64007
C	-0.08536	-0.47860	-2.76297
C	0.08751	-2.59684	-1.41332
C	2.15211	-1.34199	-2.05190
C	2.38989	0.26027	1.46454
C	3.54224	0.50477	0.47836
C	1.64980	1.56205	1.79869
C	2.86235	-0.45202	2.72222
H	1.00304	0.73222	-0.69872
H	-2.68561	2.34217	1.06327
H	-3.23377	1.84860	-0.56479
H	-1.42522	4.25819	0.05923
H	-3.14023	4.35008	-0.37763
H	-1.96074	3.76469	-1.56442
H	-2.39858	-2.17737	1.01968
H	-3.33870	-2.34601	-0.48922
H	-4.79760	-0.42458	0.23191
H	-3.86384	-0.30447	1.75143
H	-4.84885	-1.73747	1.41985
H	0.30814	0.52866	-2.93521
H	-1.15412	-0.40785	-2.54930
H	0.03609	-1.04692	-3.68908
H	0.67426	-3.19160	-0.71089
H	0.09378	-3.12351	-2.37210
H	-0.94649	-2.55785	-1.06857
H	2.74834	-1.84783	-1.28418
H	2.60839	-0.37298	-2.27807
H	2.21131	-1.95431	-2.95564
H	4.26694	1.13873	0.99517
H	4.04197	-0.42617	0.20065
H	3.22095	1.03290	-0.42216
H	2.37516	2.20770	2.30003
H	1.29493	2.09428	0.91254
H	0.81103	1.37581	2.47099
H	2.02261	-0.68766	3.38048
H	3.40660	-1.37065	2.49434
H	3.53706	0.22546	3.24941

NO+_br

N	1.34543	-0.48261	-0.07739
O	1.47792	-1.65200	-0.23927
C	0.45082	0.25517	-0.96949
P	-1.29106	0.09764	-0.25635
O	-2.32973	0.51399	-1.21217
O	-1.22291	-1.40219	0.23408
C	-2.40824	-2.04634	0.80521
C	-2.27190	-2.10299	2.30999
O	-1.21963	0.96773	1.08135
C	-2.03331	2.17732	1.21902
C	-3.43356	1.82386	1.66648
C	0.58346	-0.16586	-2.47780
C	0.01712	1.01509	-3.28473
C	-0.18051	-1.44818	-2.82853
C	2.07571	-0.31986	-2.81421
C	2.12898	0.14474	1.09366
C	3.57828	-0.31128	0.89107
C	2.01537	1.66244	1.08551
C	1.50664	-0.47119	2.35492
H	0.70428	1.31099	-0.86086
H	-2.43135	-3.03753	0.35217
H	-3.29716	-1.49542	0.48303
H	-1.37285	-2.65572	2.59314
H	-3.13796	-2.61573	2.73633
H	-2.22105	-1.09744	2.73548
H	-2.03846	2.70682	0.26272
H	-1.50191	2.77283	1.96321
H	-3.41022	1.26373	2.60457
H	-3.94450	1.23752	0.89826
H	-4.00679	2.74022	1.82951
H	0.59615	1.92956	-3.11378
H	-1.03246	1.20189	-3.04890
H	0.08860	0.77312	-4.34862
H	0.14842	-2.30287	-2.23417
H	0.00183	-1.67899	-3.88194

H	-1.25833	-1.31598	-2.70156
H	2.52122	-1.22045	-2.38168
H	2.65271	0.55668	-2.49258
H	2.18325	-0.40048	-3.89880
H	4.17508	0.11579	1.69991
H	3.66501	-1.39788	0.93088
H	3.98089	0.05295	-0.05870
H	2.59568	2.02860	1.93591
H	2.44955	2.10575	0.18437
H	0.98562	1.99977	1.21949
H	0.46429	-0.16453	2.47065
H	1.57382	-1.56092	2.32759
H	2.07747	-0.10795	3.21290

NO+_bn

N	1.06338	-0.69055	-0.35069
O	0.94366	-1.52979	-1.18230
C	0.30772	0.55837	-0.48511
P	-1.45628	0.21910	0.13329
O	-2.54466	0.53890	-0.80546
O	-1.38875	-1.31084	0.58826
C	-2.36051	-2.28729	0.08751
C	-1.82505	-2.96887	-1.15030
O	-1.35763	1.08197	1.46129
C	-2.57644	1.32581	2.23444
C	-2.21507	2.25885	3.36503
C	0.39113	1.20616	-1.91465
C	-0.24973	2.59672	-1.76343
C	-0.32482	0.42232	-3.02258
C	1.87309	1.37457	-2.27848
C	2.01385	-0.94658	0.82293
C	2.38213	-2.42240	0.79024
C	3.23458	-0.04910	0.56236
C	1.30816	-0.56828	2.12838
H	0.73620	1.24910	0.24378
H	-3.29921	-1.76685	-0.11119
H	-2.49521	-2.98160	0.91749
H	-1.68115	-2.24651	-1.95982
H	-2.54159	-3.72000	-1.49274
H	-0.87750	-3.47386	-0.94257
H	-2.93711	0.36037	2.60344
H	-3.31965	1.75896	1.56083
H	-1.83901	3.20730	2.97567
H	-1.45663	1.81147	4.01158
H	-3.10480	2.46109	3.96609
H	0.23286	3.18085	-0.97217
H	-1.32107	2.52882	-1.56059
H	-0.12125	3.14192	-2.70234
H	0.15819	-0.53381	-3.23456
H	-0.27558	1.02070	-3.93716
H	-1.37863	0.25940	-2.78990
H	2.38312	0.41284	-2.40342
H	2.41129	1.97305	-1.53608
H	1.94320	1.89677	-3.23624
H	3.03690	-2.61808	1.64167
H	1.49313	-3.05149	0.88683
H	2.91389	-2.69480	-0.12290
H	3.95432	-0.25820	1.35778
H	3.70688	-0.27877	-0.39578
H	2.98785	1.01414	0.60529
H	1.05388	0.49128	2.19157
H	0.40594	-1.16375	2.27952
H	2.01146	-0.78931	2.93509

NO+_bt

N	0.83915	-0.84854	0.76571
O	0.51748	-1.84757	1.31876
C	0.34615	-0.59056	-0.59358
P	-1.38401	0.19103	-0.42660
O	-2.43800	-0.46972	-1.21175
O	-1.50305	0.17751	1.15794
C	-2.78290	0.51670	1.78476
C	-2.61015	0.34374	3.27449
O	-1.11840	1.71908	-0.77961
C	-1.46741	2.24552	-2.09830
C	-1.54071	3.74954	-1.98242
C	0.43341	-1.82898	-1.55211
C	0.12629	-1.27481	-2.95458
C	-0.53621	-2.97225	-1.22279
C	1.87668	-2.35317	-1.53184
C	1.79486	0.11084	1.48462
C	3.16487	-0.14533	0.83310
C	1.33920	1.55619	1.27751
C	1.79024	-0.27292	2.95751
H	0.98186	0.20649	-0.98758
H	-3.54150	-0.15309	1.37373
H	-3.02197	1.54975	1.51641
H	-2.33634	-0.68673	3.51332
H	-3.55124	0.57483	3.77897
H	-1.84206	1.02002	3.65877
H	-2.41852	1.80292	-2.40180
H	-0.68704	1.93092	-2.79956
H	-0.58492	4.16397	-1.65399
H	-2.31678	4.04317	-1.27247
H	-1.78556	4.17597	-2.95821
H	0.80261	-0.45412	-3.22176
H	-0.91020	-0.93872	-3.03895
H	0.27684	-2.07308	-3.68624
H	-0.28555	-3.47051	-0.28487
H	-0.45506	-3.71688	-2.02017
H	-1.57196	-2.63127	-1.18929
H	2.15637	-2.76766	-0.55718
H	2.59793	-1.57810	-1.81260
H	1.96667	-3.16512	-2.25815
H	3.89111	0.46834	1.37193
H	3.46446	-1.19213	0.92561
H	3.18784	0.15182	-0.21808
H	2.06332	2.18687	1.79909
H	1.33012	1.86563	0.23088
H	0.35168	1.72971	1.70783
H	0.78212	-0.20214	3.37521
H	2.17405	-1.28052	3.12322
H	2.43481	0.43307	3.48499

NO+_az

N	1.12611	-0.27583	-0.03286
O	1.21575	-1.45700	-0.14311
C	0.17034	0.43453	-0.87686
P	-1.51869	0.23686	-0.04919
O	-2.64875	0.50416	-0.95152
O	-1.44346	-1.20647	0.60628
C	-2.38615	-2.27826	0.28753
C	-1.64105	-3.58798	0.38086
O	-1.26319	1.23524	1.16298
C	-2.34844	1.49442	2.10950
C	-1.87519	2.57555	3.05186
C	0.21874	-0.00718	-2.38380
C	-0.43483	1.14249	-3.16862
C	-0.52610	-1.31649	-2.66716
C	1.69086	-0.12745	-2.80810
C	2.02943	0.38982	1.02453
C	3.44825	-0.08106	0.68284
C	1.91648	1.90670	0.97496
C	1.54791	-0.17964	2.36630
H	0.40338	1.49632	-0.79624
H	-2.80006	-2.09602	-0.70679
H	-3.19243	-2.21212	1.02139
H	-0.83110	-3.63018	-0.35172
H	-2.32882	-4.41322	0.18071
H	-1.22172	-3.72443	1.38032
H	-2.56258	0.55837	2.63518
H	-3.22695	1.80338	1.53761
H	-1.65033	3.49273	2.50299
H	-0.98294	2.25559	3.59648
H	-2.66000	2.79362	3.77989
H	0.12685	2.07540	-3.05035
H	-1.47085	1.30387	-2.86303
H	-0.42934	0.88491	-4.23136
H	-0.13637	-2.15068	-2.07924
H	-0.39696	-1.56690	-3.72395
H	-1.59898	-1.20612	-2.48734
H	2.18917	-0.99921	-2.37266
H	2.25735	0.77611	-2.55030
H	1.73629	-0.24260	-3.89401
H	4.12785	0.36302	1.41345
H	3.53418	-1.16705	0.74212
H	3.75066	0.25674	-0.31268
H	2.58109	2.29855	1.74893
H	2.26016	2.31552	0.01994
H	0.90549	2.25462	1.19710
H	0.52070	0.12755	2.57572
H	1.61686	-1.26930	2.37537
H	2.20127	0.21905	3.14594

NO+_bj

N	1.28442	-0.42907	0.03762
O	1.35827	-1.59115	-0.20368
C	0.47591	0.41722	-0.83783
P	-1.31617	0.18931	-0.29450
O	-2.29685	0.69161	-1.26950
O	-1.39635	-1.35331	0.07100
C	-2.42436	-2.22545	-0.49680
C	-3.69623	-2.12723	0.31407
O	-1.19262	0.93672	1.10620
C	-2.38397	1.08594	1.94023
C	-2.02511	2.00958	3.08025
C	0.73330	0.15821	-2.36593
C	0.24670	1.42846	-3.08347
C	-0.01341	-1.06312	-2.91432
C	2.24582	0.00763	-2.59018
C	2.05991	0.06953	1.27464
C	3.50538	-0.38690	1.03887
C	1.96772	1.58184	1.41648
C	1.42061	-0.66102	2.46302

H	0.71889	1.45090	-0.59095
H	-1.98052	-3.22051	-0.45840
H	-2.58812	-1.93731	-1.53742
H	-3.50949	-2.37454	1.36208
H	-4.43421	-2.83173	-0.07816
H	-4.12212	-1.12184	0.24318
H	-2.66855	0.08932	2.29293
H	-3.18356	1.49633	1.31758
H	-1.73140	2.99135	2.70226
H	-1.20708	1.59521	3.67552
H	-2.89176	2.13691	3.73309
H	0.82454	2.30635	-2.77483
H	-0.81452	1.61427	-2.90333
H	0.39208	1.29723	-4.15933
H	0.22474	-1.97922	-2.36841
H	0.28051	-1.20935	-3.95755
H	-1.09436	-0.89777	-2.90157
H	2.64193	-0.93718	-2.20518
H	2.80189	0.84026	-2.14137
H	2.44533	0.02370	-3.66464
H	4.09676	-0.06381	1.89842
H	3.57249	-1.47296	0.95789
H	3.92837	0.07447	0.14195
H	2.53235	1.84975	2.31300
H	2.43391	2.10530	0.57634
H	0.93989	1.92320	1.55573
H	0.37704	-0.36349	2.58799
H	1.48439	-1.74356	2.33703
H	1.97728	-0.38042	3.36018

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C	-0.85499	3.28093	0.07650
C	0.32126	2.36165	0.11264
C	0.21193	0.94967	0.06710
C	-1.03858	0.28696	-0.01741
C	-1.12127	-1.09747	-0.06078
C	0.04044	-1.87204	-0.02147
C	1.29265	-1.24877	0.06201
C	1.37196	0.12832	0.10501
O	0.02148	-3.23448	-0.06085
H	-0.54134	4.32517	0.12185
H	-1.53769	3.10111	0.91840
H	-1.44560	3.14982	-0.84067
H	1.31698	2.78924	0.17701
H	-1.95391	0.86973	-0.04916
H	-2.09290	-1.58231	-0.12560
H	2.18244	-1.86873	0.09136
H	2.34637	0.60526	0.16973
H	-0.88696	-3.55133	-0.11775

N•_bk

N	0.70101	-0.11262	-1.04253
C	0.45110	-0.26653	0.36526
P	-1.29940	0.31593	0.54516
O	-2.21752	-0.60352	-0.17459
O	-1.59319	0.49002	2.11219
C	-1.98507	-0.67476	2.86752
C	-3.49421	-0.81102	2.88455
O	-1.34620	1.84573	0.10221
C	-1.75587	2.22751	-1.22904
C	-0.61264	2.93520	-1.92575
C	1.56077	0.43556	1.20923
C	1.40076	0.08705	2.69474
C	1.56655	1.95601	1.02822
C	2.90098	-0.13502	0.71882
C	0.57410	-1.25788	-1.94886
C	-0.49346	-0.86948	-2.98856
C	1.93931	-1.37161	-2.65127
C	0.20240	-2.60202	-1.31482
H	0.40938	-1.31745	0.69543
H	-1.57849	-0.51794	3.86979
H	-1.51534	-1.57125	2.44404
H	-3.94840	0.09581	3.29136
H	-3.78450	-1.65968	3.51098
H	-3.86531	-0.97317	1.87021
H	-2.61889	2.88579	-1.09937
H	-2.07947	1.33732	-1.77657
H	-0.29404	3.80673	-1.34736
H	-0.93740	3.27362	-2.91456
H	0.23424	2.25348	-2.03983
H	1.33021	-0.99793	2.84334
H	0.51701	0.55888	3.12849
H	2.27809	0.43980	3.24703
H	0.67408	2.41777	1.45937
H	1.60859	2.21744	-0.03304
H	2.44688	2.37766	1.52572
H	2.91275	-1.23043	0.78649
H	3.72052	0.24994	1.33461
H	3.08719	0.14908	-0.32109
H	-0.25952	0.10900	-3.42016
H	-0.51262	-1.61180	-3.79320
H	-1.47870	-0.83336	-2.51573
H	2.21511	-0.41326	-3.10033
H	2.72012	-1.66123	-1.94102
H	1.88905	-2.13160	-3.43757
H	0.12525	-3.35621	-2.10385
H	-0.76396	-2.54170	-0.80515
H	0.96900	-2.94417	-0.61024

N•_ba

N	0.75509	-0.36415	-0.94789
C	0.28148	-0.53795	0.40599
P	-1.28850	0.45388	0.41645
O	-2.40870	-0.20125	-0.30181
O	-1.55922	0.78097	1.96029
C	-2.82048	1.39759	2.30892
C	-3.86117	0.34053	2.61973
O	-0.92750	1.91070	-0.15670
C	-1.02741	2.18889	-1.56783
C	0.27361	2.80216	-2.04020
C	1.37955	-0.10150	1.44298
C	0.99870	-0.59784	2.84415
C	1.59491	1.41631	1.45335
C	2.70494	-0.77414	1.05488
C	0.66711	-1.49134	-1.88239
C	1.17602	-0.95473	-3.22375
C	1.56739	-2.65333	-1.42393
C	-0.77067	-2.01151	-2.04793
H	-0.03046	-1.56897	0.64359
H	-3.14247	2.05094	1.49100
H	-2.59972	2.02000	3.17878
H	-4.05524	-0.26684	1.73304
H	-4.79297	0.81926	2.93531
H	-3.51259	-0.30757	3.42799
H	-1.86960	2.87585	-1.69402
H	-1.25921	1.26639	-2.11002
H	0.50397	3.70080	-1.46154
H	0.19271	3.07960	-3.09576
H	1.08478	2.07955	-1.92181
H	0.86821	-1.68641	2.84994
H	0.08150	-0.13536	3.20894
H	1.80793	-0.35751	3.54229
H	0.72484	1.94845	1.84563
H	1.79667	1.78625	0.44373
H	2.45531	1.65180	2.08889
H	2.61600	-1.86531	1.05419
H	3.47320	-0.50285	1.78640
H	3.04224	-0.44731	0.06669
H	2.19618	-0.57341	-3.11640
H	1.17043	-1.73973	-3.98642
H	0.53935	-0.13254	-3.56641
H	2.61031	-2.33727	-1.34158
H	1.24428	-3.06132	-0.46136
H	1.50787	-3.45642	-2.16467
H	-0.76296	-2.81643	-2.78979
H	-1.44496	-1.22223	-2.38671
H	-1.18065	-2.40452	-1.11424

N•_bu

N	0.33759	-0.01063	-1.27078
C	0.34425	-0.40258	0.11315
P	-1.22686	0.34068	0.75890
O	-2.39979	-0.30732	0.11975
O	-1.18989	0.25094	2.36154
C	-1.61007	-0.98107	2.98027
C	-1.62353	-0.75742	4.47663
O	-1.11506	1.92106	0.58777
C	-1.71660	2.59767	-0.53731
C	-0.63735	3.28262	-1.34932
C	1.69169	-0.00954	0.79685
C	1.78254	-0.64048	2.19201
C	1.88224	1.50641	0.89676
C	2.81070	-0.60184	-0.07436
C	-0.13495	-0.93762	-2.30345
C	-1.31207	-0.23658	-3.00660
C	1.03497	-1.06932	-3.29533
C	-0.57715	-2.32689	-1.83331
H	0.20279	-1.48479	0.26866
H	-0.90477	-1.77754	2.70929
H	-2.59910	-1.24621	2.59627
H	-0.62627	-0.48987	4.83532
H	-1.94552	-1.66922	4.98670
H	-2.31291	0.05073	4.73135
H	-2.42041	3.31812	-0.11242
H	-2.28072	1.87496	-1.13434
H	-0.07853	3.98560	-0.72545
H	-1.09368	3.83723	-2.17508
H	0.05318	2.53838	-1.75468
H	1.63056	-1.72611	2.14673
H	1.05257	-0.20878	2.88032
H	2.78106	-0.46455	2.60589
H	1.17653	1.95706	1.60003
H	1.73973	1.97766	-0.07995
H	2.89895	1.72269	1.24281

H	2.67182	-1.68132	-0.21600
H	3.78208	-0.44679	0.40683
H	2.83194	-0.12440	-1.05829
H	-1.01974	0.77275	-3.31352
H	-1.60062	-0.80385	-3.89755
H	-2.16912	-0.17830	-2.33008
H	1.36132	-0.08031	-3.62929
H	1.88513	-1.57811	-2.83019
H	0.71831	-1.65224	-4.16615
H	-0.91868	-2.90157	-2.69959
H	-1.40633	-2.25560	-1.12307
H	0.24976	-2.88362	-1.37781

N•_bv

N	0.92668	-0.25271	-1.29115
C	0.74444	-0.34347	0.12996
P	-0.84513	0.50909	0.52469
O	-1.94146	0.19357	-0.42687
O	-1.20973	0.08929	2.04080
C	-2.10681	-1.01442	2.26702
C	-3.53930	-0.52574	2.34795
O	-0.47822	2.05301	0.69287
C	-1.56579	3.00320	0.77495
C	-1.92589	3.50997	-0.60695
C	2.03204	0.12534	0.88030
C	1.80017	0.15987	2.39444
C	2.52816	1.49250	0.39529
C	3.10753	-0.92509	0.56171
C	0.43267	-1.31360	-2.17171
C	-0.44169	-0.61288	-3.22552
C	1.68795	-1.88668	-2.85663
C	-0.35668	-2.45534	-1.51992
H	0.52606	-1.36771	0.48433
H	-1.77807	-1.46294	3.20772
H	-1.99444	-1.75613	1.46763
H	-3.63451	0.23356	3.12902
H	-4.20802	-1.35753	2.58843
H	-3.83932	-0.09837	1.38818
H	-1.19481	3.80260	1.41961
H	-2.42359	2.53205	1.26830
H	-1.05045	3.95728	-1.08407
H	-2.71026	4.26900	-0.53205
H	-2.28577	2.68568	-1.22675
H	1.39573	-0.79056	2.76198
H	1.10576	0.95414	2.68106
H	2.75414	0.34078	2.90075
H	1.82387	2.28687	0.64776
H	2.67255	1.48777	-0.68743
H	3.48729	1.71343	0.87676
H	2.79310	-1.92753	0.87779
H	4.03819	-0.68186	1.08482
H	3.31691	-0.94884	-0.51263
H	0.12211	0.19772	-3.69531
H	-0.74038	-1.33120	-3.99634
H	-1.33452	-0.19850	-2.75124
H	2.27048	-1.08208	-3.31335
H	2.32165	-2.41160	-2.13423
H	1.39150	-2.59779	-3.63454
H	-0.67449	-3.15413	-2.29969
H	-1.25338	-2.07774	-1.02000
H	0.25361	-3.02208	-0.80751

N•_bh

N	0.67301	-0.26667	-1.20268
C	0.44409	-0.15141	0.20869
P	-1.27071	0.52657	0.40710
O	-2.24009	-0.10551	-0.52241
O	-1.62134	0.33276	1.96506
C	-2.06343	-0.96015	2.41356
C	-2.47067	-0.82486	3.86486
O	-1.18913	2.11933	0.33157
C	-1.84487	2.81568	-0.75453
C	-0.96000	2.85050	-1.98443
C	1.61410	0.62086	0.89762
C	1.32369	0.83229	2.38754
C	1.90929	1.96813	0.22843
C	2.85205	-0.27798	0.75063
C	0.38882	-1.52639	-1.89474
C	-0.51900	-1.16182	-3.08143
C	1.74984	-2.01066	-2.43017
C	-0.26073	-2.64549	-1.07116
H	0.36815	-1.12679	0.72082
H	-1.24099	-1.68037	2.30561
H	-2.89631	-1.28754	1.78361
H	-1.62564	-0.48289	4.46764
H	-2.80967	-1.79035	4.24977
H	-3.28353	-0.10183	3.96321
H	-2.03769	3.81610	-0.36261
H	-2.79683	2.32163	-0.96478
H	-0.01609	3.35792	-1.77044
H	-1.47055	3.38473	-2.79125
H	-0.73545	1.83439	-2.32321
H	1.05284	-0.10950	2.88119
H	0.50868	1.54288	2.54780
H	2.22080	1.22374	2.87868
H	1.10575	2.68544	0.40542
H	2.03822	1.84144	-0.84979
H	2.83487	2.37989	0.64572
H	2.68029	-1.26848	1.19033
H	3.70964	0.17405	1.25970
H	3.11096	-0.40731	-0.30518
H	-0.05031	-0.37422	-3.67898
H	-0.67235	-2.04060	-3.71654
H	-1.48608	-0.80857	-2.71434
H	2.23374	-1.21839	-3.00781
H	2.41258	-2.29944	-1.60788
H	1.60259	-2.88263	-3.07565
H	-0.44170	-3.50412	-1.72485
H	-1.22223	-2.32466	-0.66002
H	0.39129	-2.98950	-0.26011

N•_ax

N	0.35820	-0.34735	-1.23197
C	0.33551	-0.62218	0.18611
P	-1.23901	0.19577	0.73471
O	-2.46064	-0.55273	0.35442
O	-1.04517	0.43792	2.30617
C	-2.17633	0.92623	3.05844
C	-1.78248	0.92688	4.51944
O	-1.20383	1.70235	0.17796
C	-1.75073	2.01905	-1.11788
C	-0.71305	2.77918	-1.91637
C	1.65272	-0.11175	0.87678
C	1.76231	-0.69938	2.29041
C	1.72492	1.41893	0.92670
C	2.85177	-0.62488	0.06518
C	0.08480	-1.44018	-2.17156
C	0.09690	-0.79998	-3.56299
C	1.18823	-2.51142	-2.09377
C	-1.27736	-2.10987	-1.92470
H	0.20442	-1.68894	0.43410
H	-3.03166	0.27157	2.86665
H	-2.41493	1.93558	2.70630
H	-1.53303	-0.08540	4.84698
H	-2.61129	1.29660	5.12909
H	-0.91469	1.57105	4.68220
H	-2.64812	2.61960	-0.94184
H	-2.05484	1.09740	-1.62488
H	-0.39772	3.67574	-1.37575
H	-1.13427	3.08413	-2.87936
H	0.15590	2.14022	-2.09251
H	1.73471	-1.79500	2.26020
H	0.96424	-0.34914	2.94557
H	2.72234	-0.40431	2.72793
H	0.97218	1.84016	1.59760
H	1.57515	1.84730	-0.06880
H	2.71365	1.71937	1.28979
H	2.86400	-1.71848	0.01550
H	3.77890	-0.30281	0.55065
H	2.84193	-0.22609	-0.95358
H	1.05914	-0.31225	-3.74711
H	-0.07321	-1.55129	-4.34049
H	-0.68906	-0.04114	-3.63537
H	2.17055	-2.08404	-2.31025
H	1.21940	-2.98983	-1.11013
H	0.97773	-3.28664	-2.83671
H	-1.42662	-2.87966	-2.68855
H	-2.09459	-1.38798	-1.98329
H	-1.33685	-2.58220	-0.94095

N•_ap

N	0.37242	-0.54252	-1.28873
C	0.49379	-0.64371	0.14777
P	-1.04980	0.19299	0.74941
O	-2.27715	-0.62029	0.57555
O	-0.72016	0.61749	2.25847
C	-1.79315	1.16236	3.05557
C	-1.26846	1.33622	4.46417
O	-1.12495	1.63125	0.03627
C	-1.74869	1.77764	-1.25396
C	-2.36354	3.15994	-1.31911
C	1.85084	-0.01687	0.63611
C	2.11942	-0.41639	2.09343
C	1.86727	1.50894	0.48703
C	2.98473	-0.59863	-0.22177
C	0.06272	-1.75190	-2.05943
C	-0.02495	-1.30173	-3.52065
C	1.17964	-2.80225	-1.91861
C	-1.27387	-2.38348	-1.63517
H	0.42845	-1.67509	0.53365
H	-2.64078	0.47163	3.01833
H	-2.09534	2.12009	2.61816
H	-0.41120	2.01408	4.47313
H	-0.95721	0.37310	4.87618

H	-2.05028	1.75340	5.10452
H	-2.50827	0.99719	-1.37218
H	-0.97234	1.63779	-2.01212
H	-3.13738	3.27204	-0.55550
H	-2.81659	3.32050	-2.30147
H	-1.60006	3.92532	-1.15860
H	2.12974	-1.50727	2.20282
H	1.37685	-0.00521	2.77773
H	3.10611	-0.04454	2.39063
H	1.17454	1.99224	1.18031
H	1.59507	1.80086	-0.53183
H	2.87625	1.87944	0.69766
H	3.03436	-1.68879	-0.13403
H	3.94129	-0.19255	0.12326
H	2.86097	-0.33507	-1.27645
H	0.91431	-0.83306	-3.82958
H	-0.22872	-2.15208	-4.17896
H	-0.82878	-0.56891	-3.64076
H	2.13813	-2.40939	-2.26705
H	1.29167	-3.14284	-0.88485
H	0.92153	-3.67205	-2.53017
H	-1.47294	-3.24085	-2.28609
H	-2.09581	-1.66995	-1.72478
H	-1.25997	-2.72910	-0.59852

N•_bw

N	0.82796	-0.64915	-1.08265
C	0.49797	-0.35269	0.28499
P	-1.18425	0.41327	0.25107
O	-2.12257	-0.22077	-0.70947
O	-1.60133	0.29739	1.79607
C	-2.91479	0.74893	2.18060
C	-3.08367	0.45955	3.65633
O	-1.06084	2.00476	0.03534
C	-1.51724	2.59023	-1.20616
C	-0.47300	2.45987	-2.29758
C	1.65416	0.45070	0.96225
C	1.27346	0.86927	2.38645
C	2.06407	1.68656	0.15390
C	2.84966	-0.51301	1.02432
C	0.51797	-1.96543	-1.64598
C	-0.25954	-1.69345	-2.94494
C	1.88337	-2.58824	-1.99450
C	-0.27394	-2.93488	-0.76073
H	0.32075	-1.24802	0.90373
H	-3.65829	0.21953	1.57627
H	-2.98768	1.82259	1.97376
H	-2.99572	-0.61271	3.84641
H	-4.06859	0.79483	3.99228
H	-2.31904	0.98113	4.23728
H	-1.71687	3.63543	-0.96027
H	-2.45124	2.10249	-1.49662
H	0.44338	2.99166	-2.03107
H	-0.86275	2.88079	-3.22926
H	-0.22408	1.40720	-2.46676
H	0.91217	0.01864	2.97461
H	0.49171	1.63394	2.38601
H	2.15502	1.28370	2.88693
H	1.28191	2.44829	0.17178
H	2.27270	1.41828	-0.88508
H	2.97047	2.11726	0.59355
H	2.59598	-1.42734	1.57471
H	3.69326	-0.03476	1.53283
H	3.17261	-0.79235	0.01619
H	0.31073	-1.01270	-3.58406
H	-0.42012	-2.63202	-3.48567
H	-1.22703	-1.24186	-2.71059
H	2.46677	-1.90236	-2.61487
H	2.45358	-2.81146	-1.08685
H	1.73124	-3.52308	-2.54364
H	-0.46346	-3.85252	-1.32593
H	-1.23935	-2.50907	-0.47315
H	0.28468	-3.21870	0.13800

N•_bq

N	0.71848	-0.41188	-1.08996
C	0.77746	0.08370	0.25781
P	-0.86597	0.87368	0.64772
O	-0.92846	2.34164	0.85560
O	-1.88932	0.37176	-0.49486
C	-2.44792	1.32014	-1.42955
C	-1.41728	1.81691	-2.42476
O	-1.29638	-0.01938	1.91362
C	-2.53988	0.29885	2.56893
C	-2.68191	-0.62736	3.75708
C	1.98644	1.04618	0.45993
C	2.01239	1.53687	1.91316
C	1.94316	2.23451	-0.50676
C	3.25605	0.22718	0.18946
C	0.36473	-1.81861	-1.29901
C	-0.37511	-1.87935	-2.64032
C	1.70808	-2.56679	-1.41762
C	-0.49433	-2.49136	-0.21685
H	0.86420	-0.71228	1.01395
H	-2.88039	2.15149	-0.86578
H	-3.25001	0.76808	-1.92515
H	-0.64733	2.40406	-1.91736
H	-1.90512	2.45785	-3.16538
H	-0.93341	0.98174	-2.93615
H	-3.35703	0.15589	1.85239
H	-2.51645	1.34968	2.87376
H	-2.68527	-1.67015	3.43041
H	-3.61912	-0.42152	4.28110
H	-1.85282	-0.48209	4.45359
H	2.01310	0.69298	2.61371
H	1.15662	2.17959	2.13604
H	2.92525	2.11610	2.08779
H	1.09883	2.89238	-0.28509
H	1.86744	1.88310	-1.54021
H	2.86567	2.81697	-0.40720
H	3.32024	-0.63902	0.85954
H	4.14247	0.84798	0.35654
H	3.27737	-0.13066	-0.84467
H	0.20949	-1.37485	-3.41501
H	-0.54233	-2.91872	-2.94059
H	-1.34612	-1.38151	-2.55277
H	2.32571	-2.12496	-2.20449
H	2.26193	-2.52600	-0.47409
H	1.52017	-3.61716	-1.66229
H	-0.71262	-3.51599	-0.53398
H	-1.44349	-1.96705	-0.08259
H	0.01250	-2.55264	0.75036

N•_al

N	0.65343	-0.59841	-1.06339
C	0.65694	0.03114	0.22778
P	-0.96250	0.98029	0.38278
O	-0.81791	2.41947	0.70779
O	-1.79678	0.64031	-0.93960
C	-1.52397	1.41656	-2.12959
C	-2.40512	2.64871	-2.17268
O	-1.83989	0.13016	1.42602
C	-1.59047	0.32382	2.82892
C	-2.64158	-0.45369	3.59096
C	1.93329	0.90677	0.41865
C	1.95061	1.50357	1.83171
C	2.02560	2.01497	-0.63630
C	3.14719	-0.02179	0.26998
C	0.21260	-1.99202	-1.16190
C	-0.23375	-2.19471	-2.61305
C	1.45466	-2.86014	-0.87717
C	-0.92584	-2.40954	-0.21858
H	0.62882	-0.69203	1.06293
H	-1.72898	0.73880	-2.96110
H	-0.45996	1.67514	-2.16404
H	-3.45876	2.36209	-2.12589
H	-2.23238	3.19384	-3.10547
H	-2.17753	3.30481	-1.32952
H	-1.63212	1.39427	3.05309
H	-0.58224	-0.04197	3.06785
H	-3.63881	-0.08480	3.34102
H	-2.48342	-0.34030	4.66674
H	-2.58955	-1.51561	3.33804
H	1.88357	0.71216	2.58963
H	1.13398	2.21340	1.98121
H	2.89668	2.03092	1.99411
H	1.22097	2.74496	-0.51449
H	1.98246	1.58541	-1.64209
H	2.98085	2.54071	-0.53124
H	3.11832	-0.83500	1.00545
H	4.06982	0.54482	0.43358
H	3.18604	-0.46046	-0.73151
H	0.55456	-1.87017	-3.29779
H	-0.46360	-3.24757	-2.80513
H	-1.13267	-1.60301	-2.81186
H	2.27033	-2.60460	-1.55923
H	1.80333	-2.72315	0.15154
H	1.19807	-3.91524	-1.01509
H	-1.17819	-3.45570	-0.41833
H	-1.81834	-1.80118	-0.38210
H	-0.64796	-2.33600	0.83715

N•_bb

N	0.68115	-0.30090	-1.12434
C	1.02426	-0.01932	0.24313
P	-0.50768	0.65796	1.07814
O	-0.43456	2.01561	1.67281
O	-1.70161	0.50418	0.00534
C	-1.90408	1.56038	-0.95797
C	-3.29367	1.39131	-1.53412
O	-0.84072	-0.51440	2.12052
C	-1.67315	-0.21605	3.26269
C	-3.12079	0.00362	2.86554
C	2.24444	0.94888	0.32192

C	2.61450	1.19981	1.78935
C	1.96173	2.27203	-0.39939
C	3.42221	0.24627	-0.36779
C	0.29986	-1.66950	-1.47842
C	-0.51865	-1.55650	-2.76814
C	1.61285	-2.42686	-1.76085
C	-0.51299	-2.43744	-0.42444
H	1.27191	-0.91942	0.82979
H	-1.13027	1.46877	-1.72917
H	-1.79463	2.52427	-0.45087
H	-3.39847	0.41239	-2.00934
H	-3.48253	2.16384	-2.28445
H	-4.04649	1.47635	-0.74633
H	-1.26293	0.66177	3.77057
H	-1.56517	-1.08779	3.91051
H	-3.73606	0.10290	3.76448
H	-3.48856	-0.84081	2.27694
H	-3.22830	0.91505	2.27192
H	2.79024	0.25350	2.31580
H	1.83428	1.75714	2.31259
H	3.54080	1.78222	1.83756
H	1.17707	2.83979	0.10749
H	1.66237	2.08463	-1.43499
H	2.87107	2.88274	-0.41016
H	3.65243	-0.71105	0.11538
H	4.31607	0.87592	-0.30761
H	3.20423	0.05971	-1.42374
H	0.04465	-1.00307	-3.52464
H	-0.76678	-2.54769	-3.16086
H	-1.45144	-1.01882	-2.56867
H	2.19780	-1.91429	-2.52955
H	2.22180	-2.50946	-0.85481
H	1.37989	-3.43728	-2.11138
H	-0.74527	-3.43154	-0.81923
H	-1.45240	-1.92468	-0.20482
H	0.03170	-2.57439	0.51363

N•_av

N	0.78003	-0.36359	-1.09690
C	0.84272	0.03275	0.28380
P	-0.84759	0.67529	0.75527
O	-0.96033	2.09046	1.18744
O	-1.83290	0.32702	-0.47312
C	-1.94668	1.27512	-1.55612
C	-3.19105	0.92402	-2.34293
O	-1.29025	-0.41752	1.84079
C	-2.48746	-0.16679	2.61069
C	-2.14483	0.57097	3.88963
C	1.98040	1.07337	0.51807
C	2.03299	1.45497	2.00323
C	1.79642	2.31946	-0.35606
C	3.30141	0.38955	0.13956
C	0.54738	-1.77630	-1.40442
C	-0.02921	-1.80799	-2.82312
C	1.93141	-2.45580	-1.39165
C	-0.39618	-2.53000	-0.45382
H	1.01045	-0.80767	0.97742
H	-1.04214	1.19560	-2.17066
H	-2.00769	2.28326	-1.13506
H	-3.12978	-0.09692	-2.72913
H	-3.30237	1.60881	-3.18799
H	-4.07828	1.00241	-1.70977
H	-2.90911	-1.15425	2.81031
H	-3.20141	0.39763	2.00145
H	-1.41828	-0.00112	4.47247
H	-3.04607	0.70851	4.49437
H	-1.72236	1.55056	3.65442
H	2.13185	0.56257	2.63365
H	1.14161	2.00746	2.30954
H	2.90690	2.08907	2.18665
H	0.90024	2.87586	-0.06999
H	1.72552	2.03741	-1.41076
H	2.66182	2.98002	-0.23442
H	3.46976	-0.51208	0.74092
H	4.13735	1.07363	0.31914
H	3.30903	0.10922	-0.91818
H	0.62660	-1.26395	-3.50852
H	-0.13992	-2.83828	-3.17594
H	-1.01439	-1.33026	-2.83395
H	2.61498	-1.95498	-2.08282
H	2.36994	-2.43500	-0.38879
H	1.82428	-3.50107	-1.69828
H	-0.49614	-3.56101	-0.80742
H	-1.38749	-2.07120	-0.44165
H	-0.02102	-2.56934	0.57244

N•_as

N	0.94227	-0.56245	-1.01971
C	0.77815	-0.11840	0.33927
P	-0.92448	0.63733	0.47446
O	-1.01734	2.07286	0.84103
O	-1.68367	0.29987	-0.90706
C	-1.55928	1.23997	-1.99707
C	-2.67765	2.26140	-1.94521
O	-1.63236	-0.38303	1.48727
C	-2.94226	-0.03493	1.98952
C	-2.81843	0.72063	3.29749
C	1.91832	0.86207	0.75471
C	1.72301	1.29104	2.21489
C	1.97852	2.08637	-0.16614
C	3.24110	0.09142	0.64315
C	0.69924	-1.97715	-1.31409
C	0.43871	-2.05886	-2.82086
C	2.00202	-2.72863	-0.97440
C	-0.47127	-2.62661	-0.55819
H	0.76235	-0.94046	1.07382
H	-1.60466	0.63259	-2.90405
H	-0.57400	1.71809	-1.96027
H	-3.64898	1.75960	-1.96923
H	-2.61178	2.93105	-2.80795
H	-2.60072	2.85278	-1.03000
H	-3.46212	-0.98706	2.11570
H	-3.47715	0.55354	1.23573
H	-2.26863	0.12246	4.02872
H	-3.81253	0.93620	3.70014
H	-2.28893	1.66248	3.13641
H	1.64697	0.41664	2.87303
H	0.82850	1.90585	2.33875
H	2.58804	1.87786	2.54174
H	1.08552	2.70735	-0.05818
H	2.07984	1.77282	-1.20958
H	2.85082	2.69534	0.09511
H	3.24111	-0.79585	1.28763
H	4.07077	0.73352	0.95672
H	3.42462	-0.22653	-0.38764
H	1.25287	-1.57846	-3.37033
H	0.35461	-3.10108	-3.14482
H	-0.49525	-1.54387	-3.06616
H	2.84768	-2.30734	-1.52498
H	2.22046	-2.67643	0.09692
H	1.89289	-3.78197	-1.25108
H	-0.56223	-3.66739	-0.88455
H	-1.40992	-2.11212	-0.77612
H	-0.32476	-2.63271	0.52536

N•_ad

N	0.81610	0.17450	-0.60193
C	0.61074	0.09259	0.81498
P	-1.19728	0.37053	1.11538
O	-1.58061	0.38594	2.54297
O	-1.64429	1.68048	0.32716
C	-1.78343	1.80109	-1.10179
C	-2.59494	3.05065	-1.36956
O	-1.88751	-0.81452	0.25368
C	-2.39573	-1.96813	0.95162
C	-2.99131	-2.89813	-0.08312
C	1.53621	1.09718	1.57975
C	1.48361	0.80623	3.08451
C	1.14367	2.55348	1.30909
C	2.96825	0.85907	1.08052
C	1.03371	-1.03682	-1.39606
C	2.41094	-0.85805	-2.06193
C	1.00266	-2.37238	-0.64523
C	-0.04742	-1.03722	-2.49174
H	0.79120	-0.90651	1.24492
H	-2.28459	0.90570	-1.48319
H	-0.78291	1.86050	-1.53839
H	-3.58448	2.97238	-0.91337
H	-2.71348	3.19133	-2.44765
H	-2.08978	3.92713	-0.95649
H	-3.13651	-1.63959	1.68486
H	-1.57444	-2.45104	1.49617
H	-3.79665	-2.39650	-0.62550
H	-3.39929	-3.78752	0.40442
H	-2.23188	-3.21413	-0.80424
H	1.80820	-0.21996	3.29453
H	0.47807	0.93642	3.48952
H	2.16636	1.48524	3.60681
H	0.18833	2.80737	1.77801
H	1.06269	2.74004	0.23324
H	1.90994	3.21988	1.71928
H	3.25265	-0.19559	1.18807
H	3.67152	1.45751	1.66907
H	3.07016	1.14096	0.02825
H	3.21197	-0.88867	-1.31754
H	2.58013	-1.66208	-2.78548
H	2.45573	0.10284	-2.58167
H	1.79467	-2.43718	0.10831
H	0.03667	-2.53543	-0.15769
H	1.16001	-3.18691	-1.35864
H	0.13172	-1.86023	-3.19135
H	-0.02039	-0.09449	-3.04600
H	-1.03896	-1.15802	-2.04677

N•_aq

N	1.33176	-0.05788	-0.53710
C	0.53438	-0.46888	0.58841
P	-1.01944	0.56907	0.57115
O	-1.29257	1.42212	1.75369
O	-0.99375	1.39889	-0.81134
C	-0.33853	2.68631	-0.81979
C	-1.32625	3.78649	-0.48681
O	-2.12657	-0.54462	0.24746
C	-3.50755	-0.12828	0.19840
C	-4.34485	-1.35933	-0.07051
C	1.34005	-0.35238	1.91906
C	0.47449	-0.83094	3.09174
C	1.83347	1.07896	2.16039
C	2.55508	-1.28221	1.79470
C	1.25145	-0.84940	-1.76728
C	1.74064	0.06627	-2.89308
C	2.23133	-2.02750	-1.59650
C	-0.14009	-1.39601	-2.12442
H	0.16313	-1.50449	0.51234
H	0.06622	2.79393	-1.82888
H	0.50385	2.67440	-0.11903
H	-2.16264	3.76943	-1.19109
H	-0.83499	4.76171	-0.55529
H	-1.70853	3.65121	0.52742
H	-3.61827	0.61365	-0.60013
H	-3.76506	0.33888	1.15383
H	-4.05663	-1.81728	-1.02000
H	-5.40258	-1.08722	-0.12001
H	-4.20987	-2.09355	0.72723
H	0.09720	-1.84508	2.91134
H	-0.37264	-0.16392	3.26647
H	1.08033	-0.86025	4.00367
H	0.99768	1.76147	2.33551
H	2.41779	1.42964	1.30417
H	2.47840	1.09697	3.04568
H	2.24636	-2.31939	1.61684
H	3.13486	-1.25959	2.72330
H	3.20815	-0.96758	0.97506
H	2.72069	0.48109	-2.64216
H	1.81579	-0.48363	-3.83660
H	1.03869	0.89469	-3.02997
H	3.23821	-1.66461	-1.37232
H	1.91117	-2.69334	-0.78877
H	2.26522	-2.60615	-2.52495
H	-0.06762	-1.94194	-3.07037
H	-0.85843	-0.58216	-2.24855
H	-0.52952	-2.08788	-1.37268

N•_at

N	1.21997	-0.21093	-0.52037
C	0.54092	-0.35617	0.73924
P	-0.93520	0.79049	0.70465
O	-1.02125	1.84245	1.74616
O	-1.01945	1.38505	-0.79282
C	-0.26352	2.57352	-1.10798
C	-0.81801	3.14145	-2.39668
O	-2.13750	-0.27022	0.68645
C	-3.48949	0.23367	0.68070
C	-4.41857	-0.95437	0.80136
C	1.51055	-0.07614	1.92805
C	0.77203	-0.27343	3.25795
C	2.11093	1.33234	1.84550
C	2.64399	-1.10746	1.83795
C	0.93364	-1.17418	-1.58494
C	1.32406	-0.48018	-2.89342
C	1.86101	-2.38136	-1.33986
C	-0.52019	-1.66255	-1.68161
H	0.10044	-1.35579	0.89115
H	0.78930	2.28546	-1.21163
H	-0.36307	3.28251	-0.28028
H	-0.74062	2.41079	-3.20621
H	-0.25651	4.03543	-2.68123
H	-1.86926	3.41334	-2.27339
H	-3.65177	0.77571	-0.25724
H	-3.60769	0.92889	1.51754
H	-4.26663	-1.64407	-0.03271
H	-5.45847	-0.61699	0.79115
H	-4.23375	-1.48942	1.73581
H	0.31778	-1.27066	3.30907
H	-0.00714	0.47828	3.40225
H	1.48423	-0.19119	4.08590
H	1.34276	2.09880	1.97756
H	2.60721	1.47881	0.88143
H	2.85667	1.45736	2.63809
H	2.25493	-2.13176	1.88667
H	3.33593	-0.97142	2.67565
H	3.20644	-0.99255	0.90638
H	2.35545	-0.12125	-2.83641
H	1.23016	-1.16551	-3.74182
H	0.66785	0.37910	-3.06669
H	2.90636	-2.06356	-1.29535
H	1.60880	-2.88697	-0.40214
H	1.74594	-3.09861	-2.15865
H	-0.59815	-2.36002	-2.52158
H	-1.20123	-0.82716	-1.86123
H	-0.85037	-2.18935	-0.78223

P+

C	-1.88882	1.92313	-0.27160
C	0.93622	3.26584	0.66302
O	0.31742	3.34770	1.60654
C	1.72310	3.17392	-0.46623
C	1.13636	3.34161	-1.74954
C	1.94026	3.26303	-2.85797
C	3.32466	3.01792	-2.70541
C	3.90394	2.85142	-1.42535
C	3.11821	2.92867	-0.30757
O	4.15127	2.92991	-3.72938
H	-1.88554	3.00829	-0.40735
H	-2.05634	1.69006	0.78044
H	-2.69933	1.50097	-0.86518
H	-0.94711	1.47568	-0.60317
H	0.07177	3.52398	-1.84865
H	1.51416	3.38791	-3.84840
H	4.96973	2.66523	-1.35831
H	3.54729	2.80517	0.68114
H	3.71902	3.04931	-4.58795

N+_av

N	0.54623	0.48944	0.06108
C	0.81644	0.79562	-1.16979
P	-0.92889	-0.45506	0.45590
O	-2.03286	-0.15773	-0.46651
O	-0.25799	-1.87917	0.43935
C	-1.10153	-3.06569	0.60728
C	-0.21569	-4.27495	0.43028
O	-1.23190	-0.09695	1.96229
C	-2.57491	0.37356	2.34602
C	-2.77085	1.84139	2.04085
C	0.26488	0.39278	-2.51816
C	-0.85992	1.39071	-2.88514
C	-0.19543	-1.06840	-2.65558
C	1.45086	0.61097	-3.48661
C	1.51114	0.94654	1.19252
C	2.84074	1.42176	0.60034
C	0.86472	2.09534	1.96720
C	1.79119	-0.27276	2.07760
H	1.64986	1.48698	-1.26616
H	-1.89502	-3.02194	-0.14407
H	-1.54006	-3.02366	1.60896
H	0.22529	-4.28587	-0.56884
H	-0.81256	-5.18152	0.55480
H	0.58370	-4.28095	1.17417
H	-2.61721	0.16096	3.41403
H	-3.30741	-0.24263	1.82172
H	-2.64853	2.03521	0.97195
H	-2.08623	2.47065	2.61243
H	-3.79140	2.12090	2.31615
H	-0.51283	2.42723	-2.82283
H	-1.73147	1.25415	-2.24549
H	-1.14481	1.19876	-3.92366
H	0.54106	-1.75757	-2.23048
H	-0.27548	-1.28688	-3.72365
H	-1.16929	-1.24897	-2.20604
H	2.28646	-0.05951	-3.25960
H	1.81072	1.64463	-3.46166
H	1.12037	0.39883	-4.50560
H	3.52097	1.58136	1.43917
H	3.29845	0.67304	-0.05392
H	2.76502	2.37834	0.07563
H	1.61307	2.51615	2.64377
H	0.53763	2.89014	1.28928
H	0.02114	1.75695	2.56462
H	0.90146	-0.63615	2.59054
H	2.22959	-1.08705	1.49469
H	2.51128	0.03114	2.84117

N+_ad

N	0.91195	-0.31642	0.11334
C	1.46208	-0.14031	-1.04719
P	-0.74527	0.30769	0.43223
O	-0.91586	1.61320	-0.21928
O	-1.53313	-0.96986	-0.03371
C	-2.98166	-1.06167	0.17502
C	-3.73106	-0.26651	-0.87166
O	-0.90243	0.33798	2.00066
C	-1.10640	1.61146	2.70282
C	-2.57330	1.97353	2.69739
C	0.99682	0.37648	-2.38777
C	1.31205	1.89277	-2.41087
C	-0.45998	0.09679	-2.78670
C	1.91685	-0.33624	-3.40630
C	1.70136	-1.03157	1.24033

C	0.79984	-2.13623	1.80311
C	2.96646	-1.68914	0.68331
C	2.10492	0.00909	2.28789
H	2.50776	-0.43577	-1.07735
H	-3.19837	-0.72603	1.19401
H	-3.18564	-2.12974	0.10688
H	-3.49505	0.79943	-0.80951
H	-4.80555	-0.39136	-0.71462
H	-3.48722	-0.62450	-1.87450
H	-0.49492	2.37667	2.21945
H	-0.73285	1.41942	3.70953
H	-3.16980	1.17882	3.15221
H	-2.92042	2.15994	1.67722
H	-2.72383	2.88759	3.27750
H	2.36011	2.09191	-2.16433
H	0.66258	2.43734	-1.72526
H	1.13801	2.24975	-3.43013
H	-0.72677	-0.94991	-2.61273
H	-0.54606	0.28825	-3.85957
H	-1.16970	0.74459	-2.27678
H	1.74944	-1.41830	-3.41273
H	2.97532	-0.14380	-3.20351
H	1.69680	0.04176	-4.40698
H	1.37203	-2.68495	2.55500
H	-0.09566	-1.74973	2.28713
H	0.51064	-2.83686	1.01497
H	3.40373	-2.27171	1.49652
H	2.75177	-2.38275	-0.13563
H	3.72812	-0.96885	0.37157
H	1.24913	0.42073	2.81972
H	2.75160	-0.47613	3.02346
H	2.67185	0.82306	1.82594

N+_am

N	0.70174	0.31373	-0.14305
C	1.04184	0.29894	-1.39415
P	-1.02068	0.07991	0.32407
O	-1.90886	0.73596	-0.64361
O	-0.97731	-1.48585	0.45782
C	-2.22069	-2.21834	0.71822
C	-1.88518	-3.68978	0.70467
O	-1.14164	0.62935	1.79669
C	-1.91207	1.85182	2.06565
C	-1.96435	2.01851	3.56481
C	0.34182	-0.03792	-2.68999
C	-0.26070	1.28070	-3.23478
C	-0.70252	-1.16498	-2.64839
C	1.48607	-0.48359	-3.63016
C	1.77956	0.54980	0.94712
C	3.18435	0.46489	0.34519
C	1.58040	1.94378	1.54710
C	1.63361	-0.57016	1.98337
H	2.07663	0.58589	-1.56315
H	-2.93609	-1.95092	-0.06459
H	-2.60074	-1.89332	1.69096
H	-1.49025	-3.98648	-0.26943
H	-2.79107	-4.26821	0.90084
H	-1.14907	-3.92568	1.47593
H	-2.90040	1.72905	1.62039
H	-1.40659	2.68601	1.57083
H	-2.53618	2.91767	3.80624
H	-0.96186	2.12437	3.98703
H	-2.45353	1.16147	4.03238
H	0.49441	2.07058	-3.30345
H	-1.09150	1.61793	-2.61492
H	-0.62522	1.08236	-4.24691
H	-0.32037	-2.04106	-2.11576
H	-0.90018	-1.46372	-3.68115
H	-1.64703	-0.85017	-2.20967
H	1.96377	-1.40344	-3.27695
H	2.25053	0.29278	-3.73677
H	1.07344	-0.68111	-4.62180
H	3.88832	0.51172	1.17827
H	3.35993	-0.48098	-0.17661
H	3.42422	1.30421	-0.31389
H	2.43296	2.16392	2.19463
H	1.54949	2.70594	0.76233
H	0.68019	2.00844	2.15557
H	0.68110	-0.53782	2.51079
H	1.75271	-1.55047	1.51399
H	2.42720	-0.44583	2.72422

N+_ae

N	0.66901	-0.48332	-0.00459
C	0.36676	-1.71344	-0.28130
P	-0.58599	0.80465	-0.09258
O	-1.51408	0.53309	-1.19741
O	-1.03877	0.74526	1.41023
C	-2.00840	1.71350	1.93508
C	-3.42163	1.30229	1.58586
O	0.20632	2.16157	-0.23300
C	0.15797	2.91559	-1.49295
C	0.87879	4.21999	-1.25374
C	-0.91676	-2.46980	-0.52872
C	-1.17269	-2.44729	-2.05564
C	-2.15283	-2.01441	0.26257
C	-0.58493	-3.91974	-0.10470
C	2.12933	-0.11783	0.37406
C	2.77066	0.63009	-0.79696
C	2.07842	0.72002	1.65665
C	2.94337	-1.38200	0.66314
H	1.23295	-2.36810	-0.33553
H	-1.74777	2.70224	1.54538
H	-1.82823	1.70286	3.00961
H	-3.57909	1.29517	0.50416
H	-4.12161	2.01393	2.03127
H	-3.64219	0.30953	1.98466
H	-0.89067	3.05589	-1.75936
H	0.63737	2.31068	-2.26792
H	1.92187	4.05078	-0.97477
H	0.39185	4.79161	-0.46078
H	0.85965	4.81440	-2.17029
H	-0.30442	-2.81025	-2.61529
H	-1.43689	-1.44541	-2.39400
H	-2.00574	-3.12621	-2.25979
H	-1.91311	-1.85564	1.31855
H	-2.89145	-2.81846	0.20746
H	-2.60896	-1.11616	-0.14732
H	-0.37626	-3.98879	0.96806
H	0.27116	-4.31977	-0.65756
H	-1.44558	-4.55687	-0.31912
H	3.83641	0.74982	-0.58583
H	2.67441	0.05828	-1.72512
H	2.34843	1.62405	-0.93448
H	3.10743	0.92561	1.96128
H	1.57780	1.67732	1.51803
H	1.58612	0.16788	2.46166
H	2.47900	-2.01206	1.42819
H	3.15419	-1.97611	-0.23058
H	3.90891	-1.05436	1.05324

N+_be

N	0.45346	0.45837	0.54534
C	1.17807	0.48105	-0.52677
P	-1.17028	-0.31343	0.64482
O	-1.96098	0.19379	1.77154
O	-1.78567	-0.02759	-0.78100
C	-2.90407	0.90985	-0.93773
C	-2.46744	2.34086	-0.71488
O	-0.68513	-1.80672	0.65536
C	-1.67840	-2.88574	0.69383
C	-0.92994	-4.17797	0.91251
C	1.12813	-0.15709	-1.89955
C	0.46786	0.87278	-2.84587
C	0.47936	-1.53948	-2.04783
C	2.62010	-0.29254	-2.29040
C	0.96824	1.13702	1.84742
C	2.42999	1.55818	1.69611
C	0.11255	2.37314	2.13237
C	0.87698	0.08322	2.95790
H	2.05869	1.11194	-0.43184
H	-3.68955	0.61310	-0.24050
H	-3.23837	0.73280	-1.96036
H	-2.18390	2.50334	0.32781
H	-3.30198	3.00945	-0.94125
H	-1.63304	2.60895	-1.36911
H	-2.20903	-2.87517	-0.26307
H	-2.37756	-2.67181	1.50652
H	-0.38770	-4.15386	1.85985
H	-0.22324	-4.35926	0.09962
H	-1.64206	-5.00606	0.94160
H	0.90289	1.87189	-2.73618
H	-0.60785	0.92670	-2.67520
H	0.64373	0.54543	-3.87448
H	0.89888	-2.25208	-1.33387
H	0.70960	-1.89521	-3.05572
H	-0.60320	-1.52010	-1.94434
H	3.15162	-0.97275	-1.61721
H	3.13116	0.67548	-2.28889
H	2.68641	-0.70279	-3.30040
H	2.75437	1.92206	2.67297
H	3.08401	0.72232	1.42742
H	2.57169	2.38433	0.99306
H	0.53459	2.88428	3.00162
H	0.14699	3.06759	1.28645
H	-0.92112	2.11360	2.35802
H	-0.15164	-0.20156	3.17877
H	1.45965	-0.80583	2.69884
H	1.30275	0.51541	3.86667

N+_bf

N	0.82976	0.15365	-0.30021
C	1.21455	-0.54608	-1.32161
P	-0.90168	0.16258	0.18594

O	-1.75927	0.16679	-1.00623
O	-0.83866	-1.07395	1.15235
C	-2.02075	-1.43744	1.94125
C	-1.80781	-1.02450	3.37922
O	-1.08800	1.41749	1.12235
C	-1.95236	2.53195	0.71272
C	-3.39362	2.21911	1.04215
C	0.56462	-1.56327	-2.22970
C	-0.02255	-0.77864	-3.42932
C	-0.47758	-2.50320	-1.60368
C	1.74408	-2.42705	-2.73383
C	1.85997	1.00349	0.48730
C	3.28864	0.65128	0.06605
C	1.60470	2.48223	0.18548
C	1.70147	0.65596	1.97217
H	2.25156	-0.37141	-1.59704
H	-2.10839	-2.51804	1.82446
H	-2.90542	-0.96779	1.49848
H	-0.90731	-1.49355	3.78211
H	-2.66196	-1.34561	3.98088
H	-1.71263	0.06094	3.46289
H	-1.80686	2.71165	-0.35502
H	-1.57313	3.37944	1.28530
H	-3.50263	1.97787	2.10273
H	-3.75668	1.38751	0.43287
H	-4.01300	3.09327	0.82554
H	0.73016	-0.13819	-3.90062
H	-0.87845	-0.17727	-3.12268
H	-0.34700	-1.51131	-4.17397
H	-0.10979	-2.93933	-0.67022
H	-0.64232	-3.32092	-2.31016
H	-1.43608	-2.01909	-1.42996
H	2.21230	-2.98663	-1.91739
H	2.50873	-1.82149	-3.23103
H	1.36843	-3.14966	-3.46139
H	3.95845	1.19199	0.73756
H	3.50695	-0.41538	0.17748
H	3.53409	0.97780	-0.94850
H	2.40060	3.07047	0.64934
H	1.63341	2.66796	-0.89249
H	0.65652	2.83339	0.58839
H	0.73035	0.94122	2.37431
H	1.85958	-0.41343	2.13734
H	2.46509	1.20511	2.52825

N+_cc

N	0.97246	-0.07088	0.29272
C	1.34549	-0.44238	-0.88952
P	-0.72478	0.34320	0.72640
O	-0.81545	1.08728	1.98782
O	-1.22725	1.13922	-0.54229
C	-1.60508	2.55367	-0.42629
C	-3.03670	2.67260	0.04185
O	-1.31259	-1.10852	0.63648
C	-2.74760	-1.32586	0.85169
C	-3.04302	-1.48026	2.32674
C	0.67391	-0.73130	-2.21374
C	0.75281	0.59909	-3.00334
C	-0.74917	-1.30365	-2.23432
C	1.60569	-1.76135	-2.89480
C	2.01910	0.06230	1.43543
C	3.37865	-0.47912	0.99399
C	2.15905	1.54652	1.78574
C	1.51425	-0.78863	2.60707
H	2.42332	-0.55175	-0.98077
H	-1.46574	2.94539	-1.43468
H	-0.90907	3.04412	0.25790
H	-3.70958	2.13857	-0.63382
H	-3.32907	3.72578	0.05295
H	-3.14376	2.28136	1.05729
H	-2.96289	-2.23234	0.28520
H	-3.29488	-0.49200	0.39831
H	-2.80450	-0.56514	2.87385
H	-2.46558	-2.30709	2.74602
H	-4.10549	-1.69983	2.45976
H	1.77080	1.00094	-3.02995
H	0.08158	1.34700	-2.57925
H	0.44904	0.39542	-4.03412
H	-0.82240	-2.20336	-1.61914
H	-0.96487	-1.58399	-3.26882
H	-1.50681	-0.58897	-1.92153
H	1.62073	-2.70992	-2.34905
H	2.63132	-1.38930	-2.98329
H	1.23699	-1.96145	-3.90322
H	4.03208	-0.43236	1.86730
H	3.33491	-1.52648	0.67872
H	3.85322	0.12657	0.21623
H	2.94955	1.64631	2.53411
H	2.45962	2.12104	0.90341
H	1.24236	1.96153	2.20214
H	0.58707	-0.40646	3.03293
H	1.37782	-1.82937	2.29792

H	2.27407	-0.76574	3.39198

N+_ca

N	0.88925	-0.14573	0.18340
C	1.52491	-0.37171	-0.92335
P	-0.86469	0.28279	0.15848
O	-1.18401	1.07260	-1.03826
O	-1.43357	-1.16883	0.33930
C	-2.80156	-1.51188	-0.06049
C	-3.82786	-0.79916	0.79077
O	-1.10398	1.03081	1.52372
C	-1.29352	2.48792	1.54853
C	-2.73477	2.84867	1.27570
C	1.12484	-0.56854	-2.36681
C	1.18177	0.81506	-3.05801
C	-0.21656	-1.27531	-2.61878
C	2.24973	-1.45754	-2.94742
C	1.65588	-0.22589	1.53115
C	3.01226	-0.91095	1.33871
C	1.88559	1.19189	2.05809
C	0.82080	-1.08815	2.48427
H	2.59992	-0.46567	-0.79119
H	-2.83711	-2.59286	0.06993
H	-2.90560	-1.27193	-1.12202
H	-3.64774	-0.98266	1.85245
H	-4.82326	-1.17224	0.53709
H	-3.81899	0.27841	0.60640
H	-0.61597	2.94046	0.81962
H	-0.98726	2.77201	2.55625
H	-3.39794	2.35128	1.98747
H	-3.01554	2.58124	0.25433
H	-2.85802	3.92875	1.39135
H	2.15308	1.29851	-2.91131
H	0.38693	1.46712	-2.69579
H	1.05107	0.65353	-4.13199
H	-0.33428	-2.15094	-1.97215
H	-0.21438	-1.62776	-3.65346
H	-1.06751	-0.60837	-2.49855
H	2.26494	-2.44718	-2.47873
H	3.23513	-0.99567	-2.82855
H	2.07507	-1.59683	-4.01641
H	3.42928	-1.07333	2.33450
H	2.92056	-1.89055	0.85912
H	3.73590	-0.29715	0.79498
H	2.55374	1.13386	2.92119
H	2.36984	1.81566	1.30031

H	0.96380	1.66761	2.38616
H	-0.14391	-0.64424	2.72580
H	0.66313	-2.08639	2.06716
H	1.38052	-1.19111	3.41704

N+_ao

N	0.97211	0.16305	0.42825
C	1.44172	-0.08659	-0.75172
P	-0.77058	0.48702	0.77485
O	-0.99947	1.00759	2.12747
O	-1.04055	1.46909	-0.42432
C	-2.17350	2.40134	-0.34216
C	-3.49365	1.66587	-0.26364
O	-1.44955	-0.89037	0.43164
C	-2.02661	-1.75046	1.46982
C	-3.20896	-2.46472	0.85942
C	0.88473	-0.27417	-2.14405
C	1.03609	1.11444	-2.81581
C	-0.53149	-0.82683	-2.33696
C	1.87150	-1.25638	-2.81859
C	1.93397	0.25044	1.64540
C	3.35517	-0.15129	1.25154
C	1.94385	1.69863	2.14451
C	1.42373	-0.74468	2.69468
H	2.52656	-0.15185	-0.77337
H	-2.08263	2.98949	-1.25513
H	-2.00556	3.04290	0.52544
H	-3.60510	0.96678	-1.09632
H	-4.30992	2.39102	-0.30958
H	-3.58871	1.12114	0.68101
H	-2.30833	-1.12240	2.31807
H	-1.24163	-2.44594	1.77745
H	-2.90260	-3.05678	-0.00570
H	-3.97352	-1.74992	0.54687
H	-3.64639	-3.13726	1.60140
H	2.05572	1.50347	-2.72881
H	0.33994	1.83580	-2.38614
H	0.81619	0.99521	-3.88058
H	-0.66276	-1.77965	-1.81995
H	-0.66169	-1.00301	-3.40810
H	-1.31168	-0.14137	-2.01583
H	1.83673	-2.24482	-2.34995
H	2.90175	-0.88785	-2.78815
H	1.59212	-1.37383	-3.86797
H	3.94894	-0.13625	2.16756
H	3.41290	-1.16655	0.84626

H	3.82645	0.55455	0.56127
H	2.67840	1.77484	2.95041
H	2.25352	2.37630	1.34276
H	0.97642	2.01011	2.53508
H	0.44375	-0.47316	3.08682
H	1.39769	-1.75876	2.28208
H	2.12481	-0.74451	3.53289

N+_ay

N	0.65418	0.62541	0.02542
C	0.92246	-0.25018	-0.89001
P	-0.89410	0.65786	0.95279
O	-0.99144	1.83042	1.82692
O	-1.85971	0.55624	-0.28469
C	-3.31020	0.59002	-0.05443
C	-3.97926	0.49614	-1.40408
O	-0.94470	-0.74366	1.66708
C	-0.54867	-0.91834	3.06594
C	0.61544	-1.88113	3.12062
C	0.23859	-1.43541	-1.53012
C	-0.38422	-0.82986	-2.81667
C	-0.79928	-2.26501	-0.76885
C	1.39465	-2.37914	-1.93479
C	1.65792	1.77714	0.31701
C	2.94097	1.60664	-0.49599
C	0.98493	3.09339	-0.08631
C	2.01723	1.71729	1.80585
H	1.87012	-0.06639	-1.38918
H	-3.54131	1.52506	0.46101
H	-3.56448	-0.25810	0.58889
H	-3.67732	1.32904	-2.04295
H	-5.06301	0.53788	-1.27233
H	-3.73027	-0.44613	-1.89887
H	-1.43280	-1.31416	3.56682
H	-0.31194	0.06061	3.48985
H	1.47450	-1.49133	2.56634
H	0.33769	-2.85221	2.70461
H	0.91983	-2.02867	4.15981
H	0.35444	-0.28997	-3.41786
H	-1.20846	-0.15717	-2.57254
H	-0.76413	-1.65734	-3.42300
H	-0.39119	-2.66133	0.16242
H	-1.06204	-3.11041	-1.41050
H	-1.71333	-1.71913	-0.54719
H	1.89462	-2.79754	-1.05565
H	2.14026	-1.87362	-2.55654
H	0.98748	-3.20986	-2.51553
H	3.60735	2.41924	-0.20038
H	3.46252	0.66914	-0.27800
H	2.78349	1.70601	-1.57417
H	1.71253	3.89927	0.03989
H	0.69298	3.06578	-1.14087
H	0.11621	3.32152	0.52936
H	1.16171	1.91606	2.44989
H	2.46232	0.74873	2.05630
H	2.76726	2.48680	2.00478

N+_bz

N	0.60931	-0.14620	0.70259
C	1.38853	-0.55793	-0.24526
P	-1.08757	0.40609	0.44382
O	-1.60329	1.16866	1.58594
O	-0.99862	1.21754	-0.90760
C	-0.88169	2.67926	-0.88182
C	-1.33784	3.19358	-2.22626
O	-1.71317	-0.98774	0.09807
C	-3.16973	-1.11487	-0.05571
C	-3.80529	-1.42900	1.27905
C	1.27230	-0.81591	-1.73161
C	1.75972	0.48893	-2.40798
C	-0.06722	-1.27723	-2.31949
C	2.31420	-1.92687	-2.00364
C	1.12997	-0.08572	2.16663
C	2.50464	-0.74383	2.28469
C	1.24037	1.38625	2.57386
C	0.13797	-0.87698	3.02815
H	2.40389	-0.75062	0.09236
H	0.16962	2.91642	-0.68459
H	-1.49469	3.05500	-0.06054
H	-0.73106	2.78121	-3.03609
H	-1.24425	4.28204	-2.24556
H	-2.38371	2.93357	-2.40228
H	-3.28663	-1.92349	-0.77765
H	-3.55694	-0.19104	-0.49640
H	-3.66147	-0.60542	1.98223
H	-3.37825	-2.34238	1.69929
H	-4.87840	-1.58332	1.13975
H	2.73214	0.81383	-2.02382
H	1.03396	1.29312	-2.27798
H	1.87421	0.29073	-3.47754
H	-0.45245	-2.15069	-1.78880
H	0.12306	-1.56903	-3.35583
H	-0.82589	-0.49845	-2.32953
H	2.03769	-2.86383	-1.51023
H	3.31716	-1.63755	-1.67405
H	2.35911	-2.11575	-3.07845
H	2.76276	-0.74099	3.34545
H	2.50343	-1.78763	1.95475
H	3.29523	-0.18968	1.77005
H	1.66842	1.43060	3.57871
H	1.91806	1.91933	1.89869
H	0.27190	1.88406	2.59402
H	-0.84565	-0.41049	3.06806
H	0.04571	-1.90523	2.66513
H	0.53024	-0.91240	4.04734

N+_ar

N	0.90255	-0.13174	0.11361
C	1.35520	-0.47458	-1.05179
P	-0.86490	-0.19786	0.44181
O	-1.44905	-1.39508	-0.17728
O	-1.01679	-0.12879	2.00838
C	-1.60571	-1.25251	2.74919
C	-3.11270	-1.14516	2.73839
O	-1.21574	1.24406	-0.07916
C	-2.61988	1.66357	-0.10381
C	-2.66201	3.06066	-0.67342
C	0.73493	-0.83384	-2.38156
C	-0.56644	-0.11989	-2.77818
C	0.56046	-2.37327	-2.38137
C	1.81928	-0.45842	-3.41822
C	1.88677	0.30432	1.22904
C	3.29583	0.49909	0.66468
C	1.39662	1.65374	1.76603
C	1.92940	-0.79129	2.29739
H	2.44033	-0.52062	-1.09592
H	-1.19187	-1.14971	3.75320
H	-1.25913	-2.18537	2.29868
H	-3.43420	-0.18651	3.15268
H	-3.53696	-1.94302	3.35331
H	-3.50007	-1.25829	1.72231
H	-2.99687	1.62733	0.92287
H	-3.17069	0.94892	-0.72238
H	-2.26341	3.07473	-1.69015
H	-2.08369	3.74842	-0.05310
H	-3.69774	3.40708	-0.70370
H	-0.48681	0.96134	-2.63309
H	-1.43646	-0.49999	-2.24667
H	-0.72431	-0.30283	-3.84426
H	1.49629	-2.88625	-2.13646
H	0.27441	-2.67217	-3.39402
H	-0.22014	-2.67818	-1.68399
H	2.76634	-0.97073	-3.22044
H	1.99987	0.62128	-3.44014
H	1.48002	-0.76072	-4.41127
H	3.90442	0.91142	1.47186
H	3.77343	-0.43655	0.36004
H	3.32117	1.21718	-0.16084
H	2.11550	1.99992	2.51259
H	1.35364	2.39486	0.96304
H	0.42266	1.59077	2.24885
H	0.98952	-0.88529	2.83807
H	2.19141	-1.75594	1.85225
H	2.70535	-0.53391	3.02285

N+_bw

N	0.82590	-0.07159	0.66025
C	1.50494	-0.26852	-0.42373
P	-0.92571	0.34137	0.68534
O	-1.36166	0.87408	1.98074
O	-1.05931	1.34969	-0.52315
C	-1.48277	2.73645	-0.28786
C	-2.99075	2.81610	-0.23947
O	-1.47099	-1.05289	0.20950
C	-2.91244	-1.20916	-0.00943
C	-3.17605	-2.67455	-0.25696
C	1.21577	-0.31777	-1.90769
C	1.49930	1.11657	-2.42014
C	-0.14771	-0.82070	-2.39844
C	2.29943	-1.26474	-2.47476
C	1.52769	-0.15215	2.04623
C	2.95798	-0.67158	1.90240
C	1.56168	1.25639	2.64630
C	0.73116	-1.14901	2.89634
H	2.56788	-0.40548	-0.24113
H	-1.06545	3.28480	-1.13336
H	-1.02441	3.08603	0.63983
H	-3.42809	2.41815	-1.15852
H	-3.29682	3.86057	-0.13890
H	-3.37762	2.26545	0.62213
H	-3.18065	-0.59131	-0.87262
H	-3.43079	-0.84267	0.88097
H	-2.87527	-3.27114	0.60646
H	-2.63448	-3.02293	-1.13921

H	-4.24483	-2.82450	-0.42703
H	2.48503	1.47645	-2.10814
H	0.73514	1.81429	-2.07473
H	1.48632	1.09016	-3.51349
H	-0.38052	-1.80234	-1.98000
H	-0.07767	-0.92363	-3.48463
H	-0.96330	-0.13362	-2.18455
H	2.17027	-2.28716	-2.10624
H	3.30986	-0.92545	-2.22562
H	2.21623	-1.28845	-3.56352
H	3.35319	-0.78251	2.91400
H	3.00429	-1.65674	1.42742
H	3.62146	0.02627	1.38295
H	2.12072	1.21264	3.58462
H	2.08618	1.94569	1.97648
H	0.56468	1.63768	2.86251
H	-0.27659	-0.79880	3.11649
H	0.68479	-2.12559	2.40497
H	1.25430	-1.27374	3.84751

N+_ax

N	0.81705	0.22538	0.03186
C	1.42714	0.49732	-1.07913
P	-0.94030	-0.17305	0.02989
O	-1.65480	0.59548	-0.99769
O	-0.80169	-1.73369	-0.09324
C	-1.94527	-2.54604	-0.51903
C	-3.13700	-2.37557	0.39865
O	-1.40493	0.11673	1.50759
C	-2.33552	1.21714	1.78677
C	-2.80176	1.04665	3.21219
C	1.07287	0.40217	-2.54431
C	0.47768	1.76886	-2.96234
C	0.16376	-0.76468	-2.96162
C	2.43771	0.22062	-3.24883
C	1.60490	0.26836	1.36925
C	3.11148	0.33422	1.10311
C	1.18524	1.51164	2.15715
C	1.31042	-1.03788	2.11519
H	2.43929	0.86729	-0.93595
H	-1.55429	-3.56252	-0.49796
H	-2.17707	-2.26831	-1.55072
H	-2.86278	-2.57837	1.43644
H	-3.91781	-3.07979	0.10110
H	-3.55791	-1.36756	0.32647
H	-3.15354	1.15985	1.06636
H	-1.79946	2.15809	1.63237
H	-1.96185	1.08927	3.91008
H	-3.31472	0.09053	3.33759
H	-3.49876	1.85011	3.46193
H	1.14508	2.59607	-2.69973
H	-0.50055	1.92595	-2.50777
H	0.37018	1.76273	-4.05092
H	0.48494	-1.70514	-2.50272
H	0.25203	-0.87856	-4.04514
H	-0.88374	-0.57977	-2.73360
H	2.91206	-0.72682	-2.97217
H	3.12603	1.04032	-3.01921
H	2.28021	0.21227	-4.32945
H	3.60864	0.21651	2.06788
H	3.45747	-0.47839	0.45667
H	3.43928	1.29639	0.69934
H	1.85877	1.61932	3.01125
H	1.27729	2.41246	1.54241
H	0.17079	1.43490	2.54403
H	0.26418	-1.13774	2.40080
H	1.60363	-1.90256	1.51369
H	1.90563	-1.04018	3.03157

O•

C	-1.07820	2.82406	0.61784
C	0.08959	2.17599	-0.12557
O	0.02381	2.44700	-1.48383
C	0.07251	0.65198	-0.05634
C	-1.00405	-0.06630	-0.58159
C	-1.03083	-1.45490	-0.51223
C	0.03036	-2.13965	0.08374
C	1.11860	-1.43463	0.59861
C	1.13794	-0.04755	0.51460
O	0.06101	-3.49640	0.18714
H	-1.04827	3.90968	0.49254
H	-1.01445	2.59022	1.68426
H	-2.02959	2.45408	0.22791
H	1.04642	2.52158	0.29610
H	-1.82290	0.46366	-1.05880
H	-1.87227	-2.00695	-0.92373
H	1.93538	-1.98704	1.05013
H	1.99172	0.49956	0.90462
H	-0.72839	-3.87940	-0.21184

e•

C	-0.04005	1.31107	0.05869
C	1.36190	1.32539	0.12239
C	2.08870	0.15734	0.06527
C	1.40512	-1.12217	-0.06337
C	-0.03748	-1.10842	-0.12671
C	-0.77775	0.08918	-0.06793
C	-2.18666	0.07091	-0.13222
C	-3.03905	1.29633	-0.07639
O	2.04228	-2.19628	-0.11730
H	-0.58021	2.25083	0.10663
H	1.87304	2.27844	0.21828
H	3.17183	0.14009	0.11231
H	-0.53421	-2.06922	-0.22254
H	-2.66967	-0.89643	-0.22805
H	-2.88750	1.85225	0.85816
H	-4.09759	1.04200	-0.14341
H	-2.80868	1.98711	-0.89806

T

C	0.44874	1.02097	-0.18946
C	1.82265	0.94864	-0.21534
C	2.49269	-0.26955	-0.02338
C	1.84683	-1.55051	0.21690
C	0.41723	-1.44106	0.23755
C	-0.27394	-0.20435	0.04288
C	-1.64792	-0.23018	0.08621
C	-2.60039	0.89141	-0.08134
O	2.47866	-2.60936	0.38278
H	-0.06873	1.95973	-0.33714
H	2.40798	1.84734	-0.38728
H	3.57975	-0.28880	-0.05086
H	-0.15920	-2.34643	0.41014
H	-2.10582	-1.20375	0.26774
H	-3.23134	0.96049	0.81307
H	-3.28019	0.66131	-0.91065
H	-2.12690	1.85410	-0.26183

S_ab

C	3.25260	-0.61438	-0.80605
C	2.93614	0.70565	-0.72884
C	1.58729	0.76363	-0.25493
C	1.18716	-0.53037	-0.08043
C	-0.04360	-1.16658	0.37051
C	-1.12853	-0.51013	0.71916
C	-2.20652	0.14382	1.06310
C	-3.31968	0.51888	0.11672
O	2.20063	-1.37423	-0.41551
H	4.13897	-1.15124	-1.10417
H	3.58193	1.53436	-0.97767
H	0.98724	1.64112	-0.06517
H	-0.03132	-2.25398	0.41127
H	-2.31693	0.43983	2.10706
H	-3.46034	1.60401	0.10207
H	-4.26343	0.06932	0.44053
H	-3.10079	0.18039	-0.89727

S_ad

C	2.77913	-0.00164	0.34216
C	3.03866	-1.32246	0.15645
C	1.76189	-1.96064	0.04122
C	0.82676	-0.97248	0.16677
C	-0.62707	-1.00694	0.13534
C	-1.40646	0.04344	0.27692
C	-2.18310	1.08477	0.41322
C	-2.66368	1.94865	-0.72562
O	1.44182	0.22313	0.35017
H	3.40365	0.86681	0.47901
H	4.01336	-1.78411	0.10791
H	1.55872	-3.01003	-0.11357
H	-1.06999	-1.98895	-0.01691
H	-2.50498	1.35737	1.41876
H	-2.33287	2.98222	-0.58500
H	-3.75728	1.95482	-0.76706
H	-2.27868	1.58584	-1.67997

R

C	0.47176	-1.74520	-0.23913
C	1.96777	-1.93407	-0.32318
C	2.65949	-0.83480	-0.00043
C	1.73116	0.27331	0.35299
C	0.34399	-0.30126	0.20296
C	-0.74701	0.38718	0.43631
C	-1.80558	1.11246	0.67793
C	-2.51392	1.95814	-0.34920
O	2.02661	1.39860	0.68922
H	-0.00719	-1.92609	-1.20784
H	2.40626	-2.88171	-0.61908
H	3.73565	-0.71592	0.01648
H	0.02319	-2.43918	0.48048
H	-2.19779	1.11466	1.69468
H	-2.51232	3.00675	-0.03786
H	-3.55669	1.64341	-0.45250
H	-2.02539	1.88372	-1.32185

e+

C	-1.37124	3.05811	-0.14058
C	-0.23223	2.13831	-0.20200
C	-0.23050	0.75211	-0.07786
C	-1.42594	0.00157	0.14050
C	-1.34127	-1.36876	0.25265
C	-0.09819	-2.01151	0.15314
C	1.09174	-1.29451	-0.06154
C	1.02520	0.08536	-0.17679
O	2.30065	-1.86628	-0.16310
H	-1.17295	3.79912	0.64723
H	-2.33927	2.59160	0.02337
H	-1.38966	3.64541	-1.06999
H	0.73942	2.60737	-0.36695
H	-2.38584	0.49754	0.21737
H	-2.23220	-1.96354	0.41857
H	-0.05530	-3.09470	0.24484
H	1.94059	0.64595	-0.34272
H	2.27146	-2.82764	-0.07321

e•

C	-1.39357	3.04408	-0.08867
C	-0.15402	2.21328	-0.12059
C	-0.15677	0.79284	-0.05951
C	-1.36183	0.04972	0.03796
C	-1.32601	-1.33428	0.09538
C	-0.11326	-2.02679	0.05907
C	1.08113	-1.30407	-0.03698
C	1.06546	0.08101	-0.09554
O	2.29996	-1.91838	-0.07695
H	-1.15707	4.10766	-0.14657
H	-1.96825	2.87779	0.83232
H	-2.06341	2.80331	-0.92503
H	0.80731	2.71198	-0.19436
H	-2.31503	0.56662	0.06766
H	-2.25309	-1.89443	0.16989
H	-0.09444	-3.11257	0.10464
H	2.00973	0.61189	-0.16973
H	2.18763	-2.87414	-0.03005

O• •

C	-0.99155	2.66453	0.48852
C	-0.50345	1.91415	-0.78032
C	-0.37457	0.42666	-0.50329
C	-1.47352	-0.41190	-0.70700
C	-1.37150	-1.76679	-0.40540
C	-0.18134	-2.29273	0.09282
C	0.91271	-1.44843	0.28758
C	0.81908	-0.08882	-0.00978
O	0.68193	2.52504	-1.10203
O	2.10666	-1.89831	0.76641
H	-1.94956	2.23663	0.79191
H	-1.11035	3.72857	0.27708
H	-0.26734	2.52543	1.29412
H	-1.24950	2.09097	-1.57269
H	-2.40091	-0.00724	-1.10416
H	-2.22031	-2.42468	-0.56364
H	-0.10095	-3.35223	0.32293
H	1.68304	0.55217	0.13288
H	2.06293	-2.84750	0.92731

Q

O	0.56173	2.97942	-0.79229
C	-0.21314	2.19509	-0.27824
C	-1.32746	2.68895	0.62112
C	-0.08482	0.72619	-0.52123
C	0.94764	0.27160	-1.35443
C	-0.95231	-0.20902	0.04876
C	-0.79810	-1.56877	-0.20318
C	0.23543	-2.00249	-1.03507
C	1.11221	-1.07824	-1.61331
O	0.44118	-3.31352	-1.32166
H	-1.26729	3.77488	0.68252
H	-1.23450	2.25943	1.62338
H	-2.30408	2.39795	0.22215
H	1.61556	1.00677	-1.79180
H	-1.76061	0.11329	0.69776
H	-1.47716	-2.29020	0.24405
H	1.90613	-1.44349	-2.25554
H	-0.21391	-3.86255	-0.87564

3a•_ae, SMD Methanol

N	0.38718	-1.08463	0.16233
O	0.77997	0.20045	-0.33460
C	2.19159	0.45712	-0.22362
C	2.39800	1.77751	0.51671
C	2.82991	0.57254	-1.58749
C	2.18730	1.31007	-2.61414
C	2.77968	1.46419	-3.83838
C	4.08179	0.88413	-4.10730
C	4.72242	0.14788	-3.03525
C	4.10471	0.00738	-1.81872
O	4.63507	1.01428	-5.23012
C	-0.63351	-0.86431	1.20939
P	-1.46803	0.78775	1.11165
O	-0.81659	1.93120	1.82622
O	-1.85183	1.15435	-0.40030
C	-1.26917	2.27981	-1.09492
C	-2.17633	3.48575	-0.98491
O	-2.91184	0.37489	1.68422
C	-3.94146	1.39181	1.78804
C	-5.14126	0.95670	0.97803
C	-0.09489	-1.18232	2.65005
C	0.30577	-2.66245	2.69641
C	-1.19156	-0.96431	3.70329
C	1.12946	-0.34670	3.02945
C	-0.02563	-1.95765	-0.98972
C	1.17488	-2.08661	-1.93017
C	-0.34025	-3.35797	-0.45258
C	-1.22661	-1.42888	-1.77845
H	2.64864	-0.37445	0.31973
H	1.92515	2.59665	-0.03483
H	3.46810	1.99148	0.59865
H	1.96765	1.73053	1.51764
H	1.21029	1.74335	-2.41885
H	2.30112	2.02088	-4.63884
H	5.69645	-0.28877	-3.23566
H	4.58427	-0.55294	-1.01989
H	-1.46364	-1.55911	1.03869
H	-1.16268	1.95291	-2.13278
H	-0.27669	2.48665	-0.68768
H	-3.18025	3.25022	-1.35126
H	-1.77028	4.30323	-1.58906
H	-2.24664	3.82604	0.05262
H	-3.55290	2.35303	1.43592
H	-4.17938	1.48492	2.85074
H	-5.51466	-0.00878	1.33162
H	-4.87906	0.86863	-0.08053
H	-5.94146	1.69606	1.07958
H	1.10964	-2.88051	1.98830
H	-0.54413	-3.31679	2.47430
H	0.66546	-2.90407	3.70253
H	-1.45284	0.09189	3.82402
H	-0.82623	-1.32551	4.67047
H	-2.10316	-1.51912	3.45602
H	1.48544	-0.66673	4.01527
H	0.89396	0.71824	3.08597
H	1.94834	-0.49678	2.32020
H	1.32593	-1.18081	-2.52044
H	2.09086	-2.30737	-1.37046
H	0.99424	-2.90795	-2.63025
H	0.52636	-3.79265	0.05275
H	-1.19303	-3.37701	0.23052
H	-0.59271	-3.99631	-1.30447
H	-1.02858	-0.42900	-2.17404
H	-1.41659	-2.09995	-2.62274
H	-2.13597	-1.39198	-1.16900

3a•_ac, SMD Methanol

N	0.32615	-0.81993	-0.78040
O	0.02908	-0.62084	0.60702
C	-0.77129	-1.66820	1.18454
C	-1.99900	-1.04631	1.84801
C	0.00708	-2.42411	2.23540
C	0.79543	-1.71935	3.18047
C	1.46806	-2.38944	4.16642
C	1.38034	-3.83374	4.27026
C	0.55549	-4.52704	3.30063
C	-0.10583	-3.83046	2.32162
O	1.99733	-4.46227	5.16921
C	-0.16832	0.36413	-1.51531
P	-0.41202	1.86340	-0.45304
O	-1.73747	2.01593	0.22675
O	0.81711	2.06258	0.55537
C	0.66339	1.97336	1.98973
C	0.47613	3.35337	2.58107
O	-0.07862	2.99919	-1.54129
C	-0.27383	4.39162	-1.18415
C	-1.58878	4.89513	-1.73802
C	-1.42882	0.03915	-2.39422
C	-1.03074	-1.01608	-3.43401
C	-1.90377	1.28604	-3.15521
C	-2.59793	-0.51400	-1.57653
C	1.78893	-1.12915	-0.93714
C	2.08748	-2.39599	-0.13233
C	2.06492	-1.44622	-2.41103
C	2.71968	-0.00644	-0.47103
H	-1.06197	-2.35540	0.38525
H	-1.69124	-0.35129	2.63598
H	-2.61012	-1.83190	2.30310
H	-2.60196	-0.50677	1.11685
H	0.86680	-0.63771	3.10466
H	2.08132	-1.86855	4.89602
H	0.48929	-5.60842	3.37678
H	-0.71618	-4.35532	1.59089
H	0.61050	0.69253	-2.21297
H	1.58446	1.50636	2.34904
H	-0.17832	1.31870	2.22667
H	1.30450	4.01091	2.30077
H	0.44630	3.28013	3.67282
H	-0.46327	3.79857	2.23936
H	0.57425	4.92370	-1.62019
H	-0.22588	4.50305	-0.09549
H	-1.69082	5.96237	-1.51792
H	-2.43251	4.36571	-1.28641
H	-1.62473	4.76092	-2.82323
H	-0.22229	-0.65857	-4.08092
H	-1.89711	-1.23929	-4.06616
H	-0.71148	-1.94645	-2.95713
H	-2.33491	2.04103	-2.49037
H	-2.68404	0.98828	-3.86376
H	-1.08882	1.74901	-3.72217
H	-2.31561	-1.42749	-1.04542
H	-3.41813	-0.76895	-2.25720
H	-2.97140	0.21863	-0.85762
H	2.12176	-2.19537	0.94018
H	1.33913	-3.17214	-0.32847
H	3.06813	-2.78307	-0.42536
H	1.46628	-2.29488	-2.75278
H	1.88618	-0.59801	-3.07664
H	3.12115	-1.71539	-2.50529
H	2.55071	0.23361	0.58214
H	2.59266	0.90571	-1.06362
H	3.75708	-0.33849	-0.58421

3a•_as, SMD Methanol

N	0.83504	-0.11822	-0.77320
O	0.35986	-0.71907	0.43773
C	0.50466	-2.15006	0.46889
C	-0.84987	-2.77770	0.79401
C	1.48938	-2.57286	1.53314
C	1.46015	-1.96375	2.81345
C	2.31061	-2.37773	3.80284
C	3.25278	-3.45470	3.56441
C	3.25172	-4.06838	2.25105
C	2.38985	-3.63201	1.27744
O	4.04257	-3.84209	4.46440
C	-0.28844	0.64061	-1.36347
P	-1.62949	1.05711	-0.15617
O	-2.71529	0.04654	0.04603
O	-1.01085	1.58172	1.22533
C	-1.20582	0.87535	2.47110
C	-2.38699	1.45675	3.21707
O	-2.12784	2.44378	-0.80178
C	-3.33181	3.05630	-0.27989
C	-3.57537	4.32432	-1.06422
C	-0.84693	-0.03090	-2.66917
C	0.28128	-0.07354	-3.70773
C	-1.99516	0.79799	-3.26523
C	-1.33770	-1.46222	-2.43984
C	2.08168	0.66987	-0.48259
C	3.12326	-0.29657	0.08547
C	2.63270	1.21276	-1.80566
C	1.87768	1.82581	0.50066
H	0.86592	-2.47835	-0.50966
H	-1.20230	-2.42813	1.76982
H	-0.75129	-3.86687	0.83499
H	-1.58907	-2.51630	0.03613
H	0.75964	-1.15327	2.99533
H	2.30764	-1.92008	4.78788
H	3.95750	-4.87386	2.07045
H	2.39729	-4.08957	0.29123
H	0.07701	1.62994	-1.66340
H	-0.27475	1.01067	3.02807
H	-1.34365	-0.18933	2.26859
H	-2.24514	2.52724	3.39300
H	-2.48867	0.95725	4.18571
H	-3.31315	1.30860	2.65297
H	-3.18505	3.26626	0.78540
H	-4.16105	2.35103	-0.39386
H	-4.48377	4.81128	-0.69826
H	-3.70544	4.09930	-2.12688
H	-2.73770	5.01785	-0.94815
H	0.64594	0.93111	-3.94750
H	-0.09914	-0.52506	-4.63048

H	1.12310	-0.67680	-3.35777
H	-2.89534	0.77713	-2.64224
H	-2.26093	0.37717	-4.24081
H	-1.70322	1.84322	-3.41424
H	-1.65315	-1.88724	-3.39946
H	-2.19159	-1.49421	-1.75950
H	-0.53995	-2.09808	-2.04528
H	2.90644	-0.56218	1.12179
H	3.17927	-1.21142	-0.51527
H	4.10548	0.18545	0.06879
H	2.85845	0.40184	-2.50344
H	1.95970	1.92133	-2.29492
H	3.56380	1.74516	-1.58989
H	1.48903	1.46727	1.45762
H	1.19294	2.58418	0.10678
H	2.84375	2.30838	0.68245

NO-RAD-AddTS-SG1-PROD, SMD Methanol

N	0.52782	-0.49564	-0.53928
O	0.16877	-0.45323	0.72398
C	-0.97420	-1.61950	1.35132
C	-1.93961	-0.68082	2.01845
C	-0.21618	-2.54642	2.14466
C	0.33756	-2.18838	3.40727
C	1.09070	-3.07423	4.12864
C	1.34029	-4.41800	3.64839
C	0.76970	-4.76511	2.36593
C	0.04157	-3.85444	1.64901
O	2.02817	-5.24240	4.31728
C	-0.14769	0.46866	-1.42054
P	-0.40692	2.08482	-0.53928
O	-1.75659	2.35184	0.04286
O	0.77185	2.27214	0.52196
C	0.54917	2.21389	1.95326
C	0.64647	3.60734	2.53089
O	0.04195	3.08194	-1.70823
C	-0.12457	4.51369	-1.51131
C	-1.39419	4.98656	-2.18289
C	-1.40013	-0.02999	-2.22684
C	-1.01285	-1.30503	-2.98281
C	-1.74855	1.06113	-3.25309
C	-2.65684	-0.31931	-1.39824
C	1.97185	-0.86321	-0.76936
C	2.30113	-2.07061	0.10339
C	2.20666	-1.24884	-2.23098
C	2.86739	0.32184	-0.38769
H	-1.32732	-2.05886	0.42041
H	-1.48879	-0.18449	2.88107
H	-2.79609	-1.26435	2.37410
H	-2.29757	0.07853	1.32183
H	0.17981	-1.18529	3.79569
H	1.52238	-2.79498	5.08601
H	0.94272	-5.77004	1.99066
H	-0.36863	-4.13021	0.67921
H	0.59206	0.72882	-2.18397
H	1.32553	1.55240	2.34680
H	-0.42739	1.76748	2.15149
H	1.61145	4.06159	2.28750
H	0.55129	3.55759	3.62003
H	-0.15479	4.24359	2.14252
H	0.76173	4.96740	-1.95852
H	-0.12331	4.73678	-0.43899
H	-1.47417	6.07334	-2.08243
H	-2.27483	4.52973	-1.72274
H	-1.37907	4.73784	-3.24809
H	-0.19789	-1.12201	-3.68995
H	-1.88015	-1.66142	-3.54847
H	-0.70822	-2.10088	-2.29391
H	-2.16499	1.95557	-2.77712
H	-2.50678	0.67097	-3.93960
H	-0.87332	1.35738	-3.84186
H	-2.53703	-1.18825	-0.74957
H	-3.47124	-0.55263	-2.09323
H	-2.96331	0.53761	-0.79647
H	2.18550	-1.85415	1.16794
H	1.66815	-2.92179	-0.16086
H	3.34264	-2.34816	-0.08132
H	1.60223	-2.11253	-2.51681
H	2.02065	-0.43189	-2.93292
H	3.26033	-1.52486	-2.32972
H	2.72022	0.59973	0.65936
H	2.67100	1.19464	-1.01852
H	3.91074	0.02365	-0.52956

3•_at, SMD Methanol

N	-0.07524	0.76086	0.97935
O	0.06691	1.90878	0.43866
C	-1.04335	-0.15065	0.36502
P	-0.29723	-0.85391	-1.16519
O	-1.20780	-1.74098	-1.94846
O	0.24309	0.33570	-2.08509
C	1.55502	0.95698	-2.01420
C	2.07599	1.12025	-3.42335
O	0.98965	-1.58854	-0.55964
C	1.52815	-2.78840	-1.17969
C	2.20574	-2.48410	-2.49729
C	-2.47243	0.46143	0.20260
C	-2.79148	1.28303	1.45811
C	-3.47366	-0.70128	0.12350
C	-2.62500	1.33939	-1.04593
C	0.76220	0.47698	2.19168
C	2.23170	0.54873	1.76448
C	0.45262	1.56344	3.22605
C	0.44865	-0.89712	2.77495
H	-1.13856	-1.01692	1.02315
H	2.21555	0.33140	-1.40799
H	1.42432	1.92115	-1.51978
H	1.39269	1.73446	-4.01684
H	3.04897	1.62023	-3.39049
H	2.19811	0.15102	-3.91441
H	0.71350	-3.50776	-1.30004
H	2.23553	-3.17479	-0.44417
H	2.64347	-3.40493	-2.89480
H	1.48970	-2.10378	-3.23307
H	3.00559	-1.74971	-2.36388
H	-2.17124	2.18143	1.52654
H	-2.64192	0.68638	2.36598
H	-3.84095	1.59422	1.42654
H	-4.48840	-0.29941	0.03268
H	-3.43158	-1.31586	1.03019
H	-3.28410	-1.34444	-0.73975
H	-1.91127	2.16678	-1.05076
H	-3.63751	1.75747	-1.06485
H	-2.49328	0.75873	-1.96625
H	2.46495	-0.24163	1.04470
H	2.45796	1.51988	1.31505
H	2.86886	0.41849	2.64441
H	1.07885	1.40444	4.10886
H	-0.59682	1.52055	3.53364
H	0.66462	2.55812	2.82570
H	-0.59008	-0.96874	3.11353
H	0.65545	-1.70273	2.06423
H	1.09348	-1.04419	3.64604

3•_ce, SMD Methanol

N	0.36502	0.99848	1.09469
O	-0.37584	1.91685	0.59806
C	0.22727	-0.32393	0.47491
P	0.43399	-0.02751	-1.33339
O	1.48889	0.98429	-1.64858
O	0.75593	-1.49841	-1.86680
C	0.99193	-1.69254	-3.28806
C	1.04363	-3.18029	-3.53999
O	-0.98375	0.31336	-1.99296
C	-1.25936	1.62672	-2.55402
C	-2.70943	1.96133	-2.29774
C	-1.03876	-1.09728	0.97599
C	-0.77884	-1.50302	2.43284
C	-1.24106	-2.37352	0.14860
C	-2.32006	-0.25886	0.92406
C	1.45100	1.44421	2.02823
C	2.32098	2.46512	1.28779
C	0.76518	2.09990	3.22978
C	2.30928	0.26779	2.48040
H	1.10192	-0.92788	0.73595
H	1.93565	-1.20446	-3.54767
H	0.17648	-1.22076	-3.84607
H	0.09472	-3.65083	-3.26702
H	1.23053	-3.36229	-4.60215
H	1.84912	-3.64143	-2.96148
H	-1.04018	1.56863	-3.62386
H	-0.59377	2.36128	-2.09485
H	-2.95211	2.90368	-2.79809
H	-3.36585	1.18097	-2.69405
H	-2.89957	2.07930	-1.22726
H	-0.60661	-0.62796	3.06846
H	0.08826	-2.16833	2.51230
H	-1.65302	-2.03408	2.82432
H	-2.02575	-2.97448	0.61992
H	-0.32835	-2.97722	0.10555
H	-1.55886	-2.15329	-0.87544
H	-2.26001	0.61492	1.57955
H	-3.15361	-0.88173	1.26736
H	-2.54401	0.08044	-0.09004
H	2.81925	2.00253	0.43119
H	1.72074	3.30840	0.93642
H	3.08545	2.84286	1.97344
H	1.52748	2.48625	3.91254
H	0.14828	1.37663	3.77236
H	0.13352	2.93244	2.90882
H	1.71963	-0.50853	2.97515
H	2.86600	-0.17380	1.64812
H	3.03865	0.64577	3.20253

3•_ab, SMD Methanol

N	0.49972	0.16858	1.39275
O	0.97913	1.35258	1.36707
C	-0.63681	-0.10920	0.50368
P	0.09444	-0.20559	-1.18217
O	1.07547	-1.33016	-1.29666
O	-1.16609	-0.28993	-2.15102
C	-0.95031	-0.45491	-3.58364
C	-1.17495	-1.89789	-3.97261
O	0.73643	1.21173	-1.55670
C	2.16943	1.43738	-1.48009
C	2.78489	1.28561	-2.85243
C	-1.86652	0.82377	0.75322
C	-2.00710	1.02867	2.26791
C	-3.12589	0.09842	0.25535
C	-1.76116	2.18627	0.05841
C	1.17461	-0.81578	2.30182
C	0.50909	-2.18530	2.22172
C	2.63996	-0.91611	1.86619
C	1.07756	-0.26649	3.72816
H	-0.96226	-1.13300	0.70135
H	0.05854	-0.11601	-3.84200
H	-1.67204	0.21177	-4.05887
H	-2.18334	-2.21738	-3.69482
H	-1.06424	-2.00225	-5.05621
H	-0.44698	-2.55127	-3.48367
H	2.61095	0.74240	-0.76060
H	2.27703	2.45374	-1.09580
H	3.85144	1.52606	-2.80242
H	2.67827	0.25873	-3.21493
H	2.30935	1.96612	-3.56502
H	-1.18533	1.62356	2.67736
H	-2.03650	0.06709	2.79423
H	-2.94478	1.55573	2.47287
H	-4.00363	0.72146	0.45745
H	-3.26030	-0.85561	0.77806
H	-3.08916	-0.09732	-0.81868
H	-0.86091	2.72699	0.36155
H	-2.63372	2.79008	0.33132
H	-1.75660	2.08394	-1.03194
H	-0.53695	-2.15076	2.54316
H	0.56603	-2.60827	1.21377
H	1.04379	-2.85738	2.89877
H	3.16570	-1.60423	2.53486
H	3.13079	0.05941	1.91954
H	2.71461	-1.29909	0.84382
H	1.52220	0.73013	3.79403
H	0.03542	-0.21333	4.05718
H	1.62061	-0.93308	4.40471

3•_cu, SMD Methanol

N	0.47617	0.81244	0.84515
O	1.42727	1.43177	0.26227
C	-0.72677	0.54779	0.05620
P	-0.36761	-0.83561	-1.12543
O	-1.11596	-0.83931	-2.41899
O	1.21937	-0.94387	-1.31634
C	1.88456	-0.24524	-2.40111
C	3.37145	-0.38741	-2.18028
O	-0.65020	-2.08245	-0.16645
C	-0.44402	-3.43367	-0.66679
C	-1.78025	-4.07514	-0.96312
C	-1.38134	1.83799	-0.53088
C	-1.39869	2.89641	0.58047
C	-2.83284	1.49247	-0.89605
C	-0.67170	2.40897	-1.76431
C	0.76076	0.26795	2.21276
C	1.83136	-0.81902	2.06971
C	1.28220	1.43256	3.05838
C	-0.49954	-0.30766	2.85157
H	-1.46784	0.11196	0.72992
H	1.58405	0.80625	-2.38767
H	1.56701	-0.69926	-3.34402
H	3.66155	-1.44203	-2.16691
H	3.90909	0.11113	-2.99191
H	3.66422	0.07456	-1.23272
H	0.09114	-3.95851	0.12726
H	0.19520	-3.40265	-1.55453
H	-1.62345	-5.10742	-1.29036
H	-2.40778	-4.08659	-0.06744
H	-2.30299	-3.53370	-1.75672
H	-0.38978	3.24479	0.82166
H	-1.85902	2.50301	1.49479
H	-1.98633	3.75902	0.24909
H	-3.33555	2.38987	-1.27158
H	-3.38396	1.13662	-0.01801
H	-2.88641	0.72534	-1.67341
H	-0.65981	1.69238	-2.59214
H	0.35553	2.70431	-1.53865
H	-1.21543	3.29771	-2.10388
H	1.45396	-1.66405	1.48495
H	2.72368	-0.41866	1.57960
H	2.11254	-1.18223	3.06295
H	1.51179	1.06790	4.06366
H	0.52572	2.22027	3.13925
H	2.19163	1.85798	2.62786
H	-1.29401	0.44244	2.92617
H	-0.87454	-1.18120	2.31057
H	-0.24413	-0.62812	3.86552

3•_al, SMD Methanol

N	0.92167	-0.14749	1.20311
O	1.79498	0.66375	0.73675
C	-0.38772	-0.10082	0.54754
P	-0.04175	-0.26483	-1.25823
O	1.10402	-1.17695	-1.55905
O	-1.45438	-0.76773	-1.80439
C	-1.59966	-1.09078	-3.21641
C	-1.62350	-2.59150	-3.39508
O	0.09614	1.17198	-1.95183
C	1.38713	1.78594	-2.20608
C	1.27646	2.57789	-3.48767
C	-1.26108	1.10535	1.02713
C	-1.65997	0.83246	2.48338
C	-2.54041	1.19166	0.18459
C	-0.52411	2.44754	0.96593
C	1.41962	-1.20788	2.13995
C	2.51283	-2.00164	1.41698
C	2.00124	-0.49007	3.36091
C	0.29395	-2.14625	2.56217
H	-0.93615	-1.01663	0.78818
H	-0.78577	-0.62906	-3.78455
H	-2.54062	-0.63011	-3.52353
H	-2.43533	-3.03469	-2.81141
H	-1.78574	-2.82917	-4.45080
H	-0.67512	-3.03566	-3.07990
H	2.14480	1.00174	-2.28014
H	1.62229	2.42796	-1.35267
H	2.22974	3.07540	-3.68914
H	1.04138	1.92096	-4.33015
H	0.49809	3.34203	-3.40485
H	-0.78022	0.73126	3.12769
H	-2.26035	-0.08044	2.56619
H	-2.25791	1.66897	2.86045
H	-3.20864	1.93194	0.63675
H	-3.06711	0.23196	0.15291
H	-2.33611	1.50956	-0.84245
H	0.34282	2.46425	1.63243
H	-1.21409	3.23494	1.28924
H	-0.19076	2.68747	-0.04735
H	2.10400	-2.52273	0.54668
H	3.32097	-1.34293	1.08815
H	2.92649	-2.74465	2.10543
H	2.42769	-1.23117	4.04318
H	1.22528	0.06680	3.89565
H	2.79315	0.20276	3.06442
H	-0.53268	-1.61130	3.03722
H	-0.08837	-2.73027	1.71928
H	0.70292	-2.84952	3.29321

3•_au, SMD Methanol

N	0.61299	0.59438	1.41277
O	1.08975	1.59783	0.77687
C	-0.27388	-0.27433	0.63452
P	0.65756	-0.68470	-0.90514
O	2.12960	-0.82493	-0.68729
O	-0.07542	-2.02497	-1.36721
C	0.26106	-2.62010	-2.65254
C	-0.86785	-2.39260	-3.63209
O	0.28993	0.33242	-2.08451
C	1.14429	1.44913	-2.44324
C	1.18061	1.53717	-3.95120
C	-1.71592	0.31492	0.48360
C	-2.38214	0.26052	1.86458
C	-2.53700	-0.55005	-0.48222
C	-1.72732	1.76702	-0.00653
C	1.23529	0.28275	2.74144
C	1.01151	1.50489	3.63608
C	0.60714	-0.95648	3.37018
C	2.73338	0.04940	2.52000
H	-0.36615	-1.23705	1.14697
H	0.41170	-3.68196	-2.44940
H	1.20472	-2.20064	-3.01648
H	-0.99670	-1.32714	-3.84263
H	-0.64028	-2.90695	-4.57089
H	-1.80542	-2.79422	-3.23652
H	2.14065	1.28707	-2.02475
H	0.71174	2.34756	-1.99401
H	1.79389	2.39200	-4.25145
H	1.61485	0.62892	-4.37994
H	0.17336	1.67400	-4.35565
H	-1.82271	0.84414	2.60354
H	-2.46597	-0.77085	2.22521
H	-3.39098	0.68178	1.79925

H	-3.58054	-0.22014	-0.44638
H	-2.50437	-1.60862	-0.20325
H	-2.19200	-0.45309	-1.51630
H	-1.24517	2.43982	0.70818
H	-2.77007	2.08450	-0.11846
H	-1.23541	1.87701	-0.97655
H	1.45185	2.40042	3.18994
H	-0.05663	1.67964	3.79992
H	1.48698	1.33144	4.60577
H	1.05475	-1.09172	4.35891
H	0.81387	-1.85949	2.78772
H	-0.47281	-0.84990	3.50257
H	2.90229	-0.83523	1.89961
H	3.19561	0.91467	2.03743
H	3.21539	-0.10843	3.48955

3•_ak, SMD Methanol

N	0.04163	0.73862	0.79386
O	1.05777	1.46922	0.54022
C	-0.84256	0.40968	-0.32697
P	-0.01146	-0.84098	-1.39010
O	-0.78047	-1.23640	-2.60729
O	1.44150	-0.31750	-1.81008
C	2.64494	-0.54544	-1.02645
C	3.61967	0.56295	-1.34383
O	0.22848	-2.00581	-0.32088
C	0.74708	-3.29510	-0.75531
C	-0.35894	-4.32312	-0.69889
C	-1.40426	1.66086	-1.07953
C	-1.73914	2.73800	-0.04057
C	-2.70803	1.24480	-1.77729
C	-0.43722	2.23122	-2.12474
C	-0.14041	0.30345	2.21899
C	-1.40626	-0.53046	2.38713
C	1.09074	-0.51884	2.61313
C	-0.23094	1.56878	3.07758
H	-1.69872	-0.13167	0.08159
H	3.04199	-1.52224	-1.31859
H	2.39249	-0.56388	0.03610
H	3.20846	1.53364	-1.05332
H	4.54843	0.39591	-0.79019
H	3.85166	0.57880	-2.41261
H	1.56008	-3.53159	-0.06486
H	1.16034	-3.20550	-1.76545
H	0.03993	-5.30402	-0.97427
H	-0.77058	-4.38686	0.31257
H	-1.16225	-4.06458	-1.39466
H	-0.83922	3.14508	0.42977
H	-2.39172	2.33707	0.74417
H	-2.26794	3.56013	-0.53406
H	-3.13445	2.11176	-2.29302
H	-3.44455	0.88638	-1.04899
H	-2.54110	0.45778	-2.51706
H	-0.25836	1.52061	-2.93992
H	0.52522	2.50388	-1.68439
H	-0.88156	3.13017	-2.56588
H	-2.30697	0.03980	2.13718
H	-1.37722	-1.44594	1.78839
H	-1.47731	-0.81997	3.43940
H	1.01204	-0.79847	3.66793
H	2.00599	0.06450	2.47843
H	1.15666	-1.43256	2.01444
H	0.66056	2.18938	2.95528
H	-1.11367	2.15864	2.81301
H	-0.31015	1.28003	4.12981

3•_ao, SMD Methanol

N	0.47862	-0.23324	1.34305
O	0.97902	0.93312	1.48775
C	-0.56387	-0.39146	0.31975
P	0.33356	-0.36390	-1.28685
O	1.27798	-1.51677	-1.42266
O	-0.82821	-0.29672	-2.37352
C	-0.48236	-0.30605	-3.78798
C	-1.75773	-0.08198	-4.56384
O	1.06258	1.05229	-1.44474
C	2.49229	1.18497	-1.21726
C	2.77665	2.64714	-0.97203
C	-1.78925	0.55892	0.52385
C	-2.07931	0.64295	2.02907
C	-3.00928	-0.08171	-0.15640
C	-1.58258	1.97034	-0.03884
C	1.04133	-1.32248	2.20756
C	0.36101	-2.65759	1.92545
C	2.54019	-1.41994	1.90648
C	0.81374	-0.91385	3.66571
H	-0.93492	-1.41651	0.39070
H	-0.02950	-1.27348	-4.02178
H	0.24590	0.48975	-3.97250
H	-2.20166	0.88362	-4.30540
H	-1.53587	-0.08838	-5.63477
H	-2.48136	-0.87468	-4.35370
H	3.00693	0.81429	-2.10800
H	2.78076	0.57417	-0.35722
H	3.85160	2.78808	-0.82633
H	2.46046	3.25153	-1.82721
H	2.25405	2.99665	-0.07678
H	-1.28993	1.17473	2.56830
H	-2.18603	-0.35725	2.46570
H	-3.02020	1.18160	2.18281
H	-3.88869	0.54779	0.01617
H	-3.21486	-1.07318	0.26336
H	-2.87271	-0.18404	-1.23560
H	-0.70754	2.45822	0.39790
H	-2.46562	2.57551	0.19454
H	-1.46769	1.95846	-1.12793
H	-0.71089	-2.62510	2.14628
H	0.50938	-2.98094	0.89037
H	0.81367	-3.40792	2.57983
H	2.98703	-2.18214	2.55172
H	3.03841	-0.46629	2.10139
H	2.70766	-1.70475	0.86314
H	1.26773	0.05869	3.87373
H	-0.25498	-0.86381	3.89521
H	1.27448	-1.65878	4.32124

3•_ag, SMD Methanol

N	0.73963	0.99084	1.04421
O	1.20711	0.03656	1.75761
C	0.14682	0.58310	-0.23217
P	-1.05030	-0.75898	0.18495
O	-1.74627	-0.54582	1.49075
O	-2.00897	-0.72353	-1.09185
C	-3.10746	-1.67059	-1.18722
C	-3.81265	-1.41365	-2.49724
O	-0.36594	-2.19992	0.05643
C	0.14658	-2.92085	1.20759
C	-0.07470	-4.39500	0.96320
C	1.22095	0.29814	-1.33408
C	1.85354	1.64230	-1.71871
C	0.54947	-0.29138	-2.58159
C	2.33211	-0.64671	-0.86378
C	0.60350	2.32677	1.71277
C	2.01177	2.77058	2.11750
C	-0.02834	3.35122	0.77660
C	-0.27570	2.14661	2.95454
H	-0.49222	1.39184	-0.60018
H	-3.77304	-1.51550	-0.33300
H	-2.69527	-2.68339	-1.14524
H	-3.12811	-1.55893	-3.33792
H	-4.64708	-2.11274	-2.60293
H	-4.20646	-0.39399	-2.53060
H	-0.37600	-2.57701	2.10379
H	1.20931	-2.68126	1.30164
H	0.33268	-4.96640	1.80248
H	-1.14215	-4.61740	0.87566
H	0.43157	-4.71563	0.04804
H	2.33085	2.12251	-0.85798
H	1.10659	2.32932	-2.13209
H	2.62339	1.47776	-2.48009
H	1.28798	-0.33425	-3.38891
H	-0.28833	0.32797	-2.91909
H	0.18177	-1.30796	-2.41107
H	1.94043	-1.61768	-0.54925
H	2.90587	-0.21733	-0.03763
H	3.01905	-0.81499	-1.70063
H	2.48243	2.02671	2.76573
H	2.64352	2.92359	1.23692
H	1.94705	3.71543	2.66486
H	-0.04024	4.31437	1.29469
H	-1.06328	3.09464	0.53010
H	0.54376	3.47345	-0.14697
H	-1.28670	1.83745	2.67440
H	0.14996	1.39914	3.62915
H	-0.33838	3.10078	3.48632

3•_aw, SMD Methanol

N	0.79134	0.21171	1.14754
O	1.62850	1.11696	0.80758
C	-0.48449	0.21351	0.42956
P	-0.11846	0.26337	-1.37683
O	0.06921	1.58271	-2.05419
O	1.13907	-0.71527	-1.52522
C	2.16833	-0.48623	-2.52694
C	3.26231	0.40660	-1.98723
O	-1.36676	-0.57471	-1.93890
C	-1.59967	-0.61359	-3.37113
C	-2.84735	-1.43099	-3.60634
C	-1.47301	1.32123	0.92406
C	-1.92957	0.94626	2.33875
C	-2.70812	1.35128	0.01186
C	-0.83381	2.71384	0.96092
C	1.29992	-0.86657	2.05909
C	0.23359	-1.92798	2.30665

C	2.52777	-1.50536	1.40139
C	1.70147	-0.19565	3.37580
H	-0.97305	-0.75325	0.57944
H	1.70901	-0.06211	-3.42409
H	2.54450	-1.48308	-2.76487
H	3.70171	-0.02373	-1.08292
H	4.04833	0.50437	-2.74281
H	2.87765	1.40344	-1.75488
H	-0.72662	-1.06626	-3.85387
H	-1.71803	0.41244	-3.73129
H	-3.05697	-1.47432	-4.67889
H	-2.71811	-2.45154	-3.23525
H	-3.70458	-0.97486	-3.10255
H	-1.08278	0.87773	3.02928
H	-2.46307	-0.01079	2.34391
H	-2.60874	1.71722	2.71826
H	-3.45038	2.02729	0.44862
H	-3.16337	0.35954	-0.08148
H	-2.47415	1.72213	-0.99201
H	-0.03086	2.76806	1.70161
H	-1.60285	3.44155	1.24275
H	-0.42810	3.00413	-0.01223
H	-0.67784	-1.50365	2.73694
H	-0.01756	-2.47488	1.39243
H	0.63886	-2.64775	3.02346
H	2.91732	-2.28462	2.06335
H	3.31417	-0.76340	1.24092
H	2.26683	-1.96090	0.44183
H	2.42730	0.60234	3.19782
H	0.83053	0.22488	3.88743
H	2.16038	-0.94081	4.03227

3•_as, SMD Methanol

N	-0.74075	0.91584	-0.05467
O	-0.04507	1.98179	-0.14497
C	-0.36371	-0.20092	-0.92153
P	1.16823	-0.98832	-0.23428
O	2.07758	-1.66139	-1.21029
O	1.91602	0.07204	0.70319
C	2.95586	0.93543	0.17435
C	3.32224	1.91253	1.26556
O	0.49729	-1.94671	0.85603
C	1.33029	-2.64139	1.82320
C	0.43690	-3.58072	2.59728
C	-0.36527	0.15847	-2.44048
C	-1.63344	0.97460	-2.72511
C	-0.44909	-1.16024	-3.22409
C	0.86264	0.94680	-2.91071
C	-1.73598	0.84990	1.06505
C	-0.95882	0.84615	2.38602
C	-2.61205	2.10069	0.95764
C	-2.60678	-0.39838	0.95585
H	-1.12055	-0.97810	-0.79319
H	2.57311	1.45549	-0.70819
H	3.80484	0.30965	-0.11472
H	3.67574	1.38355	2.15538
H	4.12119	2.57038	0.91170
H	2.45844	2.52712	1.53601
H	1.79163	-1.89449	2.47560
H	2.11377	-3.18345	1.28474
H	1.03309	-4.11762	3.34058
H	-0.34833	-3.02508	3.11843
H	-0.02745	-4.31147	1.92928
H	-1.58907	1.96430	-2.26042
H	-2.52806	0.45743	-2.35783
H	-1.74057	1.11103	-3.80641
H	-0.48799	-0.94326	-4.29670
H	-1.35405	-1.71788	-2.95697
H	0.41886	-1.79950	-3.04004
H	1.78901	0.38473	-2.75321
H	0.94434	1.90990	-2.40176
H	0.76955	1.13635	-3.98599
H	-0.34931	-0.05869	2.47889
H	-0.30655	1.72195	2.45199
H	-1.66611	0.87495	3.22062
H	-3.34886	2.08951	1.76584
H	-3.14555	2.11734	0.00136
H	-2.01516	3.01131	1.04572
H	-3.13665	-0.43805	-0.00176
H	-2.03013	-1.31806	1.09051
H	-3.35508	-0.35522	1.75229

3•_br, SMD Methanol

N	-0.38644	-1.35321	-0.12312
O	-0.02119	-1.95491	0.94579
C	-0.78317	0.04632	0.04009
P	0.55507	0.88370	0.99593
O	0.48316	0.86975	2.48810
O	1.93148	0.29940	0.41914
C	2.80005	-0.55628	1.20915
C	4.15013	-0.58388	0.53286
O	0.50148	2.34243	0.33797
C	1.28845	3.40447	0.94131
C	1.16125	4.62275	0.05876
C	-2.22329	0.21908	0.62153
C	-3.22200	-0.24223	-0.44657
C	-2.47469	1.70572	0.91107
C	-2.45197	-0.59868	1.89730
C	-0.11881	-2.06034	-1.41899
C	1.38495	-2.34270	-1.50079
C	-0.90830	-3.37148	-1.38730
C	-0.54880	-1.21095	-2.61050
H	-0.76102	0.53398	-0.93835
H	2.34786	-1.55071	1.25655
H	2.86806	-0.14510	2.21943
H	4.57874	0.42139	0.48314
H	4.82709	-1.22226	1.10823
H	4.07235	-0.98738	-0.48083
H	2.32909	3.07083	1.01654
H	0.89766	3.59157	1.94557
H	1.73363	5.44695	0.49378
H	1.55079	4.41827	-0.94238
H	0.11485	4.93089	-0.02221
H	-3.06304	-1.29136	-0.71805
H	-3.14506	0.36861	-1.35304
H	-4.24140	-0.14764	-0.05726
H	-3.52598	1.84011	1.18564
H	-2.27056	2.32563	0.03130
H	-1.86579	2.07353	1.74421
H	-1.72564	-0.35536	2.67763
H	-2.39985	-1.67316	1.69872
H	-3.45393	-0.37400	2.27948
H	1.95229	-1.40763	-1.50980
H	1.71679	-2.95399	-0.65693
H	1.59474	-2.88686	-2.42663
H	-0.69143	-3.94290	-2.29454
H	-1.98516	-3.17962	-1.34802
H	-0.62485	-3.97589	-0.52170
H	0.05306	-0.30151	-2.70243
H	-0.39309	-1.80375	-3.51629
H	-1.60744	-0.94172	-2.56380

F, SMD Methanol

C	0.00000	0.49906	2.31734
C	0.00000	-0.48591	3.42884
C	0.00000	0.25680	0.97955
C	0.00000	1.38441	0.05833
C	0.00000	1.21559	-1.28121
C	0.00000	-0.12445	-1.86677
C	0.00000	-1.25992	-0.94071
C	0.00000	-1.07716	0.39729
O	0.00000	-0.29652	-3.09840
H	0.87652	-0.31161	4.06445
H	0.00000	-1.52576	3.10305
H	-0.87652	-0.31161	4.06445
H	0.00000	2.38408	0.48745
H	0.00000	2.05891	-1.96558
H	0.00000	-2.25380	-1.37913
H	0.00000	-1.94054	1.05534
H	0.00000	1.54601	2.62184

3a+•_cd, SMD Methanol

N	0.38739	-1.02121	0.67386
O	1.42085	-0.39228	0.16350
C	1.36124	0.27257	-1.18195
C	1.52987	-0.80204	-2.23803
C	2.48515	1.27114	-1.16464
C	3.78297	0.88132	-0.82032
C	4.82881	1.79844	-0.84209
C	4.57989	3.11719	-1.23102
C	3.29176	3.51682	-1.59059
C	2.25174	2.59427	-1.54740
O	5.56364	4.05975	-1.27691
C	-0.93452	-0.39092	0.78194
P	-1.94014	-0.67625	-0.75383
O	-1.47523	-1.89254	-1.47846
O	-3.45366	-0.75169	-0.26629
C	-4.07682	-2.01248	0.11943
C	-4.32853	-2.03127	1.60908
O	-1.88191	0.69685	-1.54188
C	-2.48203	0.80721	-2.86914
C	-1.93561	2.06333	-3.50116
C	-0.95662	0.99706	1.51973
C	-2.43310	1.35132	1.75022
C	-0.27321	2.16023	0.79953
C	-0.27075	0.79570	2.87692
C	0.80058	-2.32526	1.32231
C	1.37296	-3.19956	0.19952
C	1.87579	-2.02840	2.37406
C	-0.40080	-3.00987	1.96313
H	0.40057	0.77972	-1.27148
H	2.50869	-1.28040	-2.14987
H	1.46952	-0.30819	-3.21349
H	0.73861	-1.55119	-2.17718

H	3.98344	-0.14610	-0.52581
H	5.83591	1.49834	-0.56519
H	3.11721	4.54571	-1.88983
H	1.24548	2.90959	-1.81277
H	6.41039	3.68448	-0.99264
H	-1.46754	-1.06047	1.46302
H	-3.43829	-2.84000	-0.20068
H	-5.00995	-2.05184	-0.44529
H	-3.39259	-2.00881	2.17595
H	-4.85969	-2.95298	1.86597
H	-4.94745	-1.18100	1.90869
H	-3.56653	0.84932	-2.73897
H	-2.21544	-0.08312	-3.44543
H	-2.17509	2.93936	-2.89179
H	-2.38580	2.19379	-4.48930
H	-0.85038	1.99442	-3.62062
H	-2.97231	0.53842	2.24807
H	-2.94790	1.59192	0.81511
H	-2.47604	2.23531	2.39367
H	-0.68645	2.33607	-0.19701
H	0.80785	2.01754	0.72982
H	-0.43902	3.06398	1.39558
H	-0.39588	1.70221	3.47730
H	0.80361	0.62331	2.75727
H	-0.70699	-0.04439	3.42926
H	0.62781	-3.37408	-0.58130
H	2.26516	-2.74723	-0.23890
H	1.65208	-4.16054	0.63923
H	2.72078	-1.48690	1.94274
H	1.46441	-1.46171	3.21209
H	2.23609	-2.98958	2.75060
H	-1.19911	-3.20437	1.23896
H	-0.79514	-2.44642	2.81430
H	-0.04958	-3.97378	2.34020

3a+•_dn, SMD Methanol

N	0.41117	-1.05839	-0.95619
O	1.03852	0.04014	-1.30988
C	0.42583	1.38845	-1.09424
C	-0.52885	1.64864	-2.24327
C	1.58002	2.35258	-1.06408
C	2.56323	2.32864	-2.05693
C	3.59777	3.25923	-2.05192
C	3.63899	4.23833	-1.05646
C	2.65806	4.27893	-0.06402
C	1.63919	3.33237	-0.07019
O	4.62038	5.18321	-1.00691
C	-0.10721	-1.25292	0.40232
P	-1.83658	-0.59702	0.57414
O	-2.51290	-0.41308	-0.74079
O	-2.42220	-1.73984	1.51119
C	-3.67048	-1.54027	2.23514
C	-3.94948	-2.80884	3.00350
O	-1.80056	0.70824	1.48407
C	-2.40648	1.97032	1.07610
C	-3.83579	2.04586	1.55798
C	0.93693	-1.02585	1.55610
C	0.29245	-1.55092	2.84840
C	1.39636	0.41569	1.77859
C	2.16418	-1.88329	1.22443
C	0.52967	-2.13235	-2.01584
C	-0.16664	-1.57954	-3.26564
C	2.01595	-2.38405	-2.29529
C	-0.15664	-3.41204	-1.55466
H	-0.07802	1.38149	-0.12558
H	0.01363	1.65034	-3.19238
H	-0.96146	2.64260	-2.09049
H	-1.33502	0.91401	-2.26998
H	2.52876	1.57730	-2.84225
H	4.36786	3.23612	-2.81838
H	2.70745	5.04531	0.70332
H	0.88027	3.35602	0.70848
H	5.22974	5.08107	-1.75307
H	-0.31395	-2.32491	0.43327
H	-4.46020	-1.32403	1.50970
H	-3.54148	-0.68311	2.90198
H	-4.06000	-3.65783	2.32354
H	-4.87902	-2.69048	3.56739
H	-3.13928	-3.01759	3.70802
H	-2.34364	2.05916	-0.01183
H	-1.77921	2.73627	1.53624
H	-4.44633	1.26826	1.08855
H	-4.25244	3.02127	1.28892
H	-3.88625	1.93477	2.64469
H	-0.07264	-2.57615	2.73006
H	-0.53758	-0.91943	3.18083
H	1.05328	-1.54504	3.63477
H	0.56201	1.10035	1.95409
H	2.00294	0.78122	0.94685
H	2.03364	0.42971	2.66916
H	1.88688	-2.92551	1.03029
H	2.85394	-1.86394	2.07396
H	2.69920	-1.49026	0.35391
H	0.34409	-0.69164	-3.64465
H	-0.12945	-2.35549	-4.03447
H	-1.21353	-1.34146	-3.05786
H	2.53649	-1.46122	-2.56118
H	2.50763	-2.85119	-1.43945
H	2.07389	-3.07130	-3.14368
H	-0.10482	-4.11625	-2.38865
H	-1.21288	-3.24864	-1.31814
H	0.35069	-3.87234	-0.70182

3a+•_cu, SMD Methanol

N	0.53949	-0.78927	0.77879
O	1.42887	-0.22786	-0.00747
C	1.09807	0.15300	-1.42103
C	1.24245	-1.09132	-2.27556
C	2.08448	1.22951	-1.78055
C	3.45264	1.05838	-1.55171
C	4.36275	2.04110	-1.92931
C	3.90317	3.19926	-2.56111
C	2.54071	3.37661	-2.80792
C	1.63985	2.39510	-2.40908
O	4.74617	4.19454	-2.95826
C	-0.78285	-0.19430	1.00414
P	-2.00407	-0.78417	-0.26434
O	-1.55451	-2.06231	-0.88480
O	-3.39515	-0.89055	0.50445
C	-3.79778	-2.10915	1.19669
C	-3.82976	-1.86590	2.68749
O	-2.23229	0.45032	-1.22988
C	-3.00733	0.27401	-2.45808
C	-2.07502	-0.00896	-3.61231
C	-0.77627	1.30304	1.47960
C	-2.21449	1.63154	1.90735
C	-0.30713	2.33445	0.45297
C	0.14181	1.38446	2.70569
C	1.13790	-1.93213	1.57129
C	1.62266	-2.96088	0.54308
C	2.31661	-1.39457	2.39132
C	0.08830	-2.55686	2.48367
H	0.08145	0.54968	-1.43991
H	2.26628	-1.47131	-2.22594
H	1.03126	-0.80240	-3.31009
H	0.53718	-1.86823	-1.97565
H	3.81622	0.15419	-1.06931
H	5.42569	1.91396	-1.74217
H	2.20168	4.28349	-3.29911
H	0.57677	2.53971	-2.58678
H	5.66248	3.97784	-2.73019
H	-1.14988	-0.74618	1.87371
H	-3.11473	-2.91902	0.92676
H	-4.78979	-2.34476	0.80697
H	-2.83202	-1.64313	3.07847
H	-4.19814	-2.76741	3.18661
H	-4.50075	-1.03725	2.93054
H	-3.54146	1.21660	-2.58311
H	-3.73787	-0.52719	-2.31002
H	-1.33673	0.79237	-3.71452
H	-2.65544	-0.06333	-4.53836
H	-1.55501	-0.96070	-3.47254
H	-2.59558	0.90403	2.63239
H	-2.89923	1.66909	1.05474
H	-2.21437	2.61810	2.38060
H	-0.88915	2.30121	-0.47120
H	0.75513	2.22342	0.22302
H	-0.43676	3.32801	0.89538
H	0.05911	2.38272	3.14681
H	1.18945	1.23030	2.42820
H	-0.13719	0.64849	3.46845
H	0.79771	-3.30355	-0.08742
H	2.41839	-2.55190	-0.08310
H	2.02042	-3.81609	1.09525
H	3.03854	-0.87131	1.75979
H	1.97558	-0.73061	3.18820
H	2.81473	-2.25448	2.84733
H	-0.78017	-2.91956	1.92308
H	-0.23459	-1.87417	3.27500
H	0.56110	-3.41783	2.96300

3a+•_bf, SMD Methanol

N	0.85366	-0.84473	-0.33309
O	1.13841	0.25007	-1.00256
C	0.12041	1.33746	-1.18185
C	-0.85954	0.89223	-2.25004
C	0.92130	2.54728	-1.57337
C	1.83133	2.49147	-2.63334
C	2.53979	3.62417	-3.02028
C	2.32429	4.83279	-2.35275
C	1.40976	4.90544	-1.30071
C	0.72004	3.76137	-0.91249
O	2.98398	5.97722	-2.68937
C	0.31597	-0.80191	1.02933

P	-1.53869	-0.66938	1.05475
O	-2.13010	0.69775	1.09315
O	-1.83809	-1.56045	-0.22833
C	-3.15265	-2.12561	-0.49961
C	-4.08527	-1.09723	-1.09927
O	-1.94538	-1.59105	2.28801
C	-2.84680	-1.13884	3.33938
C	-4.27239	-1.50393	2.99767
C	1.13295	0.06631	2.04965
C	0.56435	-0.24503	3.44284
C	1.08822	1.58006	1.83503
C	2.59134	-0.40176	1.98171
C	1.38431	-2.07604	-1.03435
C	0.66824	-2.14411	-2.38904
C	2.89549	-1.90675	-1.23451
C	1.08847	-3.32713	-0.21680
H	-0.37677	1.50036	-0.22632
H	-0.35665	0.77563	-3.21353
H	-1.61747	1.67686	-2.34206
H	-1.35831	-0.04010	-1.97917
H	1.99577	1.55542	-3.16188
H	3.25354	3.57890	-3.83844
H	1.25483	5.85305	-0.79413
H	0.01548	3.81412	-0.08590
H	3.59265	5.81847	-3.42622
H	0.43657	-1.83032	1.37636
H	-3.54397	-2.54666	0.43120
H	-2.95298	-2.94230	-1.19534
H	-4.27312	-0.27277	-0.40561
H	-5.04075	-1.57929	-1.32788
H	-3.67194	-0.69225	-2.02716
H	-2.72807	-0.06052	3.47003
H	-2.49725	-1.64894	4.23860
H	-4.59858	-0.98946	2.08749
H	-4.92762	-1.19880	3.81925
H	-4.37427	-2.58346	2.85491
H	0.50942	-1.32198	3.63462
H	-0.42998	0.19209	3.58228
H	1.22468	0.20353	4.19120
H	0.06503	1.96760	1.82452
H	1.60629	1.88099	0.92119
H	1.61405	2.05209	2.67173
H	2.67342	-1.48603	2.11971
H	3.16072	0.08864	2.77747
H	3.05220	-0.12789	1.02731
H	0.90584	-1.27563	-3.00731
H	1.02027	-3.04204	-2.90332
H	-0.41466	-2.21577	-2.25638
H	3.12909	-0.98034	-1.76420
H	3.42605	-1.92885	-0.28025
H	3.23932	-2.74926	-1.84055
H	1.42922	-4.17913	-0.81050
H	0.01748	-3.45124	-0.03065
H	1.63699	-3.34427	0.72929

3a+•_ap, SMD Methanol

N	-0.19337	1.07684	-0.89142
O	1.04830	0.98857	-0.46917
C	1.37043	0.38572	0.86419
C	1.11718	1.44427	1.92044
C	2.81429	-0.02305	0.77405
C	3.78830	0.87531	0.32861
C	5.12959	0.50754	0.29523
C	5.50591	-0.76521	0.73202
C	4.54459	-1.66886	1.18772
C	3.20469	-1.29535	1.19876
O	6.80530	-1.17792	0.73429
C	-1.07809	-0.09078	-0.94691
P	-1.94200	-0.42685	0.66439
O	-1.31328	-1.36821	1.63356
O	-2.09995	1.07616	1.16411
C	-2.43649	1.39224	2.54626
C	-3.87361	1.04576	2.86224
O	-3.38564	-0.87758	0.16043
C	-4.04926	-2.07019	0.67083
C	-5.15488	-2.41909	-0.29527
C	-0.50350	-1.31987	-1.73783
C	-1.67396	-2.29063	-1.95533
C	0.64043	-2.07074	-1.05521
C	-0.02060	-0.80501	-3.09836
C	-0.46871	2.42142	-1.52915
C	-1.87956	2.45984	-2.10136
C	-0.31564	3.46644	-0.41690
C	0.56684	2.66235	-2.63404
H	0.73437	-0.48780	1.00945
H	1.79879	2.28906	1.79097
H	1.30736	0.98637	2.89626
H	0.08611	1.80041	1.89551
H	3.50214	1.87178	0.00034
H	5.88678	1.20225	-0.05832
H	4.85509	-2.65406	1.52159
H	2.45371	-2.00220	1.54347
H	7.38823	-0.47453	0.41170
H	-1.91916	0.26116	-1.54810
H	-2.25540	2.46584	2.62152
H	-1.73466	0.86508	3.19908
H	-4.55159	1.50668	2.13840
H	-4.11778	1.42395	3.85933
H	-4.03297	-0.03649	2.86511
H	-4.43941	-1.83904	1.66517
H	-3.31482	-2.87473	0.75669
H	-5.86414	-1.59181	-0.38703
H	-5.69146	-3.29623	0.07769
H	-4.74923	-2.65322	-1.28358
H	-1.34697	-3.07238	-2.64756
H	-2.54381	-1.78751	-2.38989
H	-1.97535	-2.78474	-1.02571
H	0.37252	-2.41255	-0.05084
H	1.55169	-1.46999	-1.00778
H	0.87044	-2.95520	-1.65874
H	-0.80072	-0.23169	-3.61230
H	0.24799	-1.65956	-3.72723
H	0.87054	-0.17832	-2.99246
H	-2.00549	1.75761	-2.93044
H	-2.63847	2.27393	-1.33496
H	-2.03537	3.46811	-2.49297
H	-1.01802	3.27598	0.39910
H	0.70501	3.48487	-0.02820
H	-0.53849	4.44424	-0.85172
H	0.41491	3.68045	-3.00226
H	0.42715	1.97019	-3.46698
H	1.58772	2.58049	-2.25454

3a+•_ao, SMD Methanol

N	0.34029	-1.00717	0.47731
O	1.09452	-0.98126	-0.59857
C	0.70276	-0.19345	-1.81305
C	-0.35132	-0.98295	-2.56538
C	1.98121	-0.02039	-2.58468
C	2.78340	-1.12101	-2.90095
C	3.94351	-0.96081	-3.65174
C	4.29740	0.31145	-4.10925
C	3.50091	1.41745	-3.80836
C	2.35262	1.24625	-3.04213
O	5.41583	0.53036	-4.85737
C	-0.11965	0.22068	1.13426
P	-1.67877	0.88836	0.38014
O	-1.57197	1.86936	-0.73650
O	-2.37123	-0.49911	0.02017
C	-3.62536	-0.55497	-0.72093
C	-4.80542	-0.49252	0.22274
O	-2.44446	1.44998	1.66003
C	-3.14345	2.72838	1.61388
C	-3.68243	2.98998	2.99839
C	1.01194	1.24434	1.50783
C	0.37489	2.29575	2.42971
C	1.67387	1.96334	0.33150
C	2.08319	0.47521	2.28925
C	0.24706	-2.40579	1.04894
C	-0.55724	-2.40409	2.34200
C	-0.45500	-3.25815	-0.01597
C	1.66733	-2.92622	1.30107
H	0.32036	0.77283	-1.48633
H	0.05599	-1.93322	-2.91984
H	-0.64807	-0.38392	-3.43206
H	-1.23482	-1.16839	-1.95150
H	2.50652	-2.11466	-2.55655
H	4.57137	-1.81480	-3.89169
H	3.79217	2.39822	-4.17138
H	1.73704	2.10889	-2.79845
H	5.88825	-0.29992	-5.01836
H	-0.50467	-0.13566	2.09229
H	-3.58552	-1.50860	-1.25093
H	-3.63632	0.25565	-1.45561
H	-4.73917	-1.28759	0.97082
H	-5.72691	-0.63057	-0.35067
H	-4.86050	0.47308	0.73358
H	-3.94350	2.65586	0.87171
H	-2.43553	3.50039	1.30082
H	-4.37475	2.19915	3.30079
H	-4.21965	3.94263	3.00025
H	-2.86745	3.04846	3.72566
H	1.17569	2.91475	2.84545
H	-0.17069	1.83546	3.25967
H	-0.30333	2.96103	1.88502
H	0.94778	2.49019	-0.29540
H	2.26731	1.28239	-0.28325
H	2.36357	2.70950	0.74006
H	1.64873	-0.07321	3.13271
H	2.81607	1.18607	2.68326
H	2.61753	-0.22896	1.64364
H	-0.05839	-1.84218	3.13693
H	-1.57281	-2.02403	2.19507
H	-0.63118	-3.44439	2.66876

H	-1.44725	-2.85988	-0.24449
H	0.13809	-3.31564	-0.93151
H	-0.56513	-4.26726	0.38957
H	1.57917	-3.97315	1.60354
H	2.15488	-2.37460	2.10763
H	2.28069	-2.87710	0.39867

3a+•_an, SMD Methanol

N	0.42326	-1.01023	-0.22004
O	1.24148	-0.15857	-0.79665
C	0.78797	1.21918	-1.17475
C	-0.02583	1.11219	-2.45033
C	2.05571	2.00949	-1.34214
C	3.09109	1.54187	-2.15678
C	4.24379	2.29805	-2.34290
C	4.35673	3.54530	-1.72312
C	3.32569	4.02925	-0.91613
C	2.18544	3.25594	-0.72446
O	5.45776	4.33492	-1.87317
C	-0.31568	-0.66933	0.99934
P	-1.91408	0.20877	0.64945
O	-1.91540	1.69868	0.62167
O	-2.29357	-0.51037	-0.71991
C	-3.49649	-0.09240	-1.43180
C	-3.60429	-0.93936	-2.67588
O	-2.88625	-0.41920	1.74461
C	-3.80632	0.41233	2.51152
C	-4.32768	-0.42858	3.65054
C	0.55953	-0.12706	2.18629
C	-0.34403	-0.11911	3.42951
C	1.14680	1.27232	1.99667
C	1.70545	-1.12096	2.40623
C	0.57408	-2.39964	-0.80176
C	0.19951	-2.28835	-2.28467
C	2.03600	-2.83883	-0.65218
C	-0.35492	-3.37675	-0.09284
H	0.19608	1.62088	-0.35281
H	0.59023	0.74006	-3.27300
H	-0.37152	2.12040	-2.69987
H	-0.89695	0.46645	-2.32280
H	3.00412	0.57634	-2.64973
H	5.05239	1.93096	-2.96925
H	3.43089	5.00056	-0.44272
H	1.38581	3.62723	-0.08775
H	6.10591	3.91159	-2.45570
H	-0.69005	-1.63618	1.34366
H	-3.39826	0.97048	-1.67092
H	-4.35374	-0.23897	-0.76730
H	-2.74768	-0.77177	-3.33513
H	-4.51553	-0.66737	-3.21609
H	-3.65613	-2.00107	-2.41798
H	-4.60723	0.73346	1.84029
H	-3.26693	1.29238	2.87123
H	-4.84295	-1.31654	3.27408
H	-5.03739	0.16258	4.23626
H	-3.51042	-0.74100	4.30700
H	0.27929	0.09064	4.30390
H	-0.83653	-1.08513	3.58107
H	-1.10705	0.66497	3.37714
H	0.37782	2.02109	1.78424
H	1.90813	1.29330	1.21309
H	1.64084	1.55761	2.93146
H	1.33285	-2.14513	2.52195
H	2.24313	-0.84603	3.31897
H	2.42140	-1.09322	1.57868
H	0.88927	-1.63235	-2.82033
H	0.26631	-3.28972	-2.71772
H	-0.82347	-1.92167	-2.40318
H	2.72159	-2.10764	-1.08672
H	2.29483	-3.01034	0.39449
H	2.14689	-3.78202	-1.19395
H	-0.25121	-4.33779	-0.60276
H	-1.40287	-3.06935	-0.16244
H	-0.07711	-3.52715	0.95429

3a+•_df, SMD Methanol

N	0.66457	-0.95030	0.10467
O	1.45813	0.08332	-0.06503
C	0.94602	1.38506	-0.60809
C	0.75059	1.22775	-2.10356
C	2.00435	2.38727	-0.24205
C	3.34122	2.18098	-0.59655
C	4.31171	3.12808	-0.28694
C	3.94018	4.30547	0.36891
C	2.60773	4.52870	0.71941
C	1.64995	3.56575	0.41907
O	4.84204	5.27509	0.69265
C	-0.57730	-0.85511	0.87963
P	-2.01346	-0.26141	-0.13748
O	-2.26349	1.20525	-0.21696
O	-1.64443	-0.98723	-1.50595
C	-2.50790	-0.81561	-2.66858
C	-1.84077	-1.50174	-3.83549
O	-3.23271	-1.09510	0.45920
C	-4.48991	-0.46116	0.83502
C	-5.40814	-0.35723	-0.36019
C	-0.41346	-0.26929	2.32819
C	-1.73035	-0.54518	3.07045
C	-0.10963	1.22720	2.41296
C	0.71963	-1.04538	3.00845
C	1.33228	-2.23319	-0.34382
C	2.66171	-2.38487	0.40584
C	0.42739	-3.42880	-0.07677
C	1.58439	-2.07816	-1.84882
H	0.00869	1.61991	-0.10560
H	1.70160	1.02050	-2.60084
H	0.35751	2.17732	-2.48030
H	0.03430	0.43793	-2.33904
H	3.63336	1.27110	-1.11559
H	5.35222	2.96459	-0.55494
H	2.33804	5.44895	1.22823
H	0.61327	3.73446	0.70082
H	5.73126	5.03007	0.39668
H	-0.86279	-1.89909	1.02745
H	-2.63507	0.25637	-2.84745
H	-3.47797	-1.26480	-2.43647
H	-0.87807	-1.03549	-4.06401
H	-2.48495	-1.41620	-4.71525
H	-1.68406	-2.56300	-3.62170
H	-4.27688	0.52064	1.26525
H	-4.89905	-1.11036	1.61071
H	-4.98262	0.30168	-1.12378
H	-6.36670	0.06241	-0.03991
H	-5.58950	-1.34309	-0.79756
H	-2.04217	-1.59084	2.97964
H	-2.54230	0.09832	2.71692
H	-1.57760	-0.32265	4.13075
H	0.88630	1.46450	2.03081
H	-0.12335	1.51219	3.47033
H	-0.85811	1.83412	1.89452
H	0.75589	-0.76876	4.06666
H	1.69031	-0.79839	2.56729
H	0.56356	-2.12788	2.94076
H	3.29373	-1.50189	0.28667
H	2.50068	-2.58170	1.46751
H	3.18065	-3.24332	-0.02909
H	0.26973	-3.59703	0.99273
H	-0.53642	-3.33646	-0.58683
H	0.93843	-4.30762	-0.47799
H	2.27979	-1.26050	-2.05149
H	2.02980	-3.00990	-2.20701
H	0.64845	-1.90624	-2.38646

3a+•_fd, SMD Methanol

N	0.72480	-0.08080	1.17447
O	0.43150	1.17982	1.39394
C	1.28271	2.34701	1.01154
C	0.83577	3.41047	1.99281
C	1.00053	2.66753	-0.43145
C	-0.31752	2.82006	-0.87297
C	-0.59174	3.13254	-2.19943
C	0.46585	3.31528	-3.09467
C	1.78754	3.19435	-2.66273
C	2.04702	2.85979	-1.33688
O	0.26064	3.60544	-4.41051
C	-0.50087	-0.87339	1.06469
P	-1.18302	-0.72630	-0.65432
O	-2.29760	0.22712	-0.91768
O	0.16680	-0.44332	-1.44828
C	0.17579	-0.27378	-2.89539
C	0.44373	-1.59818	-3.57512
O	-1.57702	-2.24862	-0.94830
C	-2.78253	-2.57180	-1.69595
C	-2.89305	-4.07637	-1.73719
C	-1.54284	-0.68102	2.21801
C	-2.63258	-1.74141	1.98380
C	-2.21005	0.69983	2.29852
C	-0.82549	-0.97464	3.53992
C	2.13519	-0.63079	1.27759
C	3.00219	-0.14259	0.10227
C	2.70362	-0.20690	2.63730
C	2.06229	-2.15696	1.21273
H	2.32916	2.10182	1.16921
H	-0.22901	3.62814	1.87191
H	1.40420	4.32189	1.79060
H	1.03034	3.09080	3.02020
H	-1.14220	2.67647	-0.17902
H	-1.61723	3.23015	-2.54671
H	2.59607	3.34635	-3.37113
H	3.07703	2.75568	-1.00573
H	-0.68736	3.65052	-4.60567
H	-0.19331	-1.91696	1.10858
H	0.97585	0.44529	-3.08362
H	-0.77445	0.17023	-3.20893

H	1.38098	-2.03052	-3.21247
H	0.53113	-1.43581	-4.65363
H	-0.36767	-2.31013	-3.39801
H	-2.69454	-2.14368	-2.69919
H	-3.63658	-2.11698	-1.18669
H	-2.02513	-4.51724	-2.23576
H	-3.79269	-4.35621	-2.29263
H	-2.96793	-4.48499	-0.72522
H	-2.20614	-2.74302	1.86204
H	-3.24542	-1.51186	1.10436
H	-3.29873	-1.75517	2.85159
H	-1.53067	1.46364	2.68156
H	-3.05278	0.62474	2.99438
H	-2.60010	1.02516	1.33086
H	-1.55525	-0.95809	4.35593
H	-0.06729	-0.21477	3.75690
H	-0.34591	-1.95994	3.52769
H	2.44045	-0.14700	-0.83423
H	3.43285	0.84369	0.26836
H	3.83491	-0.84427	0.00814
H	2.67580	0.87326	2.79522
H	2.16498	-0.69861	3.45088
H	3.74865	-0.52792	2.66602
H	1.67769	-2.50577	0.24881
H	1.47215	-2.57965	2.02972
H	3.08635	-2.52186	1.31887

3a+•_fl, SMD Methanol

N	0.58451	-0.17546	1.26975
O	0.20505	1.02149	0.88173
C	1.07835	2.20033	0.63420
C	0.42781	3.30869	1.43804
C	1.08661	2.44097	-0.85321
C	-0.09928	2.41286	-1.59259
C	-0.09157	2.69550	-2.95476
C	1.11093	3.02671	-3.58402
C	2.30024	3.07298	-2.85448
C	2.28244	2.77160	-1.49583
O	1.17950	3.30940	-4.91636
C	-0.59406	-1.05233	1.28951
P	-1.35310	-1.05293	-0.40264
O	-2.39702	-0.03329	-0.70566
O	-0.02577	-0.97250	-1.28183
C	-0.12453	-0.94573	-2.73486
C	1.25167	-0.65162	-3.27971
O	-1.86667	-2.55845	-0.54909
C	-3.20736	-2.87615	-1.01737
C	-3.24669	-2.93476	-2.52689
C	-1.58503	-0.76749	2.46881
C	-2.78434	-1.71258	2.30238
C	-2.08124	0.68119	2.52851
C	-0.87028	-1.10729	3.78090
C	2.02690	-0.58592	1.49183
C	2.86018	-0.26195	0.23543
C	2.55734	0.11000	2.75366
C	2.05791	-2.09880	1.71474
H	2.07965	1.99791	0.99894
H	-0.60809	3.45664	1.11923
H	0.98559	4.23194	1.25838
H	0.45553	3.07836	2.50641
H	-1.03842	2.15882	-1.10713
H	-1.01229	2.66144	-3.53140
H	3.22592	3.33210	-3.35919
H	3.21059	2.79990	-0.92987
H	0.30184	3.25260	-5.32341
H	-0.23094	-2.07250	1.41386
H	-0.84333	-0.17081	-3.01820
H	-0.49136	-1.92217	-3.06544
H	1.62411	0.30256	-2.89423
H	1.19985	-0.58869	-4.37088
H	1.95456	-1.44541	-3.00997
H	-3.90579	-2.13167	-0.62747
H	-3.43017	-3.84459	-0.56650
H	-3.03258	-1.95337	-2.96213
H	-4.24698	-3.24178	-2.84747
H	-2.52248	-3.66100	-2.90689
H	-2.46724	-2.75138	2.16025
H	-3.42550	-1.41869	1.46471
H	-3.39320	-1.66292	3.21028
H	-1.28387	1.36953	2.82125
H	-2.86712	0.73979	3.28915
H	-2.50198	1.01351	1.57543
H	-1.55924	-0.94536	4.61622
H	0.00124	-0.46490	3.94083
H	-0.54686	-2.15362	3.80172
H	2.25558	-0.33600	-0.67098
H	3.33413	0.71867	0.27840
H	3.66057	-1.00343	0.17251
H	2.38153	1.18737	2.76801
H	2.11276	-0.32729	3.64995
H	3.63759	-0.05915	2.78663
H	1.74401	-2.64579	0.82039
H	1.46098	-2.40749	2.57611
H	3.09889	-2.35752	1.92232

3a(II) TS_dn, SMD Methanol

N	0.52933	-1.09556	-0.84375
O	1.12386	0.02011	-1.03960
C	0.32376	1.87544	-1.10024
C	-0.62896	1.70880	-2.21571
C	1.54015	2.61991	-1.20361
C	2.22966	2.76707	-2.42730
C	3.39523	3.50417	-2.49276
C	3.88598	4.12264	-1.32960
C	3.21321	3.99718	-0.10447
C	2.06211	3.23908	-0.04533
O	5.01217	4.85569	-1.33372
C	0.00007	-1.40501	0.49034
P	-1.76438	-0.85540	0.60127
O	-2.42057	-0.68693	-0.73003
O	-2.33890	-2.04093	1.50191
C	-3.66962	-1.94806	2.07997
C	-3.92462	-3.23262	2.83110
O	-1.85747	0.44247	1.52626
C	-2.54339	1.65854	1.11738
C	-3.97014	1.65402	1.61440
C	0.96439	-1.08334	1.67825
C	0.31908	-1.63295	2.96063
C	1.29453	0.39831	1.88508
C	2.27095	-1.84460	1.41865
C	0.63349	-2.09783	-1.96992
C	0.14889	-1.40517	-3.24417
C	2.10789	-2.49155	-2.10275
C	-0.22689	-3.32897	-1.69519
H	-0.09360	1.80612	-0.09693
H	-0.15151	1.61995	-3.19168
H	-1.22355	2.63652	-2.21302
H	-1.31653	0.88209	-2.03197
H	1.85764	2.28425	-3.32565
H	3.93851	3.61310	-3.42709
H	3.61472	4.49259	0.77327
H	1.53268	3.13312	0.89764
H	5.41349	4.87978	-2.21630
H	-0.11875	-2.49118	0.51016
H	-4.39181	-1.80340	1.27068
H	-3.69131	-1.08109	2.74694
H	-3.88718	-4.09093	2.15472
H	-4.91697	-3.19283	3.28903
H	-3.18128	-3.36855	3.62197
H	-2.50072	1.74271	0.02824
H	-1.96166	2.46868	1.56286
H	-4.54191	0.84445	1.15047
H	-4.44335	2.60525	1.35198
H	-4.00297	1.53866	2.70150
H	0.02995	-2.68329	2.84955
H	-0.56554	-1.05866	3.25493
H	1.04739	-1.56205	3.77455
H	0.39575	1.01383	1.97886
H	1.91448	0.78347	1.07413
H	1.86451	0.49484	2.81610
H	2.08907	-2.91701	1.28414
H	2.93976	-1.71632	2.27608
H	2.78664	-1.46133	0.53228
H	0.75296	-0.52366	-3.46978
H	0.24517	-2.11086	-4.07367
H	-0.90201	-1.11437	-3.15514
H	2.73432	-1.60864	-2.25923
H	2.45543	-3.02835	-1.21610
H	2.21359	-3.15169	-2.96863
H	-0.21157	-3.94388	-2.59912
H	-1.26879	-3.06310	-1.48986
H	0.16442	-3.94166	-0.87809

3a(II) TS_bh, SMD Methanol

N	0.64770	-0.65281	1.09762
O	1.37527	-0.04208	0.23801
C	1.05616	0.24322	-1.72801
C	1.01190	-1.16475	-2.17608
C	2.15740	1.11795	-1.99548
C	3.46838	0.63823	-2.20722
C	4.49759	1.51095	-2.49787
C	4.23024	2.88707	-2.59579
C	2.93606	3.38757	-2.38777
C	1.91800	2.50827	-2.07791
O	5.19284	3.77796	-2.89127
C	-0.66561	-0.09439	1.44655
P	-1.93894	-0.70604	0.25540
O	-1.60588	-2.07036	-0.25330
O	-3.33068	-0.64793	1.03881
C	-3.77196	-1.78090	1.83744
C	-4.76110	-2.60805	1.04902
O	-2.11478	0.43348	-0.83638
C	-3.05394	0.23283	-1.93790
C	-2.30875	-0.21159	-3.17452

C	-0.63972	1.41652	1.85104
C	-2.04430	1.79294	2.34478
C	-0.22607	2.39154	0.74394
C	0.35109	1.55390	3.01450
C	1.31664	-1.81343	1.79844
C	1.77732	-2.78928	0.71344
C	2.52373	-1.26720	2.56732
C	0.35334	-2.51289	2.75197
H	0.09480	0.73392	-1.58537
H	1.97391	-1.67376	-2.11372
H	0.72390	-1.11484	-3.23779
H	0.23827	-1.72837	-1.65264
H	3.68428	-0.42262	-2.12983
H	5.50980	1.14977	-2.65497
H	2.76017	4.45473	-2.47376
H	0.91048	2.88254	-1.91765
H	6.04881	3.34058	-3.02414
H	-0.98087	-0.62543	2.35156
H	-4.22817	-1.34116	2.72653
H	-2.90471	-2.37443	2.14467
H	-5.60984	-1.99295	0.73629
H	-5.13521	-3.42318	1.67593
H	-4.28716	-3.03939	0.16262
H	-3.53398	1.20277	-2.07582
H	-3.81442	-0.49418	-1.63573
H	-1.53284	0.51315	-3.43941
H	-3.01205	-0.28504	-4.00969
H	-1.84822	-1.19154	-3.02196
H	-2.41061	1.08875	3.10024
H	-2.76853	1.83155	1.52535
H	-1.99964	2.78807	2.79828
H	-0.85340	2.29659	-0.14571
H	0.81944	2.25539	0.46026
H	-0.33859	3.41146	1.12882
H	0.31339	2.57742	3.40138
H	1.37689	1.35916	2.68616
H	0.10680	0.86872	3.83475
H	0.92934	-3.14873	0.12340
H	2.50960	-2.32252	0.05067
H	2.25111	-3.64539	1.20150
H	3.18152	-0.69474	1.90754
H	2.20981	-0.63559	3.40227
H	3.08735	-2.11391	2.96979
H	-0.54351	-2.87260	2.23772
H	0.06563	-1.87597	3.59390
H	0.87601	-3.38130	3.16186

3a(II) TS_ap, SMD Methanol

N	-0.14174	0.99080	-1.05178
O	1.01781	0.72570	-0.57482
C	1.53715	0.11921	1.26667
C	0.99187	1.23113	2.07426
C	2.93597	-0.06394	1.02350
C	3.84941	1.01250	1.03140
C	5.19261	0.79584	0.79744
C	5.65006	-0.51110	0.55858
C	4.76190	-1.59728	0.54984
C	3.41833	-1.36742	0.76803
O	6.94810	-0.77693	0.32961
C	-1.12145	-0.09236	-1.19695
P	-1.98709	-0.38960	0.40378
O	-1.34341	-1.28144	1.41385
O	-2.18517	1.12173	0.88062
C	-2.85816	1.42032	2.13698
C	-4.32823	1.68527	1.89782
O	-3.43189	-0.88933	-0.06186
C	-4.12325	-1.94822	0.65633
C	-5.38681	-2.25650	-0.10924
C	-0.58235	-1.35271	-1.94859
C	-1.76688	-2.30199	-2.18773
C	0.52060	-2.12191	-1.21535
C	-0.04285	-0.87741	-3.30300
C	-0.31288	2.39706	-1.57790
C	-1.71982	2.61507	-2.12433
C	-0.04459	3.35068	-0.41074
C	0.72340	2.61074	-2.68600
H	0.92741	-0.78112	1.23064
H	1.55681	2.15910	1.98702
H	1.06175	0.88148	3.11613
H	-0.06393	1.40467	1.86350
H	3.50112	2.02566	1.20586
H	5.90144	1.61903	0.79364
H	5.14684	-2.59538	0.36873
H	2.71947	-2.19971	0.76451
H	7.48134	0.03318	0.35938
H	-1.92509	0.30755	-1.82034
H	-2.34967	2.30631	2.52325
H	-2.69565	0.59374	2.83599
H	-4.45770	2.49642	1.17555
H	-4.79641	1.98276	2.84094
H	-4.83887	0.79286	1.52475
H	-4.33827	-1.59566	1.66980
H	-3.46323	-2.81822	0.71441
H	-6.02930	-1.37355	-0.17104
H	-5.93542	-3.05081	0.40488
H	-5.15066	-2.59610	-1.12202
H	-1.44267	-3.09957	-2.86344
H	-2.61612	-1.78578	-2.64810
H	-2.10655	-2.77652	-1.26054
H	0.21176	-2.42256	-0.20963
H	1.43957	-1.53696	-1.14825
H	0.74202	-3.03148	-1.78489
H	-0.79801	-0.30780	-3.85736
H	0.23961	-1.74721	-3.90494
H	0.84806	-0.25376	-3.17921
H	-1.91716	2.00360	-3.00999
H	-2.48801	2.42664	-1.36863
H	-1.79218	3.66372	-2.42535
H	-0.75648	3.18422	0.40295
H	0.97382	3.23020	-0.03321
H	-0.15893	4.37646	-0.77193
H	0.68154	3.65821	-2.99816
H	0.50728	1.98412	-3.55535
H	1.73327	2.39556	-2.32687

3a(II) TS_an, SMD Methanol

N	0.54762	-1.11325	-0.09050
O	1.24416	-0.14684	-0.56245
C	0.63442	1.60057	-1.34734
C	-0.18155	1.10463	-2.47641
C	1.92367	2.20053	-1.51222
C	2.76509	1.89420	-2.60361
C	3.99796	2.50244	-2.73329
C	4.40767	3.44398	-1.77374
C	3.58700	3.76641	-0.68228
C	2.36578	3.13681	-0.55096
O	5.59325	4.07360	-1.85262
C	-0.22892	-0.90155	1.13618
P	-1.83789	-0.08455	0.74954
O	-1.88032	1.40580	0.66850
O	-2.20725	-0.83937	-0.60958
C	-3.46914	-0.52651	-1.26482
C	-3.51163	-1.29558	-2.56310
O	-2.83125	-0.69542	1.84281
C	-3.80011	0.13987	2.53620
C	-4.36602	-0.67787	3.67157
C	0.58688	-0.29319	2.32209
C	-0.31753	-0.30743	3.56419
C	1.09084	1.13587	2.09610
C	1.78960	-1.21111	2.56820
C	0.75213	-2.44704	-0.77160
C	0.42825	-2.24891	-2.25403
C	2.22232	-2.84233	-0.59993
C	-0.15602	-3.51615	-0.17287
H	0.08066	1.90543	-0.46135
H	0.40322	0.66979	-3.28727
H	-0.69469	1.99867	-2.86413
H	-0.95296	0.40960	-2.14153
H	2.45734	1.16273	-3.34417
H	4.65631	2.26519	-3.56405
H	3.92961	4.50046	0.03951
H	1.72155	3.37766	0.29027
H	6.09642	3.78797	-2.63142
H	-0.54807	-1.89317	1.46616
H	-3.51279	0.55377	-1.43485
H	-4.28235	-0.82101	-0.59392
H	-2.70189	-0.98015	-3.22770
H	-4.46506	-1.10411	-3.06368
H	-3.42520	-2.37040	-2.37896
H	-4.57302	0.43168	1.81957
H	-3.29422	1.03853	2.89931
H	-4.85138	-1.58240	3.29454
H	-5.10972	-0.08223	4.20861
H	-3.57629	-0.96306	4.37279
H	0.28578	-0.04751	4.43954
H	-0.76015	-1.29501	3.73268
H	-1.12369	0.43123	3.49297
H	0.27868	1.82018	1.83362
H	1.85491	1.17303	1.31731
H	1.54363	1.49198	3.02829
H	1.47654	-2.25038	2.72250
H	2.32152	-0.87703	3.46499
H	2.49297	-1.17504	1.73039
H	1.09977	-1.51578	-2.70730
H	0.56483	-3.20504	-2.76660
H	-0.60750	-1.92458	-2.38809
H	2.88555	-2.04990	-0.95743
H	2.45351	-3.06462	0.44492
H	2.40726	-3.74333	-1.19202
H	-0.01506	-4.42798	-0.75952
H	-1.21204	-3.23603	-0.23077
H	0.10697	-3.74793	0.86348

3a(II) TS_df, SMD Methanol

N	0.73327	-1.03360	0.28816
O	1.34970	0.08454	0.18345
C	0.79692	1.74845	-0.80565
C	0.58640	1.20031	-2.16260
C	1.91746	2.56452	-0.45221
C	3.14636	2.50026	-1.14471
C	4.20193	3.31156	-0.78007
C	4.04350	4.21435	0.28554
C	2.83122	4.29684	0.98776
C	1.78737	3.46979	0.62529
O	5.03507	5.03311	0.67803
C	-0.52267	-1.08682	1.04705
P	-1.93661	-0.55489	-0.01600
O	-2.19984	0.90780	-0.15807
O	-1.54323	-1.30683	-1.36894
C	-2.42146	-1.20880	-2.52542
C	-1.69478	-1.81224	-3.70328
O	-3.18105	-1.37892	0.55437
C	-4.44332	-0.73875	0.88996
C	-5.34993	-0.68899	-0.31820
C	-0.44058	-0.44809	2.47148
C	-1.75457	-0.76285	3.20363
C	-0.22073	1.06839	2.49119
C	0.71653	-1.12950	3.21162
C	1.48692	-2.23354	-0.23814
C	2.78283	-2.36574	0.56858
C	0.65614	-3.50649	-0.11436
C	1.80711	-1.95229	-1.70798
H	-0.10114	1.88882	-0.20807
H	1.50815	0.94356	-2.68439
H	0.08852	2.01052	-2.71801
H	-0.09657	0.35026	-2.15621
H	3.27880	1.80143	-1.96449
H	5.15213	3.26479	-1.30425
H	2.73822	5.00760	1.80220
H	0.84214	3.52543	1.15888
H	5.82765	4.91694	0.13025
H	-0.73548	-2.14728	1.20426
H	-2.65645	-0.15353	-2.69744
H	-3.34226	-1.75318	-2.29577
H	-0.78709	-1.24603	-3.93231
H	-2.34903	-1.78686	-4.57944
H	-1.42609	-2.85316	-3.50087
H	-4.24294	0.26198	1.28133
H	-4.86067	-1.35609	1.68750
H	-4.91869	-0.05984	-1.10331
H	-6.31468	-0.26273	-0.02634
H	-5.52063	-1.69299	-0.71708
H	-2.01621	-1.82448	3.13746
H	-2.59051	-0.17128	2.81641
H	-1.63658	-0.50337	4.26026
H	0.77061	1.33413	2.11975
H	-0.29456	1.41247	3.52898
H	-0.97725	1.59993	1.90605
H	0.73196	-0.78574	4.25096
H	1.68121	-0.87508	2.76169
H	0.60419	-2.22007	3.21343
H	3.35356	-1.43328	0.55044
H	2.57833	-2.64534	1.60514
H	3.39057	-3.15350	0.11402
H	0.48504	-3.78762	0.92885
H	-0.30273	-3.42247	-0.63373
H	1.22615	-4.31362	-0.58251
H	2.43355	-1.06269	-1.81045
H	2.35503	-2.80867	-2.11060
H	0.89055	-1.81904	-2.28928

a+, SMD Methanol

C	-0.83174	3.29476	0.11294
C	0.24058	2.29312	0.18889
C	0.13716	0.92231	0.09665
C	-1.11075	0.23957	-0.09880
C	-1.15282	-1.12265	-0.18266
C	0.05469	-1.86107	-0.07404
C	1.30317	-1.22095	0.11877
C	1.33831	0.14101	0.20166
O	0.07642	-3.17788	-0.14693
H	-0.58669	3.99499	-0.69686
H	-0.80261	3.89487	1.03227
H	-1.83049	2.88925	-0.03526
H	1.24472	2.69008	0.33736
H	-2.03241	0.80541	-0.18141
H	-2.08754	-1.65462	-0.33026
H	2.19673	-1.83067	0.19533
H	2.28234	0.65823	0.34949
H	-0.80678	-3.56302	-0.27922

NO+_au, SMD Methanol

N	0.94725	-1.10074	0.65401
O	0.43507	-2.15506	0.84222
C	0.46047	-0.28492	-0.47609
P	-1.20842	0.33817	0.08425
O	-2.15244	-0.74031	0.47787
O	-0.71785	1.30927	1.23984
C	-1.71412	2.09694	1.96996
C	-1.90629	1.52078	3.35203
O	-1.70522	1.30400	-1.06654
C	-2.94924	1.07896	-1.80146
C	-3.28171	2.36896	-2.50889
C	0.51570	-1.07722	-1.83578
C	0.46286	-0.02476	-2.95298
C	-0.62056	-2.08528	-2.01748
C	1.87084	-1.79570	-1.91285
C	2.06946	-0.68072	1.62359
C	3.14559	-1.76240	1.48509
C	2.60845	0.69534	1.27575
C	1.41664	-0.71196	3.00927
H	1.11114	0.58685	-0.54480
H	-2.65007	2.10980	1.40267
H	-1.30931	3.10948	1.99757
H	-2.25877	0.48668	3.29713
H	-2.65426	2.11593	3.88451
H	-0.97270	1.55299	3.91983
H	-3.72309	0.79163	-1.08670
H	-2.78222	0.26063	-2.50659
H	-2.48460	2.64792	-3.20365
H	-3.42848	3.17847	-1.78855
H	-4.20680	2.23467	-3.07667
H	1.27360	0.70383	-2.84834
H	-0.48895	0.51027	-2.97547
H	0.58572	-0.53875	-3.91118
H	-0.64140	-2.83765	-1.22497
H	-0.46428	-2.60230	-2.96982
H	-1.59816	-1.59660	-2.06101
H	1.93654	-2.63714	-1.21513
H	2.69835	-1.10445	-1.71583
H	1.99441	-2.19733	-2.92264
H	3.91775	-1.53321	2.22373
H	2.73877	-2.75419	1.69527
H	3.59782	-1.74695	0.49056
H	3.38121	0.92017	2.01540
H	3.07796	0.71448	0.28839
H	1.83978	1.46903	1.34434
H	0.58958	-0.00007	3.06544
H	1.06071	-1.71523	3.25320
H	2.18351	-0.42235	3.73161

NO+_ak, SMD Methanol

N	1.19623	-0.45080	1.14884
O	1.19313	-1.63649	1.12387
C	0.62836	0.27592	-0.00346
P	-1.21794	0.31932	0.32235
O	-1.53960	1.24670	1.43929
O	-1.91999	0.66972	-1.05327
C	-2.28864	2.05096	-1.36608
C	-2.95912	2.03334	-2.71687
O	-1.50791	-1.21509	0.54413
C	-2.88147	-1.71688	0.64026
C	-3.23259	-2.44904	-0.63221
C	1.14408	-0.29004	-1.37621
C	0.94930	0.83683	-2.40188
C	0.42110	-1.55217	-1.85504
C	2.65233	-0.56014	-1.24832
C	1.79537	0.22275	2.39734
C	3.20583	-0.36014	2.51863
C	1.82310	1.73318	2.24503
C	0.89191	-0.22610	3.55173
H	0.94794	1.31469	0.09804
H	-1.37688	2.65580	-1.36925
H	-2.95835	2.40609	-0.58032
H	-2.27799	1.66061	-3.48703
H	-3.25833	3.05189	-2.97962
H	-3.85229	1.40284	-2.69430
H	-3.55801	-0.87964	0.83493
H	-2.87794	-2.37655	1.50865
H	-2.52256	-3.26007	-0.81692
H	-3.23325	-1.76973	-1.48906
H	-4.23287	-2.88059	-0.53000
H	1.46298	1.75262	-2.09084
H	-0.10620	1.06013	-2.57029
H	1.37809	0.51146	-3.35459
H	0.50632	-2.37492	-1.14096
H	0.88340	-1.86899	-2.79560
H	-0.63831	-1.36227	-2.05129
H	2.87644	-1.43184	-0.62575
H	3.17719	0.31229	-0.84077
H	3.05271	-0.76123	-2.24613
H	3.66052	0.08818	3.40537
H	3.17827	-1.44424	2.64488
H	3.81280	-0.10266	1.64619
H	2.24546	2.12933	3.17207
H	2.47106	2.04777	1.42150
H	0.82240	2.15583	2.12434
H	-0.12661	0.15064	3.42463

H	0.87898	-1.31512	3.63613
H	1.31174	0.19606	4.46808

NO+_aq, SMD Methanol

N	1.11760	-1.30750	0.22132
O	0.74072	-2.43178	0.16761
C	0.35863	-0.28547	-0.52770
P	-1.21142	-0.06486	0.45822
O	-2.00230	-1.31277	0.62036
O	-0.55977	0.53766	1.77147
C	-1.41366	0.96407	2.88106
C	-1.29688	2.46082	3.03806
O	-1.97353	1.14940	-0.21356
C	-3.29630	1.00440	-0.82187
C	-3.78439	2.39411	-1.14620
C	0.20766	-0.66136	-2.04739
C	-0.14268	0.64218	-2.77975
C	-0.86051	-1.72044	-2.32892
C	1.57276	-1.14826	-2.55486
C	2.36679	-1.02537	1.08139
C	3.47572	-1.88474	0.46439
C	2.72311	0.45024	1.06462
C	1.99778	-1.51283	2.48651
H	0.91075	0.65054	-0.44205
H	-1.04385	0.42579	3.75538
H	-2.44462	0.65210	2.68772
H	-0.25667	2.74834	3.21497
H	-1.89575	2.78073	3.89588
H	-1.66320	2.97513	2.14517
H	-3.94593	0.49755	-0.10517
H	-3.19471	0.38987	-1.72022
H	-3.10955	2.88898	-1.85023
H	-3.86126	2.99909	-0.23857
H	-4.77515	2.32490	-1.60414
H	0.62185	1.40785	-2.61156
H	-1.11202	1.04418	-2.47675
H	-0.18498	0.43055	-3.85253
H	-0.66427	-2.65842	-1.80328
H	-0.85491	-1.92761	-3.40392
H	-1.86295	-1.37548	-2.06025
H	1.83571	-2.13492	-2.15919
H	2.36783	-0.43831	-2.29910
H	1.52933	-1.23402	-3.64447
H	4.35772	-1.76168	1.09785
H	3.19604	-2.94042	0.44981
H	3.72271	-1.54940	-0.54580
H	3.60423	0.56241	1.70177
H	2.99099	0.79595	0.06225
H	1.92490	1.07087	1.47983
H	1.16457	-0.93530	2.89459
H	2.87700	-1.36093	3.11724
H	1.74679	-2.57575	2.48011

NO+_ae, SMD Methanol

N	1.25386	-0.70980	0.55741
O	1.00619	-1.86561	0.46368
C	0.67911	0.21200	-0.44196
P	-1.03413	0.61277	0.21155
O	-0.97081	1.51795	1.38954
O	-1.85982	1.16796	-1.01823
C	-2.12837	2.59823	-1.16927
C	-3.43985	2.94153	-0.50423
O	-1.59377	-0.84457	0.45729
C	-2.86826	-1.01733	1.15697
C	-3.14811	-2.49770	1.21024
C	0.81771	-0.33201	-1.90890
C	0.70198	0.89357	-2.82861
C	-0.23332	-1.37516	-2.30037
C	2.23019	-0.91633	-2.07433
C	2.15401	-0.28203	1.73210
C	3.43581	-1.10157	1.55675
C	2.43310	1.21000	1.69987
C	1.37847	-0.69838	2.98683
H	1.23332	1.14944	-0.35441
H	-2.16371	2.75473	-2.24839
H	-1.29138	3.16488	-0.75271
H	-4.25091	2.34056	-0.92500
H	-3.66442	3.99827	-0.67758
H	-3.38843	2.76942	0.57462
H	-3.63635	-0.47322	0.59924
H	-2.76201	-0.58429	2.15483
H	-2.35406	-3.01976	1.75150
H	-3.22886	-2.91330	0.20223
H	-4.09366	-2.66412	1.73387
H	1.46514	1.64179	-2.58959
H	-0.28322	1.36069	-2.77313
H	0.85961	0.56374	-3.86010
H	-0.20101	-2.25721	-1.65647
H	-0.02553	-1.69656	-3.32607
H	-1.24488	-0.95964	-2.27933
H	2.36052	-1.86643	-1.54708
H	2.99334	-0.20988	-1.72713
H	2.40250	-1.10740	-3.13738
H	4.09954	-0.83500	2.38291
H	3.22948	-2.17297	1.59882
H	3.93411	-0.85589	0.61491
H	3.05691	1.42611	2.57101
H	2.99494	1.50045	0.80778
H	1.52030	1.80450	1.78422
H	0.43655	-0.14858	3.06853
H	1.18334	-1.77312	2.98675
H	2.00503	-0.45081	3.84712

NO+_bq, SMD Methanol

N	1.17669	-0.17248	0.04753
O	1.09280	-1.30335	-0.29954
C	0.30482	0.82535	-0.62142
P	-1.44355	0.57549	-0.00423
O	-2.47255	1.28064	-0.81069
O	-1.58912	-1.00404	0.04369
C	-2.81360	-1.68726	-0.35985
C	-2.49720	-3.16048	-0.42323
O	-1.30180	1.05807	1.49808
C	-2.42380	0.86504	2.41905
C	-2.23735	-0.40838	3.21163
C	0.41690	0.75393	-2.19743
C	-0.07642	2.11267	-2.71793
C	-0.41281	-0.37810	-2.81570
C	1.88396	0.59459	-2.61761
C	2.22923	0.19135	1.10644
C	2.79160	-1.11488	1.63965
C	3.30279	1.00566	0.37304
C	1.57239	1.01754	2.21019
H	0.62447	1.80964	-0.27004
H	-3.12578	-1.29334	-1.33029
H	-3.58206	-1.46390	0.38592
H	-1.71173	-3.35480	-1.15937
H	-3.39636	-3.70777	-0.72011
H	-2.17120	-3.53063	0.55282
H	-3.35806	0.86572	1.84899
H	-2.40809	1.74775	3.05920
H	-1.29396	-0.38348	3.76408
H	-2.24777	-1.28806	2.56206
H	-3.05622	-0.49945	3.93172
H	0.53668	2.92873	-2.32117
H	-1.12134	2.29826	-2.46282
H	0.01629	2.11539	-3.80841
H	-0.11575	-1.36155	-2.44198
H	-0.24580	-0.36518	-3.89727
H	-1.48534	-0.24083	-2.64967
H	2.31605	-0.36418	-2.31205
H	2.50189	1.40949	-2.23149
H	1.92382	0.63207	-3.71022
H	3.51902	-0.85580	2.41216
H	2.00778	-1.73070	2.08906
H	3.29994	-1.68644	0.85997
H	4.06980	1.22462	1.12102
H	3.75754	0.42933	-0.43529
H	2.91713	1.95438	-0.00722
H	1.14802	1.95383	1.84291
H	0.80466	0.44449	2.73206
H	2.37319	1.26106	2.91358

NO+_aa, SMD Methanol

N	1.14002	-0.77525	0.75041
O	0.81678	-1.91249	0.65657
C	0.61312	0.18699	-0.23737
P	-1.08398	0.65012	0.41230
O	-0.98295	1.47546	1.64497
O	-1.85789	1.33264	-0.78886
C	-1.87488	2.78959	-0.92792
C	-2.70842	3.10857	-2.14354
O	-1.73672	-0.78053	0.54861
C	-3.05068	-0.94085	1.17294
C	-3.41621	-2.39935	1.06243
C	0.74786	-0.33995	-1.71212
C	0.70478	0.90346	-2.61333
C	-0.34484	-1.32374	-2.13899
C	2.13331	-0.98864	-1.86564
C	2.08657	-0.40894	1.90874
C	3.31303	-1.30414	1.70797
C	2.45376	1.06396	1.87471
C	1.31141	-0.77948	3.17786
H	1.20831	1.09570	-0.12856
H	-0.84217	3.13501	-1.03758
H	-2.30388	3.20889	-0.01561
H	-2.27229	2.66789	-3.04441
H	-2.74993	4.19386	-2.27158
H	-3.72793	2.73317	-2.01990
H	-3.75928	-0.30048	0.64040
H	-2.96766	-0.61496	2.21271
H	-2.68049	-3.02143	1.57975
H	-3.47083	-2.70501	0.01399
H	-4.39437	-2.55938	1.52450

H	1.49100	1.61681	-2.34437
H	-0.26297	1.40760	-2.57308
H	0.87263	0.58401	-3.64639
H	-0.37330	-2.21250	-1.50391
H	-0.12750	-1.64527	-3.16274
H	-1.33408	-0.85669	-2.13779
H	2.20927	-1.95505	-1.35763
H	2.92314	-0.32662	-1.49116
H	2.31567	-1.16559	-2.92946
H	4.00452	-1.08327	2.52483
H	3.04291	-2.36135	1.74845
H	3.81044	-1.08344	0.75948
H	3.10750	1.23869	2.73312
H	3.01178	1.32633	0.97133
H	1.57939	1.71107	1.98180
H	0.40435	-0.17644	3.27375
H	1.05543	-1.84136	3.18370
H	1.96629	-0.56775	4.02651

NO+_am, SMD Methanol

N	0.79757	-0.74771	0.73091
O	0.28623	-1.78354	1.00584
C	0.39345	-0.08180	-0.52190
P	-1.25283	0.70389	-0.09550
O	-1.09329	1.61069	1.07246
O	-1.74369	1.36745	-1.44465
C	-1.25176	2.68752	-1.84593
C	-2.21502	3.75462	-1.38360
O	-2.22387	-0.52469	0.09312
C	-3.15820	-0.60525	1.21788
C	-2.52621	-1.37721	2.34931
C	0.51100	-1.02342	-1.77631
C	0.56555	-0.10119	-3.00360
C	-0.63756	-2.02034	-1.94035
C	1.84802	-1.77358	-1.67883
C	1.84420	-0.19231	1.71895
C	2.96431	-1.23864	1.73023
C	2.35008	1.16848	1.27268
C	1.13094	-0.12270	3.07133
H	1.07490	0.75962	-0.65702
H	-1.18872	2.63687	-2.93375
H	-0.24538	2.83691	-1.44124
H	-3.21400	3.56744	-1.78672
H	-1.87047	4.72744	-1.74681
H	-2.26911	3.78895	-0.29229
H	-4.02903	-1.11605	0.80610
H	-3.44272	0.40616	1.51577
H	-1.64480	-0.85270	2.73166
H	-2.23289	-2.37767	2.01788
H	-3.24919	-1.47792	3.16457
H	1.36826	0.63881	-2.91362
H	-0.38136	0.41678	-3.16906
H	0.76886	-0.71762	-3.88473
H	-0.75578	-2.66736	-1.06728
H	-0.41104	-2.65408	-2.80398
H	-1.58722	-1.51432	-2.13516
H	1.85195	-2.52119	-0.87884
H	2.68081	-1.07861	-1.52063
H	2.02012	-2.30179	-2.62100
H	3.69774	-0.90475	2.46849
H	2.58482	-2.21940	2.02625
H	3.45641	-1.30691	0.75738
H	3.04693	1.50709	2.04372
H	2.89930	1.11300	0.32857
H	1.54384	1.90359	1.20013
H	0.29902	0.58529	3.03868
H	0.77438	-1.10736	3.38137
H	1.86557	0.22954	3.79946

NO+_af, SMD Methanol

N	1.06170	-0.51175	0.79775
O	0.67700	-1.63544	0.79819
C	0.62448	0.37043	-0.30233
P	-1.11358	0.85069	0.19992
O	-1.11408	1.63874	1.46126
O	-1.61313	1.55867	-1.11536
C	-2.98804	2.05972	-1.19835
C	-3.19801	2.53633	-2.61332
O	-1.91708	-0.51543	0.28199
C	-2.37632	-1.07405	1.55285
C	-2.57865	-2.55364	1.34205
C	0.86136	-0.28108	-1.71606
C	0.95749	0.88529	-2.71165
C	-0.23591	-1.25365	-2.15545
C	2.21942	-0.99973	-1.69710
C	1.98395	-0.07964	1.95252
C	3.19970	-1.00683	1.85057
C	2.37575	1.38105	1.82136
C	1.17718	-0.34342	3.22794
H	1.21279	1.28522	-0.22246
H	-3.09241	2.86866	-0.47133
H	-3.66348	1.23941	-0.93969
H	-2.49614	3.33766	-2.85975
H	-4.21633	2.92285	-2.71182
H	-3.06711	1.71315	-3.32121
H	-3.30452	-0.56121	1.81483
H	-1.62420	-0.87391	2.32097
H	-1.63491	-3.03988	1.07777
H	-3.30951	-2.73598	0.54944
H	-2.95211	-2.99887	2.26869
H	1.77834	1.56036	-2.44732
H	0.03053	1.45923	-2.76502
H	1.16286	0.47193	-3.70392
H	-0.36525	-2.07715	-1.44823
H	0.05768	-1.67894	-3.12064
H	-1.19755	-0.74960	-2.29038
H	2.20209	-1.92217	-1.10809
H	3.00837	-0.34473	-1.30926
H	2.47932	-1.27343	-2.72368
H	3.86183	-0.75067	2.68134
H	2.90583	-2.05495	1.94135
H	3.73851	-0.85084	0.91257
H	2.99792	1.61218	2.68993
H	2.97247	1.56853	0.92440
H	1.50675	2.04398	1.84445
H	0.29021	0.29426	3.26767
H	0.88799	-1.39430	3.30100
H	1.82651	-0.09714	4.07159

NO+_bd, SMD Methanol

N	1.40725	-0.58534	0.60291
O	1.25358	-1.66391	1.06712
C	0.57357	-0.19875	-0.56151
P	-1.12004	0.16055	0.17768
O	-1.16992	-0.20483	1.62002
O	-1.20043	1.69459	-0.21470
C	-2.35627	2.49248	0.19367
C	-2.10200	3.12499	1.54245
O	-2.25021	-0.51967	-0.70122
C	-3.14014	-1.54122	-0.15142
C	-4.35086	-0.89071	0.47416
C	0.68065	-1.22006	-1.74704
C	-0.01867	-0.54805	-2.93865
C	0.06433	-2.59447	-1.47078
C	2.16515	-1.39957	-2.09194
C	2.40801	0.37241	1.24764
C	3.48021	0.68925	0.20001
C	1.62643	1.63041	1.64906
C	2.99282	-0.33458	2.45653
H	0.95456	0.76439	-0.90732
H	-3.24654	1.85595	0.19511
H	-2.46126	3.23886	-0.59430
H	-2.00602	2.36612	2.32387
H	-2.94471	3.77602	1.79402
H	-1.19215	3.73133	1.51749
H	-2.58340	-2.14697	0.56774
H	-3.40627	-2.15756	-1.01149
H	-4.87628	-0.26873	-0.25592
H	-4.06531	-0.27527	1.33287
H	-5.03496	-1.67108	0.82136
H	0.41280	0.43765	-3.14300
H	-1.09409	-0.43774	-2.78091
H	0.13084	-1.17496	-3.82302
H	0.61250	-3.14627	-0.70359
H	0.11863	-3.17527	-2.39735
H	-0.98637	-2.53630	-1.18068
H	2.72383	-1.87259	-1.27673
H	2.63758	-0.44490	-2.34160
H	2.24027	-2.05584	-2.96433
H	4.18811	1.36349	0.68958
H	4.01275	-0.21360	-0.10666
H	3.07584	1.20148	-0.67575
H	2.34800	2.28252	2.14864
H	1.22660	2.17327	0.78964
H	0.82509	1.39421	2.35298
H	2.21776	-0.58436	3.18575
H	3.52782	-1.24342	2.16993
H	3.70073	0.35616	2.91977

NO+_ac, SMD Methanol

N	1.21891	0.07443	0.58051
O	1.56185	-0.99830	0.95650
C	0.18046	0.14719	-0.46644
P	-1.41129	-0.19886	0.45695
O	-1.57470	0.77539	1.56866
O	-2.53941	-0.19167	-0.65300
C	-3.10051	1.07913	-1.11657
C	-4.15962	0.75096	-2.13837
O	-1.29564	-1.71877	0.86417
C	-1.64189	-2.18578	2.20858
C	-0.41236	-2.18366	3.08283
C	0.55372	-0.69803	-1.74102
C	-0.28312	-0.12796	-2.89543
C	0.28938	-2.19902	-1.61156

C	2.03623	-0.45084	-2.05917
C	1.89645	1.30036	1.22747
C	3.38331	1.15645	0.88513
C	1.31651	2.59407	0.68415
C	1.65112	1.15140	2.73122
H	0.10916	1.19617	-0.75721
H	-2.28854	1.67508	-1.54681
H	-3.51449	1.59843	-0.24937
H	-3.72918	0.21527	-2.98891
H	-4.60499	1.68155	-2.50116
H	-4.94735	0.13859	-1.69127
H	-2.03167	-3.19140	2.04850
H	-2.43599	-1.55301	2.61069
H	-0.02943	-1.16648	3.21162
H	0.37177	-2.81140	2.64949
H	-0.67187	-2.58178	4.06861
H	-0.09651	0.94242	-3.03270
H	-1.35319	-0.28836	-2.74513
H	0.00774	-0.64465	-3.81529
H	0.81452	-2.64236	-0.76135
H	0.65161	-2.68375	-2.52402
H	-0.77865	-2.41492	-1.51693
H	2.70591	-0.92029	-1.33114
H	2.25725	0.62190	-2.10592
H	2.25879	-0.88687	-3.03727
H	3.90174	1.97501	1.39083
H	3.78259	0.20690	1.24877
H	3.55582	1.24669	-0.18984
H	1.82043	3.40543	1.21576
H	1.51847	2.72005	-0.38339
H	0.24413	2.67783	0.88053
H	0.58301	1.19616	2.95870
H	2.07730	0.22013	3.11090
H	2.15210	1.99147	3.21850

NO+_bs, SMD Methanol

N	1.28625	-0.64992	0.11009
O	1.19819	-1.82666	-0.01071
C	0.43892	0.20359	-0.74033
P	-1.23905	0.29363	0.08056
O	-2.24992	0.94170	-0.79148
O	-1.44646	-1.21600	0.49256
C	-2.72557	-1.65148	1.05962
C	-3.59190	-2.23491	-0.03049
O	-0.99167	1.02297	1.47092
C	-1.25055	2.45136	1.62999
C	-2.66784	2.67076	2.10448
C	0.43392	-0.25911	-2.24318
C	0.02728	0.97891	-3.05688
C	-0.53100	-1.41283	-2.53492
C	1.86327	-0.65192	-2.64658
C	2.29115	-0.12915	1.15622
C	3.62594	-0.77392	0.77253
C	2.37808	1.38679	1.13289
C	1.76605	-0.65781	2.49601
H	0.84363	1.21597	-0.67258
H	-3.20148	-0.80092	1.55759
H	-2.45263	-2.39253	1.81151
H	-3.85569	-1.47516	-0.77142
H	-4.51389	-2.62065	0.41477
H	-3.07581	-3.05967	-0.52982
H	-1.04941	2.96078	0.68288
H	-0.52096	2.78032	2.37189
H	-2.82457	3.73879	2.28331
H	-2.84486	2.13278	3.04011
H	-3.38987	2.33473	1.35517
H	0.75056	1.79042	-2.92271
H	-0.96590	1.34058	-2.78140
H	0.01212	0.70596	-4.11645
H	-0.30573	-2.30124	-1.93966
H	-0.43326	-1.67877	-3.59232
H	-1.57271	-1.12470	-2.36119
H	2.17732	-1.60997	-2.22059
H	2.58381	0.12078	-2.35334
H	1.89794	-0.75251	-3.73532
H	4.36537	-0.43355	1.50146
H	3.56718	-1.86341	0.81100
H	3.94439	-0.45386	-0.22353
H	3.09456	1.66656	1.90955
H	2.75745	1.76064	0.17763
H	1.42397	1.86171	1.37234
H	0.78884	-0.22879	2.73134
H	1.70219	-1.74838	2.48578
H	2.48216	-0.35193	3.26271

NO+_av, SMD Methanol

N	1.33394	-0.64657	0.84819
O	0.96943	-1.67450	1.31381
C	0.58232	-0.11821	-0.31474
P	-1.11967	0.31401	0.34116
O	-1.13799	0.33394	1.82899
O	-1.30299	1.68652	-0.42932
C	-2.60396	2.35549	-0.39306
C	-2.41747	3.72907	-0.98709
O	-2.21380	-0.63532	-0.30353
C	-2.93148	-1.62744	0.49306
C	-4.18463	-1.01213	1.06980
C	0.66301	-1.06786	-1.56889
C	-0.12640	-0.36135	-2.68192
C	0.11778	-2.47910	-1.33399
C	2.12921	-1.18009	-2.00307
C	2.47705	0.11350	1.52391
C	3.53648	0.47385	0.48276
C	1.83027	1.37816	2.11352
C	3.03564	-0.78720	2.61019
H	1.03789	0.83765	-0.58404
H	-2.93697	2.40631	0.64772
H	-3.30408	1.74976	-0.97398
H	-1.70343	4.31200	-0.39933
H	-3.37826	4.25138	-0.98679
H	-2.06063	3.65789	-2.01825
H	-2.26448	-2.01265	1.26888
H	-3.15949	-2.42820	-0.21232
H	-4.81719	-0.61159	0.27252
H	-3.94028	-0.20973	1.77182
H	-4.74830	-1.78180	1.60574
H	0.23388	0.66125	-2.83539
H	-1.20009	-0.33240	-2.47967
H	0.02469	-0.91877	-3.61121
H	0.74359	-3.05228	-0.64414
H	0.13428	-3.00097	-2.29650
H	-0.91021	-2.48382	-0.96900
H	2.73162	-1.71333	-1.25955
H	2.57371	-0.19793	-2.18938
H	2.17068	-1.75697	-2.93212
H	4.30216	1.03738	1.02252
H	4.00070	-0.41699	0.05672
H	3.15069	1.11465	-0.31246
H	2.64135	1.92171	2.60582
H	1.40291	2.02940	1.34617
H	1.06900	1.12389	2.85224
H	2.28587	-1.01549	3.37102
H	3.42451	-1.71943	2.19161
H	3.85888	-0.24582	3.08167

NO+_br, SMD Methanol

N	1.10704	-0.45770	0.03328
O	1.10994	-1.64428	0.02609
C	0.30151	0.24893	-0.97962
P	-1.46866	0.14886	-0.40067
O	-2.38147	0.84313	-1.34212
O	-1.64586	-1.40273	-0.17981
C	-2.57439	-1.96318	0.80389
C	-1.79371	-2.43538	2.00578
O	-1.43103	0.73396	1.07600
C	-1.90095	2.08133	1.38431
C	-3.36896	2.04638	1.73833
C	0.59816	-0.24248	-2.44380
C	0.13996	0.89523	-3.36791
C	-0.12387	-1.53731	-2.82337
C	2.11488	-0.41773	-2.60116
C	1.96704	0.24067	1.10583
C	3.39440	-0.24662	0.83416
C	1.86088	1.75136	0.99666
C	1.44058	-0.27483	2.44809
H	0.55896	1.30645	-0.90200
H	-3.06619	-2.78505	0.28250
H	-3.32226	-1.20921	1.06474
H	-1.01885	-3.14640	1.70346
H	-2.47274	-2.93880	2.70072
H	-1.32697	-1.59399	2.52534
H	-1.69784	2.73461	0.53107
H	-1.28716	2.39727	2.22959
H	-3.54378	1.36962	2.57963
H	-3.97007	1.72132	0.88431
H	-3.69262	3.05069	2.02782
H	0.67865	1.82284	-3.14697
H	-0.93304	1.08181	-3.28418
H	0.35994	0.60945	-4.40112
H	0.13458	-2.36630	-2.15947
H	0.17825	-1.80927	-3.83985
H	-1.21132	-1.40997	-2.82243
H	2.49581	-1.28511	-2.05215
H	2.65433	0.47754	-2.27070
H	2.33712	-0.57744	-3.66031
H	4.03326	0.20392	1.59770
H	3.46164	-1.33410	0.91140
H	3.74277	0.07903	-0.14927
H	2.46743	2.16415	1.80687
H	2.26660	2.12506	0.05201
H	0.83483	2.10314	1.13313
H	0.41494	0.06059	2.61955
H	1.49310	-1.36472	2.50004
H	2.08484	0.14508	3.22452

NO+_bn, SMD Methanol

N	0.94770	-0.56387	-0.35675
O	0.69509	-1.45308	-1.09891
C	0.25498	0.73225	-0.55802
P	-1.52065	0.50497	0.04005
O	-2.56430	1.07113	-0.85028
O	-1.66310	-1.05505	0.32130
C	-2.30832	-1.93594	-0.65220
C	-1.94443	-3.35106	-0.27793
O	-1.38595	1.14175	1.48191
C	-2.52440	1.09753	2.39911
C	-2.05019	1.64446	3.72211
C	0.41893	1.26762	-2.02743
C	-0.08900	2.71730	-2.00067
C	-0.33779	0.45881	-3.08680
C	1.91201	1.28642	-2.37924
C	1.94786	-0.80636	0.77443
C	2.32079	-2.27726	0.73757
C	3.16262	0.08862	0.50745
C	1.24492	-0.42955	2.08238
H	0.71664	1.44584	0.12992
H	-1.95067	-1.67769	-1.65315
H	-3.38391	-1.75598	-0.59447
H	-0.86222	-3.50183	-0.33400
H	-2.42726	-4.04158	-0.97517
H	-2.28584	-3.58341	0.73455
H	-2.85226	0.05762	2.48522
H	-3.32682	1.70181	1.96855
H	-1.70131	2.67477	3.61183
H	-1.23934	1.03126	4.12548
H	-2.88180	1.63264	4.43225
H	0.44061	3.30583	-1.24399
H	-1.16233	2.77598	-1.80884
H	0.10663	3.16699	-2.97894
H	0.08360	-0.54041	-3.22149
H	-0.24015	0.98764	-4.04068
H	-1.40300	0.37216	-2.86011
H	2.34343	0.28014	-2.42055
H	2.48304	1.89199	-1.66898
H	2.02550	1.73069	-3.37280
H	3.02934	-2.44624	1.55137
H	1.44626	-2.91406	0.89677
H	2.80139	-2.54820	-0.20535
H	3.86635	-0.11203	1.31990
H	3.64057	-0.16677	-0.44078
H	2.91662	1.15215	0.52804
H	1.02854	0.63740	2.15202
H	0.32728	-1.00746	2.22267
H	1.94383	-0.68785	2.88255

NO+_bt, SMD Methanol

N	0.81184	-0.74993	0.73465
O	0.50121	-1.71349	1.34942
C	0.24706	-0.56801	-0.62250
P	-1.49608	0.12912	-0.41490
O	-2.51129	-0.48778	-1.30425
O	-1.69088	-0.03299	1.14632
C	-2.95355	0.35415	1.77893
C	-2.78804	0.14366	3.26252
O	-1.33580	1.69971	-0.60107
C	-1.25344	2.26244	-1.94321
C	-1.12628	3.75856	-1.79511
C	0.37624	-1.86014	-1.50433
C	0.05688	-1.41493	-2.94002
C	-0.54365	-3.01451	-1.08790
C	1.83463	-2.33734	-1.46431
C	1.79580	0.24011	1.35758
C	3.10803	0.07177	0.57864
C	1.22798	1.65031	1.19973
C	1.95531	-0.14835	2.81685
H	0.82986	0.23221	-1.08834
H	-3.74196	-0.27571	1.36023
H	-3.14688	1.40167	1.53232
H	-2.55747	-0.90291	3.48010
H	-3.72237	0.40629	3.76650
H	-1.98953	0.77768	3.65756
H	-2.15801	1.98093	-2.48813
H	-0.37960	1.83080	-2.44436
H	-0.22222	4.01923	-1.23791
H	-1.99693	4.16812	-1.27570
H	-1.06716	4.21368	-2.78767
H	0.72185	-0.60416	-3.25655
H	-0.97980	-1.08912	-3.05239
H	0.21974	-2.26602	-3.60832
H	-0.24837	-3.44860	-0.13017
H	-0.45967	-3.79877	-1.84729
H	-1.59171	-2.71162	-1.03343
H	2.13589	-2.67582	-0.46704
H	2.52125	-1.55290	-1.79763
H	1.93614	-3.18962	-2.14301
H	3.82989	0.73757	1.05958
H	3.47818	-0.95398	0.64484
H	3.01245	0.36987	-0.46781
H	1.94399	2.31953	1.68404
H	1.13837	1.95416	0.15481
H	0.26212	1.75155	1.70109
H	0.99521	-0.11598	3.34002
H	2.39368	-1.14265	2.92542
H	2.62770	0.58193	3.27214

NO+_az, SMD Methanol

N	1.10874	-0.23583	-0.00766
O	1.16280	-1.41875	-0.08329
C	0.18990	0.47639	-0.91314
P	-1.51307	0.30572	-0.15805
O	-2.62056	0.60951	-1.09745
O	-1.51627	-1.15095	0.46777
C	-2.51121	-2.17129	0.15101
C	-1.87784	-3.51125	0.43078
O	-1.32492	1.28175	1.07822
C	-2.30841	1.28156	2.15923
C	-1.91526	2.37466	3.12207
C	0.32821	-0.00228	-2.40062
C	-0.25387	1.13219	-3.25660
C	-0.40821	-1.31055	-2.70267
C	1.82122	-0.14529	-2.73111
C	2.00100	0.43924	1.05103
C	3.41270	-0.07479	0.75807
C	1.92679	1.95341	0.95343
C	1.47188	-0.08295	2.39304
H	0.43776	1.53656	-0.84682
H	-2.80331	-2.06665	-0.89656
H	-3.37803	-1.98199	0.78877
H	-1.00512	-3.66930	-0.20976
H	-2.60624	-4.30159	0.22835
H	-1.57016	-3.58253	1.47780
H	-2.28766	0.29416	2.62977
H	-3.29549	1.45915	1.72334
H	-1.92203	3.34858	2.62525
H	-0.91901	2.18924	3.53374
H	-2.63217	2.39939	3.94758
H	0.30992	2.05988	-3.11346
H	-1.30576	1.31880	-3.02727
H	-0.17884	0.84459	-4.30988
H	-0.06672	-2.13583	-2.07218
H	-0.21199	-1.58042	-3.74536
H	-1.49079	-1.19680	-2.59147
H	2.27737	-1.01997	-2.25696
H	2.37860	0.75169	-2.43687
H	1.92461	-0.26972	-3.81306
H	4.07577	0.37332	1.50188
H	3.46641	-1.16165	0.84556
H	3.74450	0.23476	-0.23687
H	2.58958	2.34486	1.72960
H	2.29164	2.31960	-0.01094
H	0.92073	2.33247	1.14718
H	0.44036	0.23753	2.56193
H	1.53499	-1.17266	2.43958
H	2.10734	0.34398	3.17298

NO+_bj, SMD Methanol

N	1.22827	-0.38552	0.06134
O	1.23442	-1.55699	-0.12660
C	0.45368	0.46342	-0.86251
P	-1.33283	0.30619	-0.33829
O	-2.29232	0.86072	-1.32524
O	-1.51346	-1.22920	0.01307
C	-2.52785	-2.08505	-0.59567
C	-3.72304	-2.17916	0.32182
O	-1.22703	1.03758	1.06462
C	-2.31761	0.93761	2.03174
C	-1.99684	1.88182	3.16379
C	0.75540	0.13404	-2.36712
C	0.34521	1.38624	-3.15576
C	-0.00385	-1.08617	-2.89718
C	2.26864	-0.07067	-2.53104
C	2.03719	0.13378	1.26473
C	3.45559	-0.40080	1.04545
C	2.01672	1.65088	1.32781
C	1.37305	-0.51019	2.48754
H	0.73266	1.49689	-0.65170
H	-2.03247	-3.04761	-0.73108
H	-2.79729	-1.67586	-1.57170
H	-3.43026	-2.56061	1.30395
H	-4.45525	-2.86587	-0.11361
H	-4.19693	-1.20000	0.44240
H	-2.37015	-0.10262	2.36604
H	-3.25042	1.21000	1.53020
H	-1.93643	2.91172	2.80188
H	-1.04858	1.61266	3.63783
H	-2.78963	1.82185	3.91470
H	0.93432	2.25538	-2.84494
H	-0.71592	1.61592	-3.03270

H	0.53667	1.20455	-4.21780
H	0.19221	-1.98691	-2.30968
H	0.32675	-1.27507	-3.92356
H	-1.08308	-0.90639	-2.93019
H	2.61391	-1.02171	-2.11261
H	2.83132	0.74757	-2.06654
H	2.50259	-0.08029	-3.59959
H	4.05516	-0.06895	1.89657
H	3.46711	-1.49190	1.00870
H	3.89259	0.00665	0.12967
H	2.61217	1.93178	2.20031
H	2.48310	2.09976	0.44582
H	1.00766	2.04644	1.46584
H	0.33304	-0.18838	2.58550
H	1.42077	-1.59983	2.42724
H	1.93073	-0.17800	3.36672

a•, SMD Methanol

C	-0.85470	3.28178	0.07670
C	0.32215	2.36494	0.11271
C	0.21342	0.95147	0.06717
C	-1.03951	0.28797	-0.01739
C	-1.12415	-1.09688	-0.06091
C	0.03951	-1.87032	-0.02159
C	1.29324	-1.24878	0.06186
C	1.37512	0.13065	0.10508
O	0.01705	-3.23694	-0.06133
H	-0.53937	4.32622	0.12267
H	-1.53964	3.10023	0.91698
H	-1.44735	3.14965	-0.83952
H	1.31900	2.79176	0.17733
H	-1.95575	0.87051	-0.04907
H	-2.09195	-1.58837	-0.12561
H	2.18783	-1.86433	0.09152
H	2.35080	0.60627	0.16980
H	-0.89343	-3.56307	-0.11849

N•_bk, SMD Methanol

N	0.76642	-0.15372	-1.13392
C	0.52072	-0.11721	0.28274
P	-1.20947	0.50327	0.50231
O	-2.14896	-0.03405	-0.52923
O	-1.62399	0.13905	2.00767
C	-1.94747	-1.23559	2.34924
C	-3.43744	-1.36299	2.57113
O	-1.17548	2.09474	0.59999
C	-1.89003	2.92353	-0.35895
C	-1.15002	3.00595	-1.67551
C	1.65064	0.66164	1.03505
C	1.31101	0.79969	2.52290
C	1.93717	2.04520	0.44148
C	2.91761	-0.19585	0.89688
C	0.60943	-1.41449	-1.86855
C	-0.20127	-1.07989	-3.12986
C	2.03070	-1.83338	-2.29147
C	-0.04926	-2.57755	-1.11853
H	0.47086	-1.11599	0.74590
H	-1.38145	-1.45633	3.25709
H	-1.60737	-1.90864	1.55456
H	-3.76781	-0.67747	3.35668
H	-3.67402	-2.38566	2.88015
H	-3.98506	-1.14025	1.65091
H	-1.95385	3.89810	0.12732
H	-2.89984	2.52520	-0.48459
H	-0.13851	3.39545	-1.53060
H	-1.68907	3.68191	-2.34671
H	-1.08723	2.02436	-2.15599
H	1.04208	-0.16739	2.96440
H	0.48544	1.49780	2.69327
H	2.18708	1.18303	3.05709
H	1.10127	2.73336	0.58408
H	2.16036	1.98154	-0.62716
H	2.81312	2.46932	0.94563
H	2.75702	-1.21003	1.28248
H	3.73795	0.25869	1.46291
H	3.22947	-0.26952	-0.15028
H	0.26819	-0.25659	-3.67766
H	-0.24483	-1.95515	-3.78631
H	-1.22321	-0.78918	-2.86912
H	2.53383	-1.02031	-2.82406
H	2.63285	-2.11079	-1.42080
H	1.96653	-2.70107	-2.95661
H	-0.15672	-3.42139	-1.80731
H	-1.04602	-2.31115	-0.75364
H	0.55882	-2.92052	-0.27470

N•_ba, SMD Methanol

N	0.81287	-0.39925	-0.95480
C	0.27781	-0.60235	0.37570
P	-1.26490	0.42463	0.38227
O	-2.42966	-0.21586	-0.30402
O	-1.53329	0.80166	1.90681
C	-2.75401	1.51779	2.25292
C	-3.72350	0.57058	2.92106
O	-0.88715	1.84728	-0.26020
C	-1.09136	2.08010	-1.67845
C	-0.08488	3.11121	-2.12926
C	1.34703	-0.22039	1.46761
C	0.90353	-0.74225	2.84055
C	1.61418	1.28812	1.52738
C	2.66359	-0.92846	1.11627
C	0.75791	-1.50489	-1.91976
C	1.34633	-0.95578	-3.22137
C	1.59933	-2.70141	-1.44313
C	-0.68105	-1.98190	-2.17122
H	-0.06194	-1.63150	0.57202
H	-3.18454	1.96914	1.35353
H	-2.43779	2.31763	2.92538
H	-4.02345	-0.22610	2.23448
H	-4.61771	1.12156	3.22793
H	-3.27029	0.12221	3.80984
H	-2.11958	2.42893	-1.81042
H	-0.96472	1.14109	-2.22570
H	-0.19614	4.03711	-1.55745
H	-0.24422	3.33603	-3.18803
H	0.93518	2.73617	-2.00273
H	0.71429	-1.82143	2.80231
H	0.00537	-0.24601	3.21014
H	1.70840	-0.57006	3.56400
H	0.74965	1.84832	1.89525
H	1.89102	1.68213	0.54396
H	2.44803	1.47523	2.21279
H	2.53740	-2.01528	1.09006
H	3.40779	-0.69434	1.88518
H	3.05797	-0.59780	0.15045
H	2.37547	-0.61661	-3.06216
H	1.35081	-1.72634	-3.99898
H	0.75489	-0.10529	-3.57880
H	2.64799	-2.42148	-1.31272
H	1.22199	-3.11615	-0.50345
H	1.54545	-3.48577	-2.20483
H	-0.65556	-2.76747	-2.93329
H	-1.30915	-1.16525	-2.53787
H	-1.13931	-2.39729	-1.26925

N•_bu, SMD Methanol

N	0.56842	-0.19093	-1.52151
C	0.56909	-0.25347	-0.08234
P	-0.95192	0.62776	0.47993
O	-2.13473	0.39808	-0.40704
O	-1.22918	0.16936	1.99634
C	-1.90954	-1.08696	2.24995
C	-2.03827	-1.24031	3.74682
O	-0.54288	2.15459	0.66687
C	-1.58109	3.14448	0.92546
C	-1.89048	3.90110	-0.34561
C	1.93319	0.21983	0.51880
C	1.85189	0.27330	2.04847
C	2.40323	1.57274	-0.02593
C	2.96528	-0.84500	0.11921
C	0.06154	-1.33187	-2.29509
C	-0.84127	-0.74260	-3.38846
C	1.29598	-1.96884	-2.96206
C	-0.69880	-2.41502	-1.52117
H	0.39572	-1.26791	0.31076
H	-1.31799	-1.90215	1.81733
H	-2.88772	-1.05796	1.76175
H	-1.05275	-1.25862	4.22091
H	-2.55081	-2.17971	3.97249
H	-2.62006	-0.41609	4.16913
H	-1.16667	3.79663	1.69629
H	-2.46864	2.64760	1.32892
H	-0.98707	4.37771	-0.73665
H	-2.63050	4.67903	-0.13457
H	-2.29662	3.23056	-1.10812
H	1.46842	-0.66747	2.46160
H	1.21218	1.08930	2.39849
H	2.85545	0.43687	2.45556
H	1.73819	2.38820	0.26519
H	2.47830	1.55639	-1.11661
H	3.39930	1.78699	0.37786
H	2.66358	-1.84206	0.46232
H	3.93566	-0.60841	0.56905
H	3.09603	-0.87737	-0.96745
H	-0.30233	0.02194	-3.95677
H	-1.15577	-1.53305	-4.07755
H	-1.73414	-0.28676	-2.95026
H	1.86977	-1.21961	-3.51630
H	1.94817	-2.43339	-2.21636
H	0.96517	-2.74450	-3.66085
H	-1.07252	-3.15519	-2.23555
H	-1.55772	-2.00279	-0.98248
H	-0.05507	-2.94435	-0.81089

N•_bv, SMD Methanol

N	0.82584	-0.23466	-1.35043
C	0.67706	-0.30561	0.08001
P	-0.88912	0.57835	0.48730
O	-1.98678	0.30414	-0.49149
O	-1.28551	0.15965	1.98631
C	-2.03388	-1.06148	2.22147
C	-3.49811	-0.73898	2.41773
O	-0.51250	2.11512	0.66360
C	-1.58556	3.08537	0.84709
C	-1.83113	3.82316	-0.44854
C	1.97734	0.15875	0.81682
C	1.74730	0.21251	2.33092
C	2.50425	1.51084	0.32502
C	3.03875	-0.91045	0.51817
C	0.41632	-1.37058	-2.18538
C	-0.40830	-0.77893	-3.33858
C	1.71741	-1.96143	-2.76138
C	-0.37662	-2.48780	-1.49905
H	0.45420	-1.31964	0.45301
H	-1.59384	-1.50089	3.11929
H	-1.88317	-1.75429	1.38665
H	-3.62585	-0.03571	3.24585
H	-4.04636	-1.65620	2.65367
H	-3.92449	-0.30117	1.51067
H	-1.23463	3.75318	1.63582
H	-2.48600	2.57220	1.19995
H	-0.91592	4.31730	-0.78675
H	-2.60037	4.58562	-0.29245
H	-2.17307	3.13668	-1.22820
H	1.31789	-0.72456	2.70483
H	1.08291	1.03378	2.61683
H	2.70787	0.36870	2.83350
H	1.81376	2.32725	0.54656
H	2.69222	1.49611	-0.75189
H	3.45297	1.72309	0.83093
H	2.70105	-1.90642	0.82928
H	3.96198	-0.67834	1.06015
H	3.27394	-0.94252	-0.55076
H	0.15859	0.00607	-3.84883
H	-0.64862	-1.56334	-4.06354
H	-1.34290	-0.34892	-2.96626
H	2.31949	-1.18332	-3.24085
H	2.31386	-2.43623	-1.97649
H	1.46636	-2.72071	-3.50960
H	-0.65937	-3.22829	-2.25385
H	-1.29478	-2.10984	-1.03865
H	0.21539	-3.00735	-0.73828

N•_bh, SMD Methanol

N	0.64040	-0.27322	-1.24443
C	0.43792	-0.13516	0.17289
P	-1.25799	0.57407	0.39348
O	-2.25030	0.02448	-0.58026
O	-1.65678	0.32396	1.92771
C	-2.03903	-1.00589	2.36559
C	-2.44400	-0.90491	3.81701
O	-1.14412	2.16489	0.39125
C	-1.84869	2.96949	-0.59534
C	-1.14938	2.93411	-1.93605
C	1.61860	0.63906	0.84737
C	1.31976	0.88404	2.33035
C	1.95143	1.96792	0.16075
C	2.84264	-0.28231	0.73756
C	0.40255	-1.57113	-1.88752
C	-0.43374	-1.28342	-3.14374
C	1.78935	-2.08197	-2.32342
C	-0.28063	-2.65122	-1.04074
H	0.36470	-1.10053	0.69751
H	-1.18471	-1.68021	2.23942
H	-2.86618	-1.35467	1.74029
H	-1.61141	-0.54084	4.42580
H	-2.73580	-1.89382	4.18181
H	-3.29328	-0.22590	3.93320
H	-1.84845	3.97377	-0.16901
H	-2.88029	2.61614	-0.66563
H	-0.11512	3.27758	-1.84542
H	-1.67508	3.59604	-2.63130
H	-1.15242	1.92343	-2.35655
H	1.01712	-0.04081	2.83637
H	0.53043	1.62854	2.47365
H	2.22418	1.25788	2.82237
H	1.14997	2.70077	0.27539
H	2.14690	1.82605	-0.90587
H	2.85680	2.38286	0.61839
H	2.64705	-1.26095	1.19261
H	3.69629	0.16976	1.25412
H	3.12431	-0.43767	-0.30928
H	0.05311	-0.52015	-3.75912
H	-0.53627	-2.19700	-3.73848
H	-1.43317	-0.93015	-2.87334
H	2.30904	-1.33046	-2.92588
H	2.40732	-2.32663	-1.45400
H	1.66603	-2.98925	-2.92430
H	-0.45590	-3.52928	-1.67020
H	-1.24807	-2.31537	-0.65451
H	0.34481	-2.97172	-0.20089

N•_ax, SMD Methanol

N	0.40990	-0.39274	-1.24325
C	0.34478	-0.69907	0.17096
P	-1.20254	0.15279	0.73060
O	-2.46352	-0.58027	0.39879
O	-1.00422	0.42754	2.28839
C	-2.10001	1.01336	3.04462
C	-1.60264	1.24150	4.45179
O	-1.17288	1.63382	0.11153
C	-1.85324	1.90922	-1.14090
C	-1.21276	3.13263	-1.75138
C	1.66524	-0.24177	0.90035
C	1.72984	-0.85599	2.30508
C	1.79876	1.28367	0.97675
C	2.86149	-0.79108	0.10931
C	0.16027	-1.46741	-2.21323
C	0.27907	-0.82296	-3.59609
C	1.19874	-2.59492	-2.08486
C	-1.24450	-2.06891	-2.04868
H	0.18190	-1.76548	0.39247
H	-2.94407	0.31868	3.02116
H	-2.39107	1.95235	2.56339
H	-1.30456	0.29597	4.91368
H	-2.40307	1.68382	5.05178
H	-0.74791	1.92394	4.45350
H	-2.91142	2.07153	-0.91710
H	-1.75924	1.04369	-1.80396
H	-1.28107	3.98610	-1.07057
H	-1.72939	3.38798	-2.68123
H	-0.15939	2.94320	-1.97895
H	1.62289	-1.94603	2.25749
H	0.96362	-0.46121	2.97365
H	2.70916	-0.63551	2.74454
H	1.04551	1.73387	1.62993
H	1.71654	1.74058	-0.01488
H	2.78452	1.53484	1.38343
H	2.83604	-1.88400	0.05652
H	3.78671	-0.50024	0.61840
H	2.89410	-0.39159	-0.90913
H	1.27553	-0.38892	-3.73102
H	0.11429	-1.56526	-4.38363
H	-0.46280	-0.02486	-3.71099
H	2.21142	-2.22306	-2.26142
H	1.16167	-3.07508	-1.10228
H	0.97600	-3.35526	-2.84028
H	-1.39584	-2.81278	-2.83745
H	-2.01652	-1.30007	-2.14454
H	-1.36525	-2.56653	-1.08219

N•_ap, SMD Methanol

N	0.45742	-0.51774	-1.31897
C	0.49900	-0.67417	0.12094
P	-0.98144	0.27692	0.69871
O	-2.27787	-0.45020	0.53026
O	-0.66795	0.70025	2.20398
C	-1.68933	1.41517	2.95325
C	-1.07173	1.83903	4.26425
O	-0.95999	1.68850	-0.06255
C	-1.75488	1.90427	-1.25635
C	-2.99975	2.68608	-0.90188
C	1.88100	-0.18143	0.69653
C	2.03859	-0.64441	2.15098
C	2.05108	1.33914	0.59820
C	3.00238	-0.84487	-0.11615
C	0.12857	-1.68501	-2.14807
C	0.16968	-1.19813	-3.59812
C	1.14601	-2.82340	-1.96377
C	-1.27586	-2.22234	-1.83020
H	0.33086	-1.70670	0.46454
H	-2.53805	0.74221	3.10348
H	-2.01391	2.27914	2.36389
H	-0.21594	2.49813	4.09230
H	-0.74052	0.96683	4.83502
H	-1.81480	2.38011	4.85702
H	-2.00313	0.94186	-1.71371
H	-1.10724	2.45781	-1.94013
H	-3.63661	2.11143	-0.22250
H	-3.56871	2.90344	-1.81112
H	-2.73464	3.63370	-0.42361
H	1.90955	-1.73025	2.22889
H	1.33022	-0.16166	2.82576
H	3.05128	-0.40302	2.49302
H	1.36369	1.87673	1.25794
H	1.89616	1.69123	-0.42690
H	3.07196	1.60290	0.89536
H	2.95072	-1.93600	-0.04997

H	3.96910	-0.52845	0.29021
H	2.96685	-0.55546	-1.17117
H	1.16279	-0.80590	-3.84183
H	-0.05795	-2.01807	-4.28681
H	-0.56419	-0.39995	-3.75431
H	2.15185	-2.50649	-2.25135
H	1.16903	-3.18975	-0.93302
H	0.85091	-3.65584	-2.61053
H	-1.49835	-3.03925	-2.52411
H	-2.03383	-1.44397	-1.95713
H	-1.34232	-2.61241	-0.81049

N•_bw, SMD Methanol

N	0.79433	-0.67910	-1.14565
C	0.49476	-0.37095	0.22897
P	-1.16736	0.43374	0.22604
O	-2.11449	-0.10399	-0.79962
O	-1.63285	0.19735	1.73949
C	-2.92033	0.71898	2.16541
C	-3.00764	0.54419	3.66274
O	-1.00221	2.02524	0.12477
C	-1.54313	2.77158	-0.99859
C	-0.70480	2.59361	-2.24557
C	1.66545	0.42372	0.89811
C	1.28469	0.85470	2.31871
C	2.10685	1.64829	0.08992
C	2.84621	-0.55506	0.98035
C	0.53382	-2.02822	-1.66045
C	-0.17017	-1.84288	-3.01311
C	1.91885	-2.65756	-1.90550
C	-0.28773	-2.96458	-0.76794
H	0.31699	-1.26016	0.85305
H	-3.70496	0.16096	1.64637
H	-2.98134	1.77496	1.88220
H	-2.92717	-0.51250	3.93286
H	-3.97120	0.92122	4.01723
H	-2.20978	1.10115	4.16235
H	-1.53790	3.80840	-0.65786
H	-2.57786	2.45883	-1.15956
H	0.32428	2.92141	-2.07600
H	-1.13222	3.19744	-3.05226
H	-0.69576	1.54777	-2.56941
H	0.92747	0.00626	2.91346
H	0.50855	1.62691	2.32039
H	2.16843	1.26932	2.81560
H	1.33566	2.42105	0.06435
H	2.36406	1.37609	-0.93743
H	2.99897	2.07727	0.56040
H	2.57116	-1.46727	1.52336
H	3.68351	-0.08378	1.50644
H	3.19187	-0.83822	-0.01944
H	0.41233	-1.17706	-3.65784
H	-0.27315	-2.81111	-3.51376
H	-1.16738	-1.41404	-2.87690
H	2.53449	-2.00996	-2.53750
H	2.44278	-2.83051	-0.96042
H	1.79089	-3.62114	-2.40998
H	-0.47050	-3.89560	-1.31362
H	-1.25893	-2.53159	-0.50818
H	0.24265	-3.22545	0.15381

N•_bq, SMD Methanol

N	0.67095	-0.29282	-1.24641
C	0.69981	0.01524	0.16278
P	-0.87612	0.88253	0.61964
O	-0.90793	2.37774	0.58996
O	-2.04870	0.24765	-0.26765
C	-2.89348	1.06417	-1.11901
C	-2.19913	1.41352	-2.41617
O	-1.12358	0.24773	2.07306
C	-2.22178	0.76710	2.86937
C	-2.37692	-0.13003	4.07398
C	1.95684	0.87860	0.54433
C	1.87734	1.28575	2.02222
C	2.10614	2.12060	-0.34160
C	3.20380	0.00545	0.35921
C	0.52355	-1.70430	-1.63450
C	0.50861	-1.73277	-3.16406
C	1.71211	-2.54231	-1.12993
C	-0.77897	-2.32668	-1.10219
H	0.70364	-0.87282	0.81386
H	-3.19246	1.95851	-0.56659
H	-3.77668	0.44660	-1.29336
H	-1.30951	2.02525	-2.23561
H	-2.88587	1.98371	-3.04966
H	-1.90313	0.50766	-2.95324
H	-3.12995	0.77287	2.25651
H	-1.97855	1.79341	3.15897
H	-2.61664	-1.15185	3.76695
H	-3.18891	0.24452	4.70374
H	-1.45670	-0.14266	4.66507
H	1.73062	0.41127	2.66660
H	1.07082	1.99964	2.21747
H	2.81848	1.76463	2.31251
H	1.25345	2.79718	-0.25159
H	2.21998	1.84253	-1.39318
H	3.00667	2.66570	-0.03685
H	3.15126	-0.90659	0.96390
H	4.08886	0.57064	0.67137
H	3.33910	-0.27684	-0.68904
H	1.43960	-1.31691	-3.56370
H	0.40338	-2.75985	-3.52831
H	-0.32749	-1.14128	-3.55101
H	2.65837	-2.16830	-1.52968
H	1.77047	-2.56228	-0.03784
H	1.57804	-3.57118	-1.47851
H	-0.79724	-3.38275	-1.38986
H	-1.65444	-1.83432	-1.53155
H	-0.84806	-2.27368	-0.01040

N•_al, SMD Methanol

N	0.62902	-0.56187	-1.06987
C	0.65725	0.06525	0.22843
P	-0.93586	1.04215	0.39285
O	-0.78253	2.49367	0.71086
O	-1.79713	0.74799	-0.92226
C	-1.52125	1.51114	-2.12971
C	-2.59052	2.56236	-2.32106
O	-1.85312	0.23770	1.43150
C	-1.51224	0.26433	2.84138
C	-2.59061	-0.49006	3.58201
C	1.95869	0.90210	0.43035
C	1.99623	1.46015	1.85867
C	2.09762	2.02845	-0.59877
C	3.14695	-0.05687	0.27009
C	0.19085	-1.96016	-1.15170
C	-0.21927	-2.20100	-2.60633
C	1.41602	-2.82980	-0.80840
C	-0.97068	-2.35023	-0.22627
H	0.61338	-0.66341	1.05438
H	-1.51830	0.78035	-2.94092
H	-0.52429	1.95998	-2.06735
H	-3.57968	2.09802	-2.36911
H	-2.41152	3.09648	-3.25925
H	-2.57671	3.28502	-1.50027
H	-1.45332	1.30684	3.16854
H	-0.53334	-0.20981	2.97611
H	-3.56354	-0.01266	3.43661
H	-2.36048	-0.49502	4.65114
H	-2.64613	-1.52517	3.23298
H	1.91301	0.65055	2.59373
H	1.19798	2.18272	2.04562
H	2.95388	1.96514	2.02701
H	1.31354	2.78222	-0.48910
H	2.06457	1.63270	-1.61882
H	3.06461	2.52578	-0.46294
H	3.08826	-0.88436	0.98649
H	4.08118	0.48498	0.45407
H	3.18978	-0.47635	-0.73995
H	0.59685	-1.93269	-3.28485
H	-0.47251	-3.25435	-2.76376
H	-1.09546	-1.59449	-2.86062
H	2.25869	-2.59874	-1.46694
H	1.72675	-2.67912	0.23033
H	1.14920	-3.88356	-0.93952
H	-1.20658	-3.40565	-0.39560
H	-1.86805	-1.76418	-0.44324
H	-0.72140	-2.23653	0.83325

N•_bb, SMD Methanol

N	0.66137	-0.06063	-1.30066
C	0.89773	-0.04497	0.12239
P	-0.57758	0.73681	0.92896
O	-0.58302	2.22790	1.04097
O	-1.89575	0.17983	0.20604
C	-2.50897	0.90076	-0.89265
C	-3.91615	0.37508	-1.05357
O	-0.62194	-0.04501	2.32439
C	-1.25546	0.56783	3.48008
C	-2.75352	0.69930	3.30507
C	2.22202	0.71870	0.49504
C	2.32158	0.88619	2.01818
C	2.32390	2.08647	-0.18933
C	3.40930	-0.13683	0.03642
C	0.42051	-1.36040	-1.94642
C	0.10433	-1.06237	-3.41349
C	1.68692	-2.23206	-1.87131
C	-0.75019	-2.14154	-1.32622
H	0.95488	-1.04604	0.57903
H	-1.90855	0.73068	-1.79263
H	-2.50529	1.96866	-0.65787
H	-3.91063	-0.69728	-1.26976
H	-4.40395	0.89384	-1.88392
H	-4.49802	0.54929	-0.14375

H	-0.78235	1.53822	3.65820
H	-1.00766	-0.10121	4.30536
H	-3.18938	1.06157	4.24108
H	-3.20185	-0.26905	3.06446
H	-3.00484	1.41313	2.51452
H	2.20458	-0.07351	2.53423
H	1.57673	1.58533	2.41240
H	3.31024	1.28553	2.26780
H	1.50515	2.75055	0.09610
H	2.32567	1.98434	-1.27802
H	3.26679	2.55939	0.10780
H	3.38701	-1.13420	0.48953
H	4.34241	0.35235	0.33700
H	3.42524	-0.24677	-1.05144
H	0.93671	-0.52901	-3.88429
H	-0.06873	-1.99191	-3.96544
H	-0.79391	-0.44097	-3.49426
H	2.53457	-1.73948	-2.35524
H	1.95560	-2.47406	-0.83885
H	1.49054	-3.17026	-2.39981
H	-0.81792	-3.11151	-1.82904
H	-1.69627	-1.61534	-1.47059
H	-0.61175	-2.32753	-0.25648

N•_av, SMD Methanol

N	0.75163	-0.14836	-1.25621
C	0.74670	-0.01664	0.18092
P	-0.88958	0.70664	0.67157
O	-0.99892	2.19772	0.70433
O	-2.03541	0.05066	-0.23873
C	-2.45451	0.67138	-1.48052
C	-3.79500	0.08432	-1.85510
O	-1.13945	-0.03089	2.06755
C	-2.25243	0.39241	2.90468
C	-1.76430	1.34313	3.97434
C	1.94512	0.86080	0.69700
C	1.78823	1.12255	2.20152
C	2.07152	2.18897	-0.05740
C	3.23907	0.06513	0.48595
C	0.69081	-1.50503	-1.82203
C	0.62848	-1.33843	-3.34157
C	1.95938	-2.29449	-1.45272
C	-0.53755	-2.30150	-1.34989
H	0.78716	-0.97667	0.71945
H	-1.69496	0.46041	-2.24058
H	-2.51847	1.75235	-1.33010
H	-3.72365	-0.99931	-1.98725
H	-4.13394	0.52684	-2.79630
H	-4.53829	0.29854	-1.08174
H	-2.65034	-0.52866	3.33428
H	-3.02758	0.84705	2.27944
H	-0.96932	0.87869	4.56529
H	-2.59348	1.59178	4.64388
H	-1.38541	2.26905	3.53283
H	1.63961	0.18860	2.75576
H	0.95264	1.79417	2.42282
H	2.70041	1.59716	2.57836
H	1.17831	2.80865	0.04693
H	2.25661	2.02226	-1.12219
H	2.92272	2.74586	0.35039
H	3.20704	-0.90158	1.00072
H	4.08254	0.63696	0.88816
H	3.42981	-0.11021	-0.57660
H	1.50878	-0.79761	-3.70436
H	0.59465	-2.31583	-3.83369
H	-0.26578	-0.77576	-3.63015
H	2.85860	-1.79220	-1.81936
H	2.04841	-2.44213	-0.37244
H	1.90119	-3.27977	-1.92584
H	-0.47176	-3.31101	-1.76793
H	-1.46432	-1.84455	-1.70373
H	-0.58479	-2.39154	-0.25995

N•_as, SMD Methanol

N	0.96243	-0.38818	-1.13312
C	0.71967	-0.18499	0.27440
P	-0.91730	0.67422	0.41816
O	-0.91080	2.16877	0.36672
O	-1.90218	0.04751	-0.68005
C	-2.08638	0.69378	-1.96577
C	-3.35111	1.52299	-1.94916
O	-1.48714	0.03229	1.76640
C	-2.70862	0.57299	2.34469
C	-2.37071	1.55234	3.44597
C	1.86847	0.62914	0.96935
C	1.45360	0.99280	2.40237
C	2.24618	1.89539	0.19324
C	3.10472	-0.27486	1.04934
C	0.86362	-1.75781	-1.65860
C	0.92480	-1.64104	-3.18286
C	2.07709	-2.56589	-1.16238
C	-0.42069	-2.50295	-1.25887
H	0.58897	-1.11861	0.84386
H	-2.15126	-0.12171	-2.69037
H	-1.20856	1.30228	-2.20319
H	-4.21284	0.90098	-1.68946
H	-3.51971	1.95213	-2.94167
H	-3.27113	2.34003	-1.22646
H	-3.24956	-0.29449	2.72686
H	-3.31069	1.03775	1.55672
H	-1.74130	1.07447	4.20250
H	-3.29399	1.89051	3.92638
H	-1.84717	2.42569	3.04717
H	1.12415	0.10778	2.95905
H	0.65106	1.73693	2.42791
H	2.31502	1.41984	2.92668
H	1.40100	2.57916	0.08600
H	2.62283	1.64943	-0.80351
H	3.04179	2.41825	0.73598
H	2.89105	-1.19995	1.59663
H	3.90590	0.25475	1.57657
H	3.47387	-0.53554	0.05345
H	1.85570	-1.15552	-3.49364
H	0.87800	-2.63199	-3.64600
H	0.08384	-1.04594	-3.55490
H	3.01574	-2.08682	-1.45517
H	2.06272	-2.68814	-0.07511
H	2.04128	-3.55987	-1.61946
H	-0.34515	-3.53372	-1.61933
H	-1.30147	-2.04458	-1.71282
H	-0.56576	-2.53981	-0.17459

N•_ad, SMD Methanol

N	0.79730	0.19017	-0.60347
C	0.57213	0.10104	0.81570
P	-1.21434	0.48055	1.07165
O	-1.62058	0.60494	2.50343
O	-1.60330	1.79327	0.25790
C	-1.76429	1.89227	-1.18255
C	-2.77429	2.98277	-1.45329
O	-1.99009	-0.67820	0.27503
C	-2.36795	-1.89297	0.97651
C	-2.90091	-2.86479	-0.04897
C	1.54750	1.04139	1.60450
C	1.50709	0.69355	3.09669
C	1.21597	2.52297	1.40287
C	2.96453	0.76309	1.08529
C	1.02969	-1.02356	-1.39513
C	2.39829	-0.83574	-2.07396
C	1.02139	-2.35005	-0.63272
C	-0.05582	-1.04518	-2.48606
H	0.68783	-0.91182	1.23035
H	-2.10264	0.92815	-1.56990
H	-0.78686	2.12794	-1.60824
H	-3.74600	2.72860	-1.02080
H	-2.89364	3.10286	-2.53418
H	-2.43650	3.93506	-1.03450
H	-3.12807	-1.63490	1.71854
H	-1.49078	-2.29608	1.49498
H	-3.75780	-2.43428	-0.57525
H	-3.22652	-3.77930	0.45514
H	-2.13063	-3.12668	-0.78040
H	1.76030	-0.36065	3.25945
H	0.52648	0.88496	3.53792
H	2.24584	1.30321	3.62884
H	0.27756	2.79937	1.89658
H	1.13522	2.77322	0.33950
H	2.01248	3.13700	1.83737
H	3.20121	-0.30664	1.13994
H	3.69305	1.30390	1.69923
H	3.08185	1.09036	0.04767
H	3.20831	-0.86118	-1.33905
H	2.56036	-1.64465	-2.79402
H	2.43712	0.11963	-2.60657
H	1.81479	-2.39133	0.12165
H	0.06069	-2.53115	-0.14051
H	1.19281	-3.16631	-1.34130
H	0.13356	-1.87793	-3.17153
H	-0.04354	-0.11241	-3.05886
H	-1.04881	-1.17459	-2.04569

N•_aq, SMD Methanol

N	1.47206	0.15209	-0.49560
C	0.54950	-0.45479	0.43290
P	-0.93194	0.65527	0.50465
O	-0.88523	1.79129	1.47585
O	-1.24109	1.15301	-0.98619
C	-0.82464	2.46595	-1.44005
C	-1.98375	3.43286	-1.34518
O	-2.10888	-0.40144	0.74453
C	-3.43771	0.10601	1.04694
C	-4.38731	-1.06747	1.03191
C	1.18401	-0.67238	1.85341
C	0.09807	-1.10786	2.84753

C	1.90388	0.57568	2.37553
C	2.20747	-1.80928	1.74423
C	1.67207	-0.49601	-1.80006
C	2.48747	0.48396	-2.64616
C	2.48622	-1.78645	-1.59139
C	0.37486	-0.84900	-2.54643
H	0.15008	-1.42567	0.09963
H	-0.50424	2.32414	-2.47517
H	0.03277	2.80556	-0.85167
H	-2.83659	3.06523	-1.92354
H	-1.68375	4.40478	-1.74894
H	-2.29171	3.56858	-0.30438
H	-3.70914	0.85155	0.29185
H	-3.40374	0.58564	2.02935
H	-4.40525	-1.53819	0.04504
H	-5.39646	-0.71997	1.27088
H	-4.09084	-1.81169	1.77657
H	-0.46432	-1.96987	2.47086
H	-0.60981	-0.30330	3.07252
H	0.57341	-1.40038	3.78970
H	1.23097	1.43155	2.46429
H	2.73555	0.85411	1.72242
H	2.31219	0.35775	3.36887
H	1.74605	-2.73089	1.37186
H	2.62544	-2.01484	2.73589
H	3.03449	-1.53989	1.08146
H	3.43984	0.71337	-2.15709
H	2.69668	0.05777	-3.63270
H	1.93576	1.42017	-2.78431
H	3.43706	-1.57681	-1.09316
H	1.92952	-2.52306	-1.00417
H	2.70133	-2.22234	-2.57218
H	0.64200	-1.40089	-3.45322
H	-0.16958	0.05037	-2.84066
H	-0.29280	-1.48452	-1.95622

N•_at, SMD Methanol

N	1.21849	-0.19228	-0.51698
C	0.55851	-0.32871	0.75725
P	-0.92152	0.80877	0.73494
O	-1.00404	1.88091	1.77369
O	-1.04569	1.40511	-0.75270
C	-0.33182	2.61801	-1.10733
C	-0.87073	3.09239	-2.43621
O	-2.12503	-0.24225	0.77001
C	-3.49369	0.24963	0.77002
C	-4.40120	-0.94392	0.59326
C	1.54424	-0.06501	1.93673
C	0.81609	-0.26271	3.27211
C	2.17834	1.32789	1.86321
C	2.65541	-1.11936	1.84018
C	0.92293	-1.17601	-1.56346
C	1.28444	-0.50615	-2.89146
C	1.86018	-2.37323	-1.31106
C	-0.52561	-1.68251	-1.62690
H	0.11881	-1.32612	0.91442
H	0.73585	2.38092	-1.16450
H	-0.49419	3.36266	-0.32297
H	-0.72383	2.33392	-3.21051
H	-0.34315	4.00203	-2.73727
H	-1.93818	3.31843	-2.35936
H	-3.60899	0.96449	-0.05062
H	-3.67354	0.75914	1.72069
H	-4.19803	-1.44464	-0.35779
H	-5.44310	-0.61128	0.59663
H	-4.26199	-1.65885	1.40907
H	0.32731	-1.24389	3.30757
H	0.06117	0.50664	3.45118
H	1.54096	-0.22052	4.09241
H	1.43153	2.12321	1.94053
H	2.73129	1.45821	0.92804
H	2.88499	1.44881	2.69196
H	2.24412	-2.13409	1.89418
H	3.35531	-0.99178	2.67329
H	3.21724	-1.02309	0.90568
H	2.32145	-0.15576	-2.87454
H	1.16564	-1.20930	-3.72210
H	0.63056	0.35495	-3.07089
H	2.90677	-2.05464	-1.29201
H	1.62235	-2.86403	-0.36165
H	1.73125	-3.10112	-2.11883
H	-0.60584	-2.39001	-2.45829
H	-1.22758	-0.86430	-1.81157
H	-0.82800	-2.21039	-0.71784

P+, SMD Methanol

C	-1.83469	1.85694	-0.27022
C	0.92525	3.35553	0.65332
O	0.28720	3.45346	1.58194
C	1.71580	3.23671	-0.47005
C	1.13770	3.44353	-1.74900
C	1.93845	3.32210	-2.85688
C	3.30234	2.99727	-2.69891
C	3.87033	2.79038	-1.42411
C	3.08745	2.90835	-0.30475
O	4.11684	2.87112	-3.74004
H	-1.79528	2.93754	-0.42892
H	-2.08980	1.65033	0.77147
H	-2.59676	1.42597	-0.92327
H	-0.86660	1.40676	-0.50565
H	0.08534	3.68960	-1.83981
H	1.53479	3.47531	-3.85268
H	4.92309	2.54146	-1.35001
H	3.49659	2.75634	0.68816
H	3.65825	3.03103	-4.58151

N+_av, SMD Methanol

N	0.41213	0.37878	0.01732
C	0.91014	0.33860	-1.18132
P	-1.29822	-0.06657	0.26343
O	-2.17492	0.80573	-0.54412
O	-1.38543	-1.58625	-0.13167
C	-0.76715	-2.66387	0.64405
C	0.45785	-3.17787	-0.07492
O	-1.43760	0.02207	1.82298
C	-2.77772	0.01217	2.42802
C	-3.15141	1.41401	2.84173
C	0.40213	0.06838	-2.57551
C	0.11886	1.50704	-3.08710
C	-0.80099	-0.83271	-2.85878
C	1.61550	-0.50368	-3.33678
C	1.28599	0.92249	1.18824
C	2.67601	1.31566	0.69004
C	0.60342	2.18172	1.72804
C	1.45428	-0.18726	2.22805
H	1.94284	0.66628	-1.23406
H	-1.54430	-3.42548	0.71816
H	-0.53751	-2.29544	1.64686
H	0.19735	-3.55850	-1.06596
H	0.88668	-3.99845	0.50848
H	1.22067	-2.40000	-0.17813
H	-2.68355	-0.66255	3.27945
H	-3.49084	-0.41168	1.71592
H	-3.19676	2.07816	1.97406
H	-2.43112	1.81007	3.56248
H	-4.13784	1.39136	3.31456
H	0.97397	2.17342	-2.93424
H	-0.75930	1.93074	-2.59239
H	-0.07382	1.43961	-4.16242
H	-0.62659	-1.85306	-2.51226
H	-0.91642	-0.85925	-3.94662
H	-1.73403	-0.46185	-2.43752
H	1.88288	-1.49543	-2.95730
H	2.48893	0.15120	-3.25739
H	1.35286	-0.59858	-4.39377
H	3.21667	1.68391	1.56478
H	3.23851	0.46610	0.29090
H	2.64919	2.12715	-0.04362
H	1.26006	2.61804	2.48593
H	0.47396	2.91382	0.92448
H	-0.36095	1.98225	2.19287
H	0.52616	-0.44663	2.73342
H	1.87737	-1.08230	1.75996
H	2.16205	0.16875	2.98168

N+_ad, SMD Methanol

N	0.74908	-0.19391	0.10987
C	1.23669	-0.26137	-1.09106
P	-0.66697	0.85632	0.43350
O	-0.36920	2.23952	0.01283
O	-1.83825	0.17041	-0.35350
C	-2.28493	-1.19975	-0.11203
C	-3.62041	-1.35880	-0.79440
O	-0.96156	0.62917	1.95685
C	-1.18257	1.75306	2.87433
C	-2.59294	2.27112	2.73020
C	0.93475	0.36413	-2.42975
C	1.88247	1.59171	-2.45267
C	-0.48524	0.77994	-2.81811
C	1.43089	-0.66535	-3.46639
C	1.49316	-0.91281	1.27298
C	0.53943	-1.92601	1.90811
C	2.70928	-1.67589	0.75037
C	1.98577	0.16228	2.24554
H	2.14166	-0.85536	-1.15929
H	-2.35814	-1.35488	0.96757
H	-1.52778	-1.86891	-0.53251
H	-4.35428	-0.66897	-0.36939
H	-3.97538	-2.38228	-0.64502
H	-3.53285	-1.17319	-1.86819
H	-0.43240	2.51927	2.66586
H	-0.99929	1.32283	3.85933
H	-3.31709	1.47026	2.90257
H	-2.75794	2.69696	1.73572

H	-2.75952	3.05797	3.47176
H	2.91339	1.31450	-2.20962
H	1.54374	2.36142	-1.75492
H	1.86795	1.99803	-3.46893
H	-1.17479	-0.06644	-2.76887
H	-0.43729	1.11944	-3.85721
H	-0.87778	1.60208	-2.22143
H	0.82435	-1.57632	-3.43630
H	2.47863	-0.93486	-3.29949
H	1.34537	-0.22751	-4.46437
H	1.08356	-2.43571	2.70807
H	-0.34760	-1.46882	2.34393
H	0.23748	-2.67552	1.16988
H	3.14804	-2.17733	1.61597
H	2.44166	-2.44946	0.02430
H	3.47503	-1.01660	0.33084
H	1.18167	0.65010	2.79459
H	2.63884	-0.32222	2.97662
H	2.57160	0.91763	1.71197

N+_am, SMD Methanol

N	0.44274	0.22765	-0.11202
C	0.85370	-0.08034	-1.30391
P	-1.31129	0.45213	0.18188
O	-1.82629	1.51306	-0.70627
O	-1.91418	-0.97436	-0.06550
C	-1.68452	-2.13863	0.79520
C	-0.71144	-3.08560	0.13341
O	-1.41050	0.71848	1.72444
C	-2.17035	1.85637	2.25913
C	-1.93478	1.87590	3.74776
C	0.22869	-0.27627	-2.66347
C	0.46062	1.11061	-3.32086
C	-1.22770	-0.70479	-2.85286
C	1.12344	-1.31870	-3.36542
C	1.48552	0.51631	1.00484
C	2.90815	0.31702	0.48456
C	1.32813	1.98275	1.41198
C	1.26107	-0.46776	2.15538
H	1.93365	-0.13863	-1.39065
H	-2.67184	-2.58684	0.91033
H	-1.33732	-1.79771	1.77343
H	-1.09487	-3.42645	-0.83181
H	-0.58090	-3.95835	0.78077
H	0.26927	-2.62286	-0.01264
H	-3.22113	1.69629	2.00970
H	-1.81250	2.76506	1.76952
H	-2.50159	2.70364	4.18322
H	-0.87487	2.02287	3.97414
H	-2.27379	0.94288	4.20579
H	1.50396	1.43187	-3.24070
H	-0.18438	1.86918	-2.86934
H	0.21238	1.01641	-4.38265
H	-1.41896	-1.68323	-2.40853
H	-1.38585	-0.78652	-3.93267
H	-1.94938	0.01427	-2.46870
H	1.03632	-2.29789	-2.88307
H	2.17596	-1.01796	-3.36498
H	0.79636	-1.41670	-4.40399
H	3.57209	0.53015	1.32529
H	3.09954	-0.71277	0.16688
H	3.16676	1.01177	-0.32011
H	2.12539	2.22167	2.12132
H	1.43890	2.63290	0.53839
H	0.37924	2.19736	1.90179
H	0.30905	-0.32396	2.66353
H	1.32763	-1.49844	1.79186
H	2.06008	-0.31192	2.88551

N+_ae, SMD Methanol

N	0.50976	-0.38020	-0.10228
C	0.18898	-1.63764	-0.07165
P	-0.67594	0.81976	-0.70674
O	-1.08731	0.47509	-2.08189
O	-1.82609	0.76791	0.35962
C	-1.61258	0.98571	1.78904
C	-2.97141	1.14104	2.42448
O	0.04064	2.20251	-0.51612
C	0.10433	3.17885	-1.61272
C	0.89273	4.35693	-1.10083
C	-1.00179	-2.47226	-0.47243
C	-0.61091	-2.93589	-1.90076
C	-2.42518	-1.91196	-0.46966
C	-0.96987	-3.68920	0.47470
C	1.95955	0.04518	0.26718
C	2.58849	0.67684	-0.97719
C	1.89958	0.98852	1.46945
C	2.79832	-1.16954	0.66009
H	1.00013	-2.28586	0.24308
H	-0.99998	1.88244	1.91448
H	-1.07829	0.11270	2.17673
H	-3.49406	2.00724	2.01069
H	-2.84375	1.29121	3.50016
H	-3.57895	0.24588	2.26743
H	-0.92040	3.45060	-1.87351
H	0.58535	2.69678	-2.46712
H	1.90946	4.05862	-0.82988
H	0.40415	4.79995	-0.22894
H	0.94981	5.11226	-1.88969
H	0.39182	-3.37468	-1.92712
H	-0.65712	-2.10347	-2.60762
H	-1.32897	-3.70418	-2.20421
H	-2.71262	-1.55859	0.52340
H	-3.08510	-2.74237	-0.73831
H	-2.58411	-1.11699	-1.19671
H	-1.17925	-3.38784	1.50620
H	-0.00217	-4.19982	0.44720
H	-1.74001	-4.39836	0.15992
H	3.65461	0.81717	-0.77961
H	2.48527	0.00835	-1.83793
H	2.17039	1.65145	-1.22340
H	2.92741	1.25583	1.73102
H	1.35454	1.90973	1.26788
H	1.45088	0.47953	2.32818
H	2.40767	-1.68551	1.54225
H	2.92430	-1.87903	-0.16338
H	3.78784	-0.78460	0.91634

N+_be, SMD Methanol

N	0.40883	0.30798	0.58541
C	1.21493	0.14188	-0.41770
P	-1.34255	-0.01279	0.47684
O	-2.07068	0.36273	1.70500
O	-1.63679	0.81907	-0.81881
C	-3.01222	0.96817	-1.31219
C	-3.52043	2.34121	-0.94822
O	-1.45380	-1.52723	0.06992
C	-1.32213	-2.59641	1.06440
C	-0.01726	-3.32385	0.84042
C	1.11887	-0.27669	-1.86529
C	1.07889	1.08228	-2.61224
C	0.01331	-1.19808	-2.38453
C	2.47391	-0.95972	-2.15430
C	0.95320	0.86563	1.92821
C	2.47089	1.01991	1.88026
C	0.32479	2.24310	2.14521
C	0.60876	-0.13982	3.02986
H	2.23528	0.44165	-0.19973
H	-3.63292	0.17151	-0.89317
H	-2.93272	0.82621	-2.39107
H	-3.57148	2.46252	0.13735
H	-4.52499	2.47059	-1.36162
H	-2.86981	3.11416	-1.36621
H	-2.18645	-3.24053	0.89973
H	-1.38981	-2.16406	2.06623
H	0.83477	-2.64127	0.92507
H	0.00164	-3.79718	-0.14466
H	0.08914	-4.10309	1.60116
H	1.87815	1.75379	-2.28207
H	0.11481	1.57733	-2.47318
H	1.22506	0.87509	-3.67700
H	0.02108	-2.16089	-1.87010
H	0.23287	-1.37743	-3.44159
H	-0.98382	-0.76649	-2.32328
H	2.56952	-1.89547	-1.59373
H	3.31723	-0.31010	-1.90066
H	2.52834	-1.19091	-3.22136
H	2.77457	1.36785	2.87032
H	2.98212	0.07060	1.69069
H	2.79884	1.77183	1.15649
H	0.74866	2.66663	3.06020
H	0.57407	2.90665	1.31096
H	-0.75795	2.19833	2.26049
H	-0.46293	-0.22356	3.20641
H	1.01805	-1.12630	2.78685
H	1.07774	0.20505	3.95525

N+_bf, SMD Methanol

N	0.85101	-0.16715	-0.07653
C	1.18663	-0.27652	-1.32509
P	-0.83032	-0.42850	0.45009
O	-1.19345	-1.85855	0.53945
O	-0.95423	0.37551	1.79615
C	-1.59386	-0.20337	2.98179
C	-1.35656	0.75847	4.11801
O	-1.50833	0.47628	-0.64505
C	-2.96482	0.50703	-0.80442
C	-3.57556	1.54033	0.11337
C	0.51144	-0.74684	-2.58918
C	0.08731	0.52864	-3.35126
C	-0.63969	-1.75225	-2.49321
C	1.65985	-1.42522	-3.37345
C	1.94089	0.19009	0.97218
C	3.33426	0.03648	0.36258

C	1.74556	1.63988	1.41253
C	1.81657	-0.81909	2.11635
H	2.20713	0.03444	-1.52750
H	-1.15431	-1.18587	3.17011
H	-2.65652	-0.32117	2.75632
H	-0.28724	0.86683	4.32101
H	-1.84405	0.37179	5.01736
H	-1.77888	1.74043	3.88742
H	-3.35779	-0.49758	-0.62246
H	-3.10871	0.75924	-1.85597
H	-3.12073	2.52006	-0.05547
H	-3.45459	1.26535	1.16492
H	-4.64580	1.61121	-0.10205
H	0.92012	1.23231	-3.44997
H	-0.74555	1.02952	-2.85415
H	-0.22497	0.22565	-4.35562
H	-0.37108	-2.60515	-1.86442
H	-0.82310	-2.12455	-3.50547
H	-1.57310	-1.32148	-2.13490
H	2.02536	-2.31347	-2.84771
H	2.49782	-0.73950	-3.53162
H	1.27844	-1.73476	-4.35008
H	4.04598	0.16919	1.18051
H	3.49084	-0.95964	-0.06406
H	3.56008	0.80111	-0.38536
H	2.55680	1.89331	2.10126
H	1.80951	2.30662	0.54696
H	0.79721	1.80269	1.92323
H	0.91075	-0.69444	2.70759
H	1.86677	-1.84395	1.73561
H	2.66303	-0.66352	2.79012

N+_cc, SMD Methanol

N	0.93157	-0.02917	0.32687
C	1.32249	-0.40424	-0.85144
P	-0.76525	0.34507	0.72226
O	-0.89908	1.10824	1.97920
O	-1.29571	1.09967	-0.55375
C	-1.48387	2.55410	-0.54333
C	-2.88775	2.88439	-0.09791
O	-1.34244	-1.11183	0.67574
C	-2.78212	-1.33270	0.85596
C	-3.04014	-1.80888	2.26458
C	0.65867	-0.76160	-2.15972
C	0.71448	0.53381	-3.00231
C	-0.74640	-1.37306	-2.17188
C	1.61901	-1.79607	-2.78928
C	1.97197	0.13728	1.46714
C	3.34280	-0.37117	1.02739
C	2.08258	1.62227	1.81402
C	1.49277	-0.72810	2.63644
H	2.40295	-0.46058	-0.94828
H	-1.30348	2.85498	-1.57594
H	-0.72387	3.00477	0.09986
H	-3.61965	2.39297	-0.74505
H	-3.03698	3.96624	-0.16461
H	-3.05629	2.57475	0.93724
H	-3.03927	-2.08378	0.10768
H	-3.31840	-0.40642	0.62710
H	-2.75645	-1.04366	2.99252
H	-2.47864	-2.72440	2.46924
H	-4.10705	-2.02155	2.37943
H	1.72451	0.95554	-3.02450
H	0.02208	1.28545	-2.61883
H	0.42909	0.27601	-4.02713
H	-0.79454	-2.26172	-1.53747
H	-0.94286	-1.68269	-3.20290
H	-1.53259	-0.67886	-1.88228
H	1.65578	-2.71317	-2.19235
H	2.63372	-1.39786	-2.88398
H	1.25395	-2.04952	-3.78803
H	3.98817	-0.31301	1.90695
H	3.31530	-1.41553	0.70109
H	3.79688	0.25033	0.25030
H	2.89516	1.73839	2.53679
H	2.33534	2.20023	0.91918
H	1.17003	2.01928	2.25668
H	0.53962	-0.39762	3.05023
H	1.41163	-1.77493	2.32712
H	2.24188	-0.66130	3.42996

N+_ca, SMD Methanol

N	0.89226	-0.11520	0.15936
C	1.53487	-0.36181	-0.94035
P	-0.83619	0.33117	0.12228
O	-1.13412	1.17361	-1.05388
O	-1.45017	-1.11045	0.22691
C	-2.83436	-1.38676	-0.17144
C	-3.80495	-0.92283	0.88835
O	-1.12186	1.03010	1.50314
C	-1.31351	2.48328	1.59181
C	-2.76450	2.83597	1.37346
C	1.13429	-0.59126	-2.37744
C	1.27275	0.76116	-3.10966
C	-0.22787	-1.24780	-2.63656
C	2.22376	-1.54933	-2.91129
C	1.65134	-0.19134	1.51382
C	3.01301	-0.86031	1.32299
C	1.86263	1.22322	2.05068
C	0.82265	-1.07547	2.44955
H	2.61002	-0.44365	-0.80786
H	-2.85117	-2.46902	-0.29879
H	-3.01079	-0.90767	-1.13821
H	-3.55353	-1.35925	1.85892
H	-4.81130	-1.24841	0.60890
H	-3.81142	0.16717	0.97609
H	-0.65414	2.97039	0.86959
H	-0.98712	2.73163	2.60232
H	-3.39923	2.33048	2.10615
H	-3.09116	2.56887	0.36475
H	-2.88350	3.91637	1.50061
H	2.26128	1.20195	-2.94521
H	0.50622	1.46724	-2.78671
H	1.15737	0.57205	-4.18172
H	-0.36576	-2.13134	-2.00546
H	-0.23483	-1.57715	-3.67982
H	-1.06798	-0.56917	-2.50145
H	2.19231	-2.51246	-2.39082
H	3.22438	-1.12078	-2.79745
H	2.04314	-1.72652	-3.97474
H	3.42330	-1.01730	2.32319
H	2.92880	-1.83697	0.83568
H	3.72397	-0.23405	0.77720
H	2.55689	1.16327	2.89359
H	2.31107	1.86055	1.28222
H	0.94245	1.67976	2.41119
H	-0.15550	-0.65769	2.68732
H	0.69826	-2.07499	2.02208
H	1.37787	-1.16964	3.38669

N+_ao, SMD Methanol

N	0.62272	0.08877	0.46384
C	1.13750	-0.19342	-0.69339
P	-1.14380	0.31526	0.71500
O	-1.40401	0.83677	2.06974
O	-1.56233	1.22898	-0.49106
C	-1.55737	2.68980	-0.33923
C	-2.92040	3.16572	0.10059
O	-1.77943	-1.06117	0.32372
C	-1.46755	-2.29020	1.05422
C	-2.49034	-3.32063	0.64816
C	0.63763	-0.47115	-2.09045
C	0.76542	0.89776	-2.80255
C	-0.74271	-1.08139	-2.34020
C	1.69153	-1.43329	-2.68233
C	1.56868	0.33589	1.67353
C	3.01736	0.01203	1.31214
C	1.47694	1.81576	2.04872
C	1.14739	-0.60496	2.80490
H	2.22293	-0.18876	-0.69246
H	-1.29753	3.06087	-1.33085
H	-0.76873	2.97164	0.36446
H	-3.68464	2.84739	-0.61349
H	-2.91637	4.25904	0.14148
H	-3.17253	2.78163	1.09247
H	-1.50857	-2.07701	2.12576
H	-0.45202	-2.58705	0.77318
H	-2.45541	-3.49968	-0.42979
H	-3.49615	-2.99553	0.92621
H	-2.27080	-4.25908	1.16484
H	1.75586	1.34137	-2.65825
H	0.00475	1.59677	-2.44844
H	0.62015	0.72754	-3.87403
H	-0.85783	-2.03202	-1.81313
H	-0.80384	-1.28194	-3.41419
H	-1.56727	-0.42116	-2.07954
H	1.68284	-2.39536	-2.15958
H	2.69927	-1.01053	-2.62489
H	1.45221	-1.61028	-3.73420
H	3.59621	0.13440	2.23056
H	3.14261	-1.02198	0.97508
H	3.43639	0.69828	0.57081
H	2.20103	2.00571	2.84630
H	1.74418	2.43950	1.18946
H	0.48905	2.09822	2.41088
H	0.14210	-0.40596	3.17343
H	1.21944	-1.64747	2.47879
H	1.84531	-0.45940	3.63391

N+_ay, SMD Methanol

N	0.61048	0.66101	0.09087
C	0.89251	-0.24916	-0.79007
P	-0.95572	0.72769	0.94436
O	-1.08192	1.92407	1.79972

O	-1.89697	0.63349	-0.30803
C	-3.35302	0.56382	-0.13294
C	-3.95477	0.40496	-1.50581
O	-1.07552	-0.65099	1.68972
C	-0.41438	-0.89163	2.97600
C	0.72112	-1.86604	2.77144
C	0.19754	-1.42210	-1.43797
C	-0.32810	-0.81460	-2.76501
C	-0.90881	-2.20984	-0.73331
C	1.33770	-2.41073	-1.76639
C	1.63986	1.78322	0.39493
C	2.94758	1.54316	-0.35496
C	1.03528	3.10531	-0.08055
C	1.93839	1.75709	1.89592
H	1.86446	-0.10980	-1.25309
H	-3.67218	1.48823	0.35396
H	-3.57353	-0.29085	0.51291
H	-3.68108	1.24712	-2.14721
H	-5.04411	0.37824	-1.41251
H	-3.62222	-0.52673	-1.97188
H	-1.19461	-1.29685	3.62110
H	-0.07529	0.06247	3.38764
H	1.44904	-1.47688	2.05208
H	0.34817	-2.82967	2.41466
H	1.23069	-2.02358	3.72678
H	0.46362	-0.29722	-3.31668
H	-1.14926	-0.11799	-2.58123
H	-0.69084	-1.64218	-3.38302
H	-0.55728	-2.63280	0.20986
H	-1.17143	-3.03746	-1.39938
H	-1.81384	-1.63433	-0.55163
H	1.78049	-2.81655	-0.85083
H	2.12631	-1.93763	-2.35963
H	0.92505	-3.24063	-2.34622
H	3.62507	2.34462	-0.05160
H	3.41672	0.59183	-0.08418
H	2.83255	1.60811	-1.44082
H	1.77997	3.89124	0.07399
H	0.80746	3.05249	-1.14995
H	0.13425	3.37707	0.46876
H	1.07963	2.03839	2.50367
H	2.29216	0.76553	2.19757
H	2.73858	2.47668	2.08909

N+_bz, SMD Methanol

N	0.19338	0.02670	0.69118
C	0.91601	-0.58413	-0.19660
P	-1.38331	0.79125	0.29567
O	-1.88422	1.55503	1.45353
O	-1.07047	1.60463	-1.00996
C	-0.42899	2.91971	-0.91205
C	-0.59045	3.59199	-2.25200
O	-2.26945	-0.38231	-0.24210
C	-2.87952	-1.35385	0.67502
C	-2.14943	-2.67232	0.57993
C	0.84130	-0.89996	-1.67128
C	1.70755	0.21636	-2.30750
C	-0.48641	-1.02877	-2.41984
C	1.58946	-2.24471	-1.80438
C	0.73453	0.17380	2.14110
C	2.01900	-0.63111	2.32934
C	1.04052	1.65397	2.37301
C	-0.31431	-0.38633	3.10592
H	1.87189	-0.92395	0.18809
H	0.62244	2.75411	-0.65744
H	-0.91803	3.48141	-0.11283
H	-0.12513	3.00116	-3.04590
H	-0.10511	4.57133	-2.21684
H	-1.64887	3.73432	-2.48512
H	-3.91400	-1.43167	0.34026
H	-2.86717	-0.94275	1.68779
H	-1.08997	-2.56156	0.83173
H	-2.23700	-3.09674	-0.42330
H	-2.59888	-3.37219	1.29107
H	2.67018	0.33064	-1.79845
H	1.18092	1.17353	-2.29606
H	1.90148	-0.06783	-3.34661
H	-1.11457	-1.80961	-1.98748
H	-0.23557	-1.32533	-3.44316
H	-1.05169	-0.10081	-2.47471
H	1.04277	-3.04924	-1.30123
H	2.59920	-2.18978	-1.38557
H	1.67135	-2.49592	-2.86515
H	2.29450	-0.52679	3.38117
H	1.87447	-1.69779	2.12795
H	2.85579	-0.24868	1.73778
H	1.46021	1.75904	3.37772
H	1.78725	2.00152	1.65165
H	0.15146	2.28153	2.30785
H	-1.22845	0.20450	3.13014
H	-0.55503	-1.42335	2.84839
H	0.12017	-0.37906	4.10916

N+_ar, SMD Methanol

N	0.96490	-0.09761	0.15833
C	1.32049	0.02955	-1.08288
P	-0.71591	-0.48657	0.59987
O	-1.02784	-1.91772	0.40232
O	-0.90558	0.04520	2.06649
C	-1.42683	-0.78696	3.15325
C	-2.92840	-0.65156	3.21801
O	-1.40684	0.60459	-0.30277
C	-2.87089	0.68180	-0.31668
C	-3.26075	1.65122	-1.40393
C	0.67287	-0.19789	-2.42500
C	0.30778	1.20992	-2.94741
C	-0.50686	-1.16611	-2.55196
C	1.82965	-0.75575	-3.28863
C	2.02856	0.07117	1.27821
C	3.43488	0.09431	0.68104
C	1.77690	1.38987	2.00786
C	1.92463	-1.15807	2.18362
H	2.33900	0.38453	-1.20987
H	-0.93634	-0.39960	4.04748
H	-1.11774	-1.82106	2.98495
H	-3.21900	0.39368	3.35363
H	-3.29960	-1.22964	4.06956
H	-3.39425	-1.04076	2.30725
H	-3.18985	1.02327	0.67182
H	-3.26497	-0.32103	-0.50635
H	-2.94447	1.28613	-2.38482
H	-2.81628	2.63387	-1.22364
H	-4.34923	1.75727	-1.40649
H	1.17278	1.88040	-2.92615
H	-0.50061	1.65291	-2.36266
H	-0.01949	1.10448	-3.98673
H	-0.27777	-2.13374	-2.09831
H	-0.67114	-1.32685	-3.62168
H	-1.43778	-0.78383	-2.13607
H	2.15321	-1.73729	-2.92709
H	2.69050	-0.08017	-3.29410
H	1.47173	-0.86692	-4.31562
H	4.12797	0.07647	1.52507
H	3.63657	-0.78513	0.06093
H	3.64283	1.00562	0.11395
H	2.58714	1.53348	2.72840
H	1.79857	2.22205	1.29732
H	0.83099	1.40141	2.54777
H	0.99545	-1.20489	2.74976
H	2.04150	-2.07714	1.60127
H	2.73929	-1.10673	2.91054

N+_bw, SMD Methanol

N	0.79340	-0.06239	0.69095
C	1.48164	-0.24878	-0.39257
P	-0.95008	0.30666	0.69334
O	-1.40402	0.86105	1.98401
O	-1.13609	1.27233	-0.53468
C	-1.40531	2.70007	-0.34158
C	-2.89495	2.92833	-0.25590
O	-1.49757	-1.10122	0.26377
C	-2.91017	-1.23319	-0.11190
C	-3.18214	-2.70216	-0.31160
C	1.18800	-0.35451	-1.86955
C	1.44791	1.06298	-2.43075
C	-0.15935	-0.90607	-2.34753
C	2.29242	-1.29693	-2.39968
C	1.50547	-0.11015	2.07044
C	2.93975	-0.61337	1.92288
C	1.53204	1.30515	2.64773
C	0.73808	-1.11088	2.93910
H	2.54968	-0.32845	-0.21304
H	-0.96895	3.17513	-1.22087
H	-0.87709	3.04121	0.55194
H	-3.39182	2.55112	-1.15415
H	-3.08824	4.00232	-0.17712
H	-3.31822	2.43431	0.62331
H	-3.05970	-0.65749	-1.02972
H	-3.51818	-0.81080	0.69281
H	-3.00134	-3.25795	0.61215
H	-2.55140	-3.10902	-1.10654
H	-4.22962	-2.83218	-0.59760
H	2.42526	1.44515	-2.11862
H	0.67326	1.76395	-2.11437
H	1.44141	0.99323	-3.52309
H	-0.36577	-1.88212	-1.90135
H	-0.07811	-1.03927	-3.43061
H	-0.99766	-0.23738	-2.16255
H	2.18899	-2.30201	-1.97789
H	3.29156	-0.91707	-2.16430
H	2.19933	-1.36789	-3.48649
H	3.33352	-0.71931	2.93631
H	2.98895	-1.59473	1.44047
H	3.58784	0.09329	1.39693

H	2.11515	1.28056	3.57281
H	2.02768	1.98667	1.94881
H	0.53675	1.68292	2.87905
H	-0.28165	-0.79389	3.15676
H	0.72056	-2.09507	2.46026
H	1.26907	-1.20205	3.89035

N+_ax, SMD Methanol

N	0.76153	-0.16440	-0.13567
C	1.44988	0.18211	-1.17895
P	-1.01742	-0.06410	-0.14694
O	-1.55532	-0.48950	-1.45526
O	-1.53575	-0.92924	1.06136
C	-2.26419	-2.18233	0.82960
C	-2.66620	-2.70890	2.18398
O	-1.15292	1.42867	0.32243
C	-2.48205	1.99583	0.58291
C	-2.65828	2.16916	2.07147
C	1.12600	0.85231	-2.49329
C	0.01461	1.91009	-2.50029
C	0.85773	-0.27453	-3.51566
C	2.44378	1.55809	-2.88238
C	1.49816	-0.67735	1.13310
C	3.00446	-0.45717	1.00104
C	0.99809	0.15203	2.31927
C	1.22949	-2.17358	1.28878
H	2.50789	-0.05061	-1.10136
H	-1.60054	-2.86853	0.29700
H	-3.12929	-1.95270	0.20516
H	-1.78795	-2.91108	2.80357
H	-3.22034	-3.64220	2.05032
H	-3.31052	-1.99219	2.70054
H	-3.24585	1.34400	0.14801
H	-2.48609	2.94699	0.04897
H	-1.86079	2.79505	2.48140
H	-2.65423	1.20202	2.58165
H	-3.61746	2.65954	2.26218
H	0.16836	2.64481	-1.70419
H	-0.98756	1.49326	-2.41955
H	0.07768	2.43481	-3.45834
H	1.67027	-1.00845	-3.51922
H	0.80797	0.18402	-4.50841
H	-0.08473	-0.78283	-3.30789
H	3.27318	0.84640	-2.94286
H	2.70237	2.33874	-2.15921
H	2.31701	2.02465	-3.86270
H	3.43997	-0.72495	1.96639
H	3.46411	-1.10473	0.24880
H	3.25688	0.58836	0.79844
H	1.55764	-0.16888	3.20207
H	1.19559	1.21564	2.15453
H	-0.06143	0.00785	2.53128
H	0.20385	-2.39073	1.58344
H	1.46405	-2.70233	0.35978
H	1.88838	-2.55311	2.07479

O•, SMD Methanol

C	-1.21583	2.87787	0.12007
C	0.11979	2.14526	0.23392
O	1.06266	2.67667	-0.62433
C	0.06344	0.62637	0.15474
C	-1.12911	-0.07589	-0.01958
C	-1.13548	-1.46979	-0.10155
C	0.06403	-2.17143	-0.00671
C	1.26858	-1.48499	0.17057
C	1.25803	-0.09853	0.25088
O	0.12233	-3.53470	-0.07949
H	-1.04455	3.95186	0.21981
H	-1.89986	2.55605	0.90918
H	-1.67834	2.68080	-0.85146
H	0.56200	2.41825	1.22047
H	-2.07455	0.45204	-0.09750
H	-2.06794	-2.01085	-0.24087
H	2.19520	-2.04627	0.24538
H	2.19599	0.43445	0.38911
H	-0.76457	-3.90473	-0.20053

e•, SMD Methanol

C	-0.04017	1.31240	0.05881
C	1.36511	1.32447	0.12190
C	2.09106	0.15829	0.06452
C	1.40010	-1.11468	-0.06373
C	-0.04178	-1.10765	-0.12701
C	-0.77997	0.08958	-0.06778
C	-2.18958	0.06873	-0.13184
C	-3.03870	1.29292	-0.07580
O	2.03901	-2.19735	-0.11862
H	-0.57626	2.25451	0.10739
H	1.87629	2.27772	0.21765
H	3.17519	0.14582	0.11150
H	-0.54492	-2.06600	-0.22282
H	-2.66881	-0.90118	-0.22748
H	-2.88196	1.84954	0.85805
H	-4.09737	1.03679	-0.14302
H	-2.80321	1.98452	-0.89599

T, SMD Methanol

C	0.69412	1.03857	0.90063
C	2.04068	0.72629	0.86499
C	2.48482	-0.35941	0.10898
C	1.61951	-1.21021	-0.66285
C	0.25013	-0.87314	-0.61567
C	-0.21488	0.23145	0.14963
C	-1.55652	0.59469	0.21222
C	-2.69614	-0.03502	-0.45668
O	2.08565	-2.20213	-1.34131
H	0.31501	1.87580	1.47816
H	2.75860	1.32030	1.42184
H	3.54731	-0.59415	0.08923
H	-0.44906	-1.48287	-1.17918
H	-1.79588	1.45515	0.83721
H	-3.22910	0.74045	-1.02383
H	-3.40687	-0.35240	0.32010
H	-2.44726	-0.87337	-1.10346

S_ab, SMD Methanol

C	3.26391	-0.61515	-0.79825
C	2.93685	0.70229	-0.73919
C	1.58260	0.76067	-0.27338
C	1.18441	-0.53156	-0.08255
C	-0.04560	-1.17089	0.36889
C	-1.12995	-0.51077	0.71838
C	-2.20774	0.14283	1.06551
C	-3.32143	0.52359	0.12438
O	2.20800	-1.37765	-0.40189
H	4.15575	-1.15264	-1.08448
H	3.57925	1.53282	-0.99607
H	0.98051	1.64234	-0.10239
H	-0.03395	-2.25959	0.40802
H	-2.31698	0.43665	2.11101
H	-3.45746	1.60988	0.12058
H	-4.26428	0.07689	0.45631
H	-3.11309	0.19039	-0.89448

S_ad, SMD Methanol

C	2.77769	0.00282	0.34707
C	3.03786	-1.31679	0.15981
C	1.76249	-1.96290	0.04212
C	0.82088	-0.98242	0.16715
C	-0.63315	-1.01817	0.13328
C	-1.40625	0.03911	0.27314
C	-2.17691	1.08668	0.40839
C	-2.65788	1.95047	-0.72890
O	1.43240	0.22196	0.35386
H	3.39925	0.87506	0.48591
H	4.01534	-1.77552	0.11096
H	1.56417	-3.01416	-0.11432
H	-1.07463	-2.00163	-0.01981
H	-2.50111	1.36167	1.41357
H	-2.33201	2.98514	-0.58085
H	-3.75222	1.95402	-0.76351
H	-2.27602	1.59447	-1.68809

R, SMD Methanol

C	0.47321	-1.74986	-0.23922
C	1.96369	-1.93340	-0.32334
C	2.65549	-0.82889	0.00138
C	1.72306	0.25614	0.35172
C	0.34540	-0.30767	0.20378
C	-0.74061	0.39433	0.43725
C	-1.79717	1.12311	0.67649
C	-2.50973	1.96087	-0.35246
O	2.01144	1.39825	0.69725
H	-0.00155	-1.93283	-1.20955
H	2.40495	-2.87945	-0.62119
H	3.73237	-0.70849	0.01786
H	0.02987	-2.44866	0.47882
H	-2.19370	1.12356	1.69283
H	-2.51695	3.00933	-0.03878
H	-3.55116	1.63682	-0.44323
H	-2.02860	1.88685	-1.32961

e+, SMD Methanol

C	-1.37680	3.04552	-0.13912
C	-0.23275	2.14529	-0.20382
C	-0.22636	0.75343	-0.07888
C	-1.41745	0.00700	0.14061
C	-1.33285	-1.36596	0.25382
C	-0.09235	-2.00683	0.15334
C	1.08968	-1.28322	-0.06297
C	1.02947	0.09450	-0.17973
O	2.29893	-1.88529	-0.16289
H	-1.16901	3.78764	0.64609
H	-2.33998	2.56930	0.02693

H	-1.38813	3.63236	-1.06971
H	0.73427	2.62042	-0.37024
H	-2.37565	0.50712	0.21780
H	-2.22373	-1.96088	0.42132
H	-0.03436	-3.08894	0.24371
H	1.93543	0.67048	-0.34742
H	2.21612	-2.84643	-0.06587

e•, SMD Methanol

C	-1.39419	3.04576	-0.08922
C	-0.15512	2.21700	-0.12107
C	-0.15741	0.79608	-0.05972
C	-1.36271	0.05082	0.03817
C	-1.32533	-1.33546	0.09587
C	-0.11282	-2.02987	0.05964
C	1.07990	-1.30290	-0.03676
C	1.06774	0.08278	-0.09583
O	2.29909	-1.92575	-0.07642
H	-1.15489	4.10929	-0.14805
H	-1.97044	2.87919	0.83138
H	-2.06611	2.80361	-0.92420
H	0.80737	2.71512	-0.19505
H	-2.31736	0.56652	0.06803
H	-2.25293	-1.89608	0.17064
H	-0.08449	-3.11502	0.10487
H	2.00960	0.62054	-0.17040
H	2.18457	-2.88610	-0.02893

O , SMD Methanol

C	-0.91849	2.68020	0.51321
C	-0.55305	1.90651	-0.78425
C	-0.40532	0.42240	-0.51105
C	-1.48023	-0.43577	-0.75479
C	-1.35915	-1.79377	-0.46122
C	-0.17556	-2.30373	0.06873
C	0.89253	-1.43661	0.30829
C	0.78265	-0.07630	0.02061
O	0.60459	2.50526	-1.22643
O	2.07917	-1.87140	0.82911
H	-1.84833	2.25720	0.90117
H	-1.06058	3.74016	0.29348
H	-0.12515	2.55472	1.25423
H	-1.36333	2.09055	-1.50667
H	-2.40367	-0.04286	-1.17246
H	-2.19075	-2.46621	-0.65087
H	-0.07429	-3.36186	0.29485
H	1.62719	0.58029	0.21299
H	2.04328	-2.82327	1.00434

Q, SMD Methanol

O	0.56180	2.99026	-0.78763
C	-0.21769	2.19193	-0.27283
C	-1.32588	2.67894	0.62100
C	-0.07864	0.73350	-0.52451
C	0.95391	0.27521	-1.35809
C	-0.95130	-0.20153	0.04801
C	-0.80154	-1.56043	-0.20183
C	0.23268	-1.99585	-1.03437
C	1.11425	-1.07628	-1.61527
O	0.42980	-3.30868	-1.31568
H	-1.27856	3.76586	0.69314
H	-1.23033	2.23985	1.61911
H	-2.29869	2.37929	0.21849
H	1.63402	0.99356	-1.80533
H	-1.75909	0.12243	0.69664
H	-1.47752	-2.28629	0.24156
H	1.90994	-1.43888	-2.25856
H	-0.23065	-3.85756	-0.8665