Supplementary Information

Combined computational and experimental study about the incorporation of phosphorus into the structure of graphene oxide

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Details about the characterization methods

Solid-state NMR experiments

Solid-state NMR experiments were conducted at room temperature in a Varian/Agilent VNMR 400 MHz spectrometer (operating at a magnetic field of 9.4 T) using a triple-resonance probehead; the powdered samples were packed into 4 mm diameter zirconia rotors for magic angle spinning (MAS) experiments at the frequency of 14 kHz. For ^{13}C nuclei (NMR frequency of 100.52 MHz), the pulse sequence comprised a $\pi/2$ pulse (4.3 μs) immediately followed by a pair of π pulses (8.6 μs), in order to avoid probe background signals, and the subsequent detection of the free induction decay (FID); the recycle delay was 15 s and the spectral window was 250 kHz; the spectra were obtained by Fourier transform of the FIDs, after accumulation of ca. 4000 transients; the ^{13}C chemical shifts were referenced to tetramethylsilane (TMS), using hexamethylbenzene as a secondary reference (signal at 17.3 ppm). For ^{31}P nuclei (NMR frequency of 161.81 MHz), the single pulse experiments were performed using a $\pi/2$ pulse with duration of 4.0 μs, a recycle delay of 60 s (adjusted to avoid saturation issues), a spectral window of 100 kHz and ca. 500 scans; the ^{31}P chemical shifts were referenced to a 85 wt. % aqueous H_3PO_4 solution, using $NH_4H_2PO_4$ as the secondary reference (signal at 0.9 ppm).

XPS experiments

The samples for the XPS experiments were glued to a Mo-plate sample-holder with conductive carbon tape. The samples were degassed in a load-lock chamber for 12 h before transferring to the XPS chamber. The obtained data were fitted assuming Shirley-type background and Lorentzian

peaks numerically convoluted with a normalized Gaussian function with a fixed full-width at half maximum of ~0.9 eV that describes the instrumental broadening. The atomic concentrations were obtained from the XPS spectra assuming that the analysed samples are primarily carbon-based materials and are chemically homogeneous. As the inelastic mean free path (IMFP) of photoelectrons is different for distinct chemical elements, the IMFP for each core-level peak was calculated using the TPP-2M formula[1], as provided in the software Quases-IMFP[2]. The TPP-2M formula has been proven to be an excellent approximation for IMFP calculations for homogenous materials. Having this information, as well as the analyser transmission and photoemission cross-sections[3] the atomic concentrations (at. %) were determined using the method reported by Wagner et al.[4] Finally, the atomic concentrations were easily converted to weight concentrations (wt. %), as reported in Table 2 of the main text.

Details about the computational methods

The DFT calculations were carried out using the Quantum Espresso package (version 5.1) using periodic boundary conditions.[5] The exchange-correlation term was described within the generalized gradient approximation (GGA), using the Perdew-Burke-Ernzerhof (PBE) scheme.[6] The Kohn-Sham orbitals were expanded in a plane wave basis set with an energy cutoff of 1088 eV.[7,8] The van der Waals interaction was taken into account following the semi-empirical approach described by Grimme et al.[9] The supercells were constructed with a vacuum region of 25 Å along the direction perpendicular to the graphene plane. All the structures were relaxed keeping the supercell lattice parameter fix until the atomic forces were lower than 0.01 eV /Å.[7,8] The NMR spectral parameters were determined using the GIPAW approach,[10] also implemented in Quantum

Espresso,[5] which is based on an extension of the projector augmented-wave (PAW) method proposed by Blöchl.[11,12]

Results

Elemental P contents

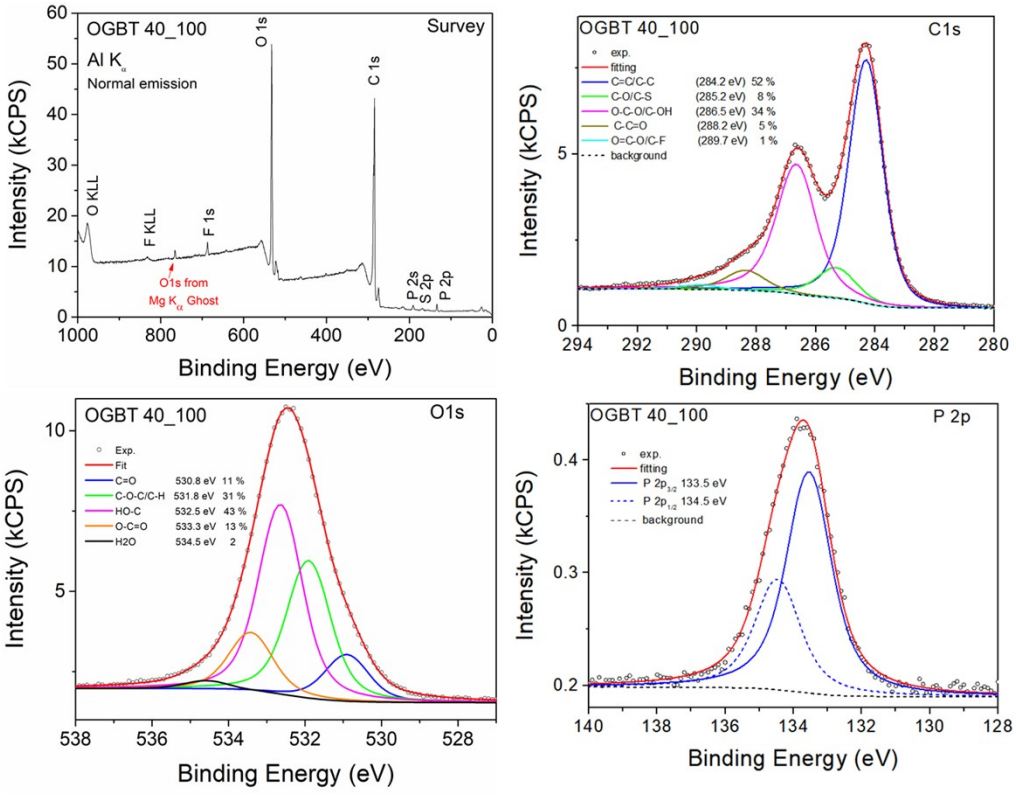
Table S1. Bulk elemental P and S contents obtained by XRF for all produced samples.

Sample	**H_2SO_4 volume** (mL)	**H_3PO_4 volume** (mL)	**P content** (wt. %)	**S content** (wt. %)
GO 120:20	120	20	0.53(3)	11.3
GO 100:40	100	40	0.90(3)	10.5
GO 90:50	90	50	1.06 (2)	4.36
GO 80:60	80	60	0.97(1)	4.51
GO 70:70	70	70	1.68(3)	7.36
GO 60:80	60	80	2.86(3)	2.10
GO 50:90	50	90	5.50(2)	3.22
GO 40:100	40	100	5.01(2)	2.24
GO 20:120	20	120	4.94(2)	0.54
GO 0:140	0	140	0.96(1)	0.009

Table S2. Surface elemental contents obtained by XPS for a set of P/GO hybrids.

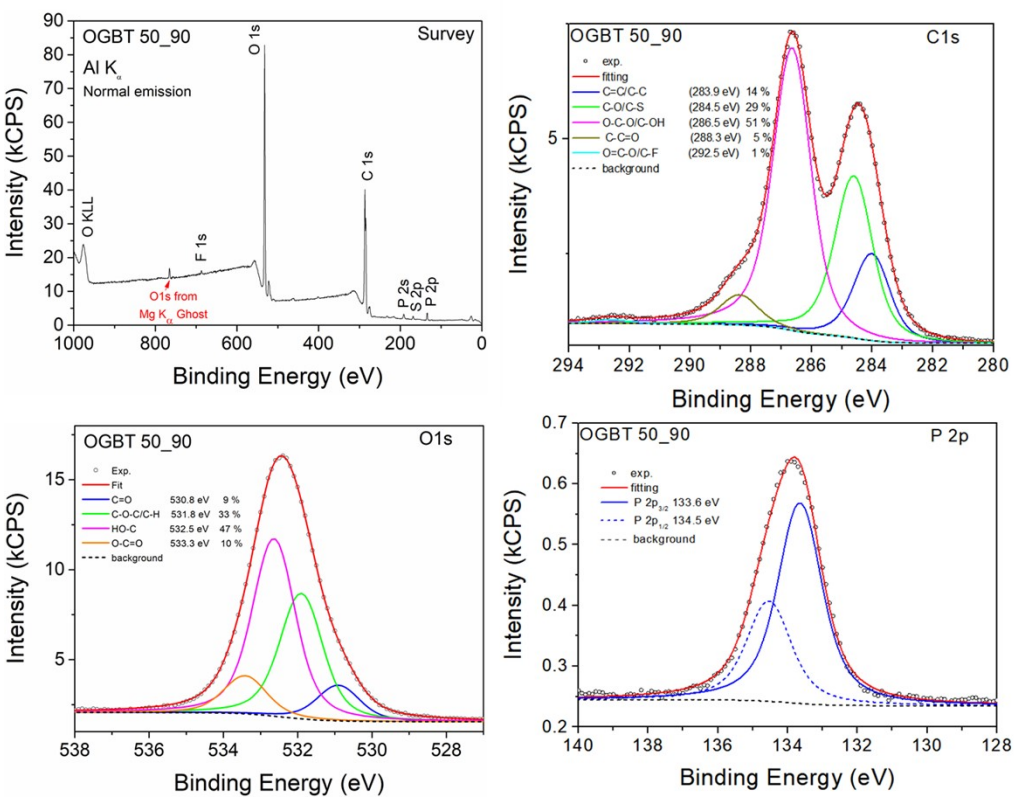
Contents (wt. %)	GO 40:100	GO 50:90	GO 60:80	GO 70:70	GO 80:60	GO 90:50	GO 100:40
C	60.5	52.4	57.4	59.1	69.0	56.0	54.0
O	32.5	41.1	39.0	38.3	27.7	41.0	41.4
P	3.6	4.9	2.6	1.6	1.0	0.9	0.7
F	2.0	0.0	0.0	0.0	0.0	0.0	0.0
S	1.2	1.6	1.1	1.0	2.3	2.1	3.9

XPS spectra



GO 40:100

Figure S1 (a): Survey and high-resolution C 1s, O 1s and P 2p XPS spectra obtained for the GO 40:100 sample.



GO 50:90

Figure S1 (b): Survey and high-resolution C 1s, O 1s and P 2p XPS spectra obtained for the GO 50:90 sample.

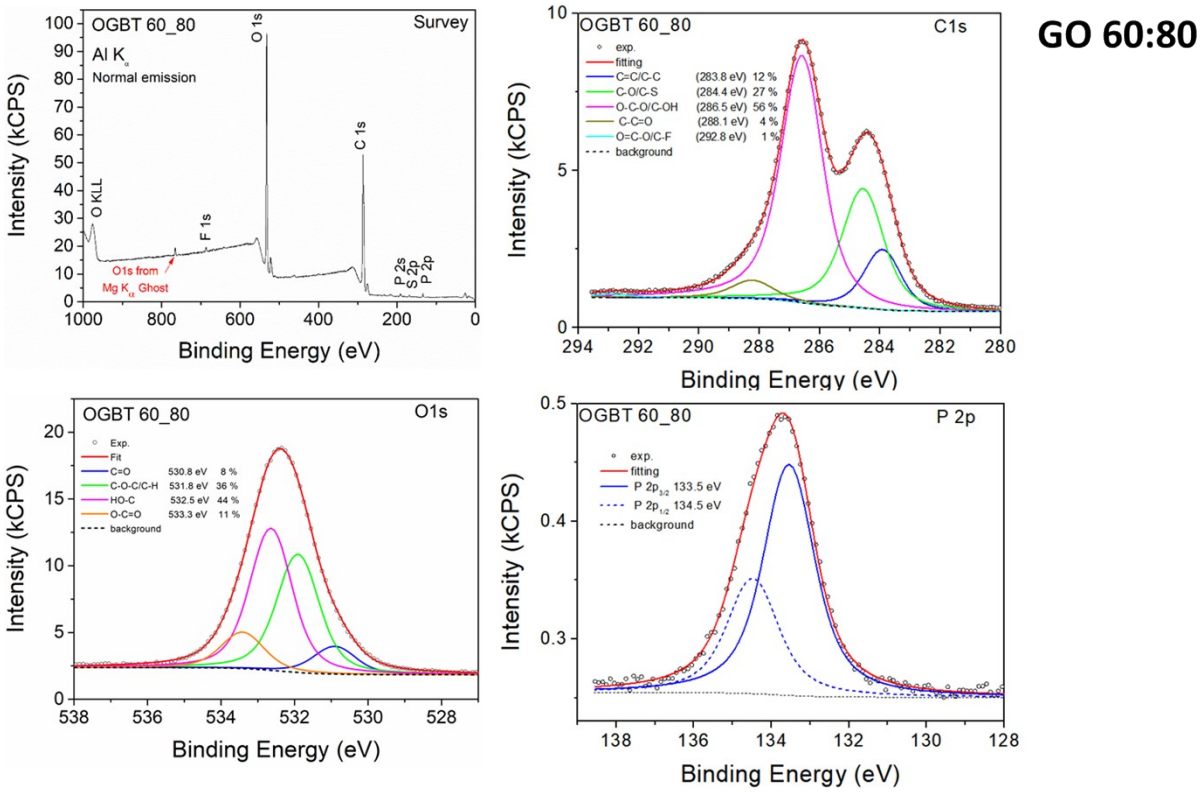
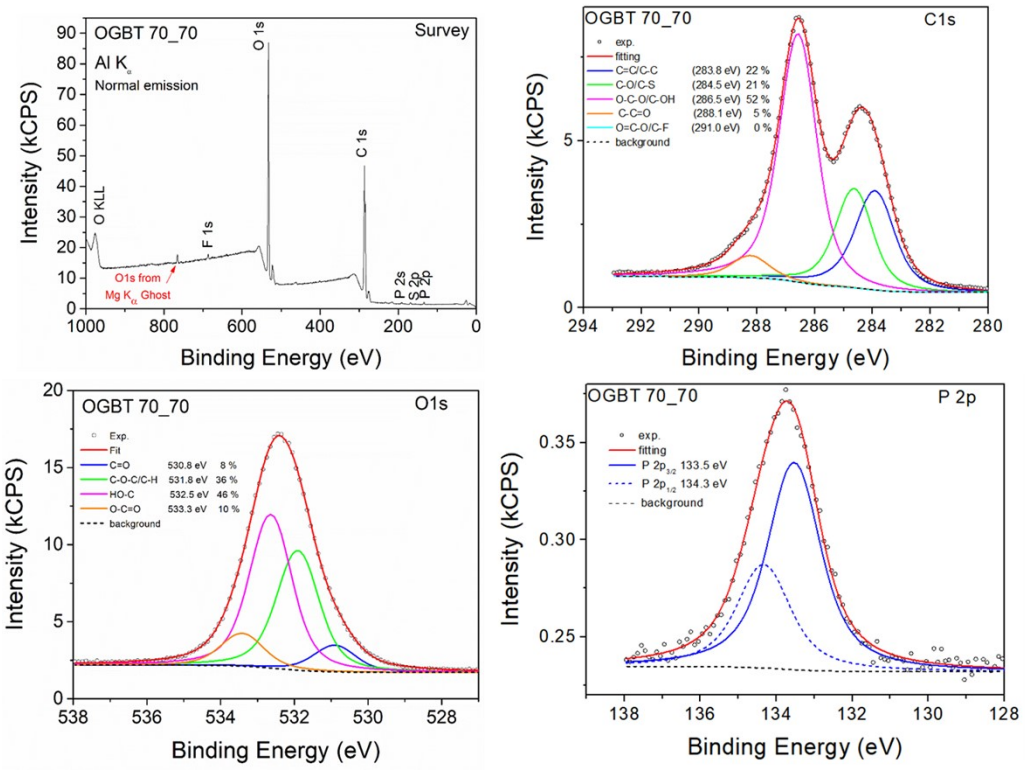


Figure S1 (c): Survey and high-resolution C 1s, O 1s and P 2p XPS spectra obtained for the GO 60:80 sample.



GO 70:70

Figure S1 (d): Survey and high-resolution C 1s, O 1s and P 2p XPS spectra obtained for the GO 70:70 sample.

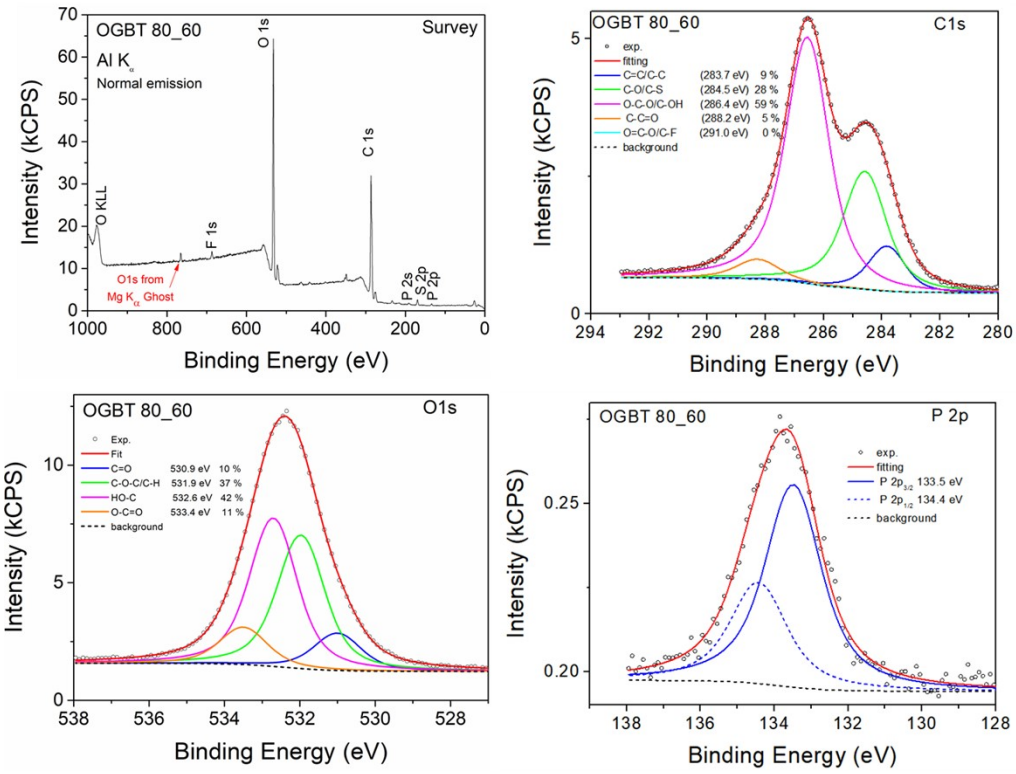
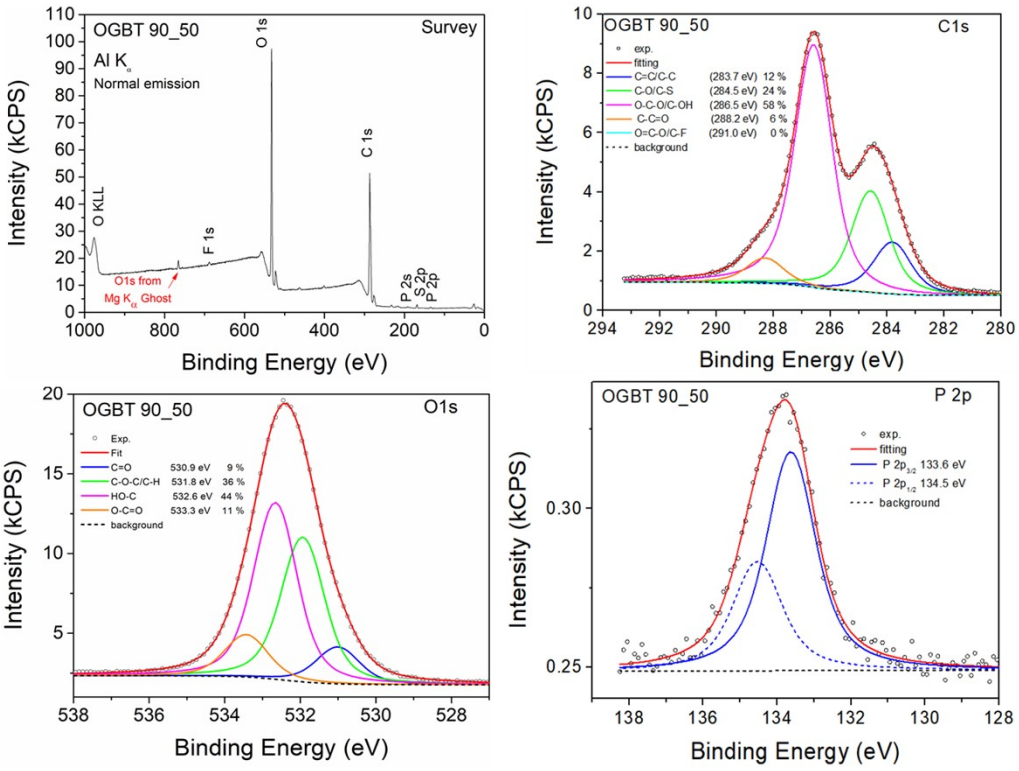
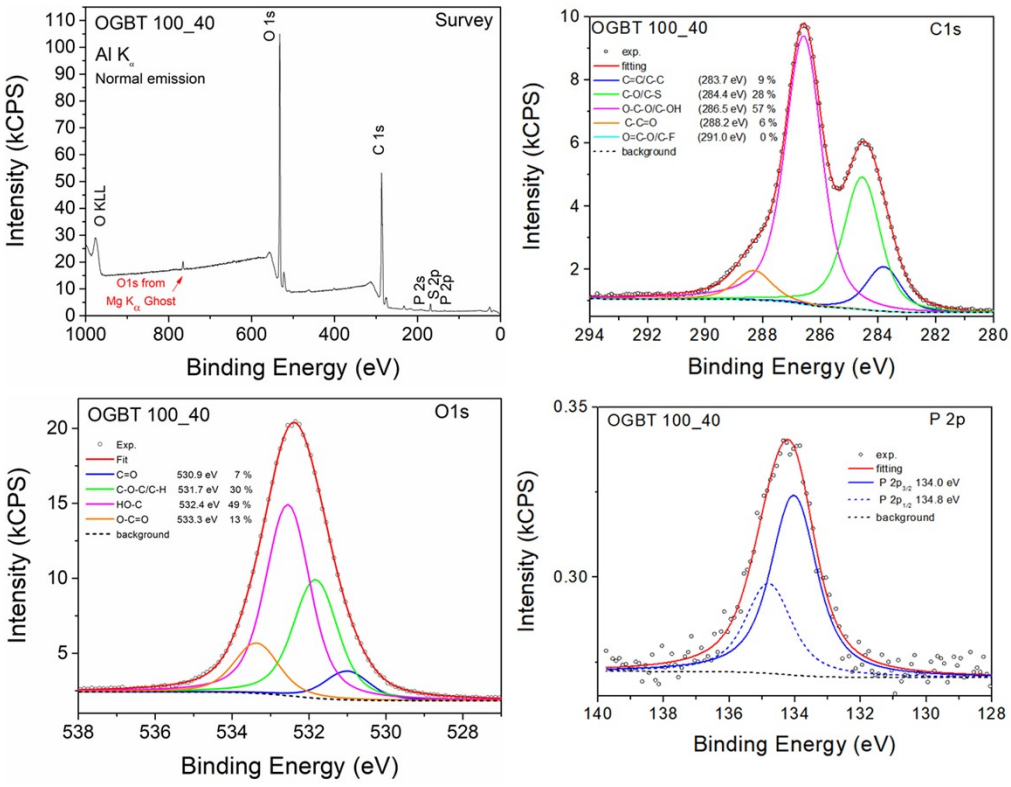


Figure S1 (e): Survey and high-resolution C 1s, O 1s and P 2p XPS spectra obtained for the GO 80:60 sample.



GO 90:50

Figure S1 (f): Survey and high-resolution C 1s, O 1s and P 2p XPS spectra obtained for the GO 90:50 sample.



GO 100:40

Figure S1 (g): Survey and high-resolution C 1s, O 1s and P 2p XPS spectra obtained for the GO 100:40 sample

XRD results

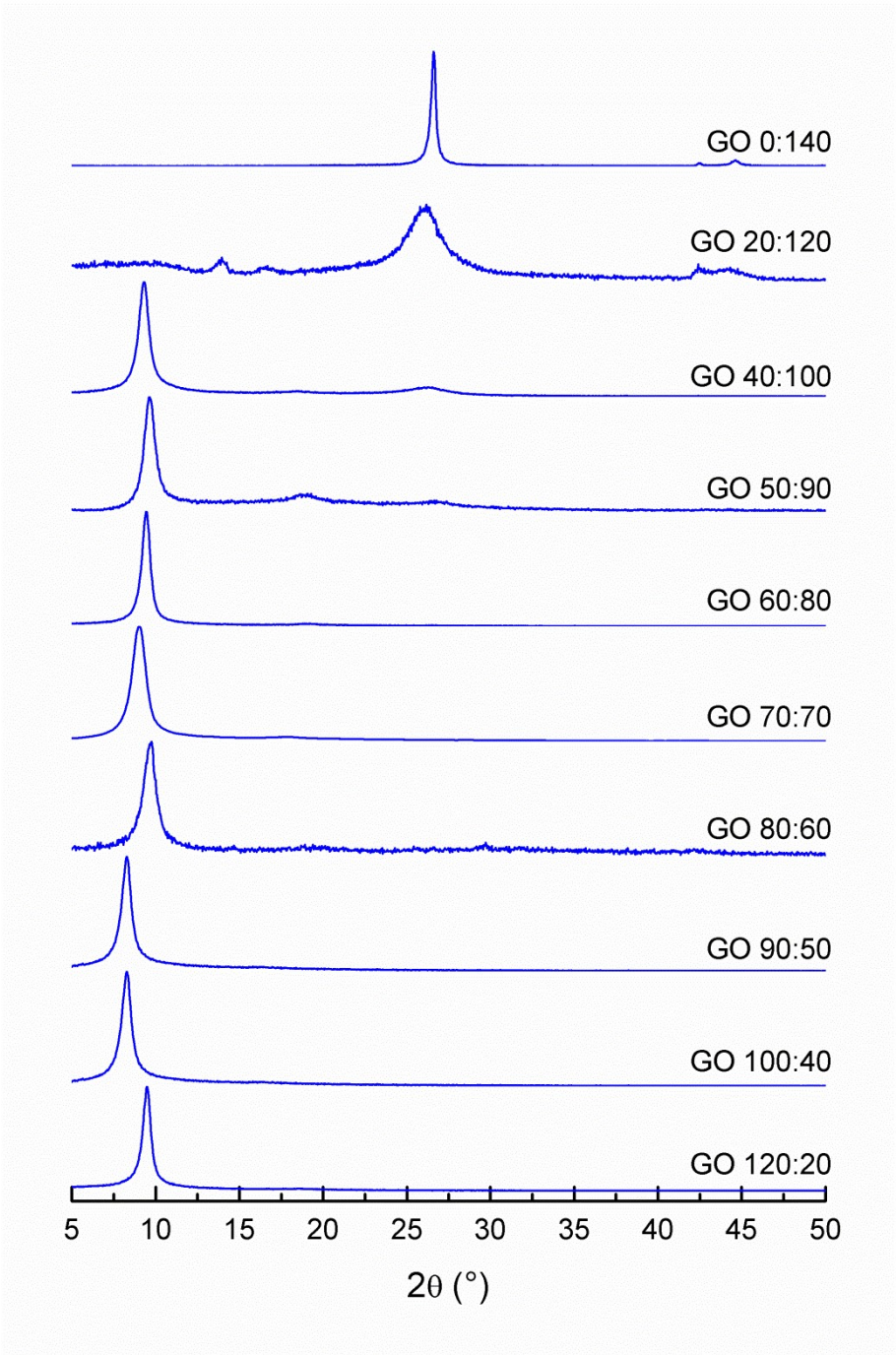


Figure S2. XRD patterns of the synthesized P/GO hybrids.

TG results

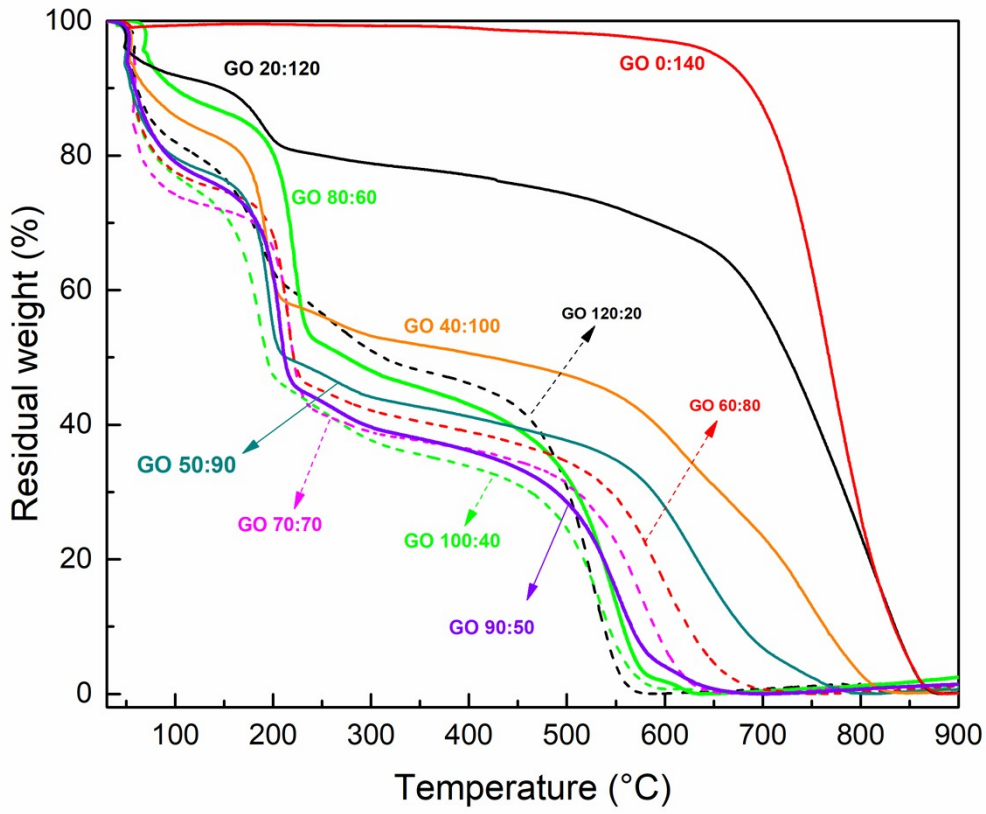


Figure S3. TG curves recorded under O_2 flow for the synthesized P/GO hybrids.

Solid-state ^{13}C NMR results

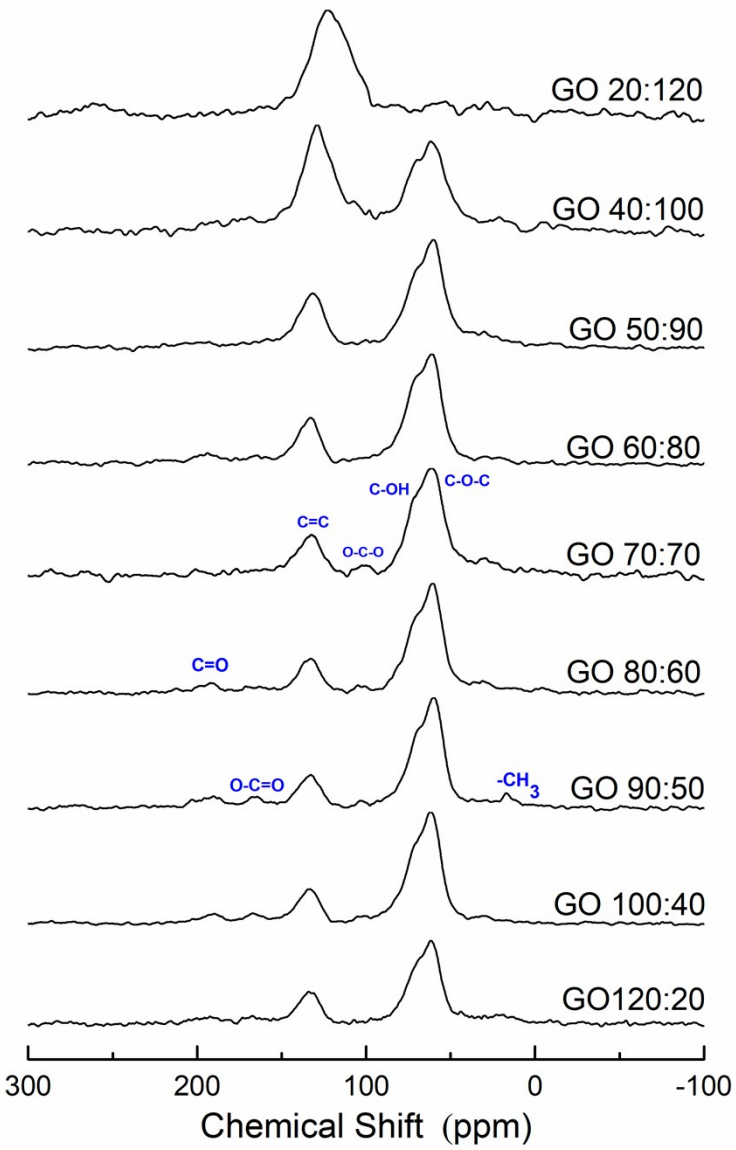


Figure S4. Solid-state ^{13}C NMR spectra of the whole set of synthesized P/GO hybrids.

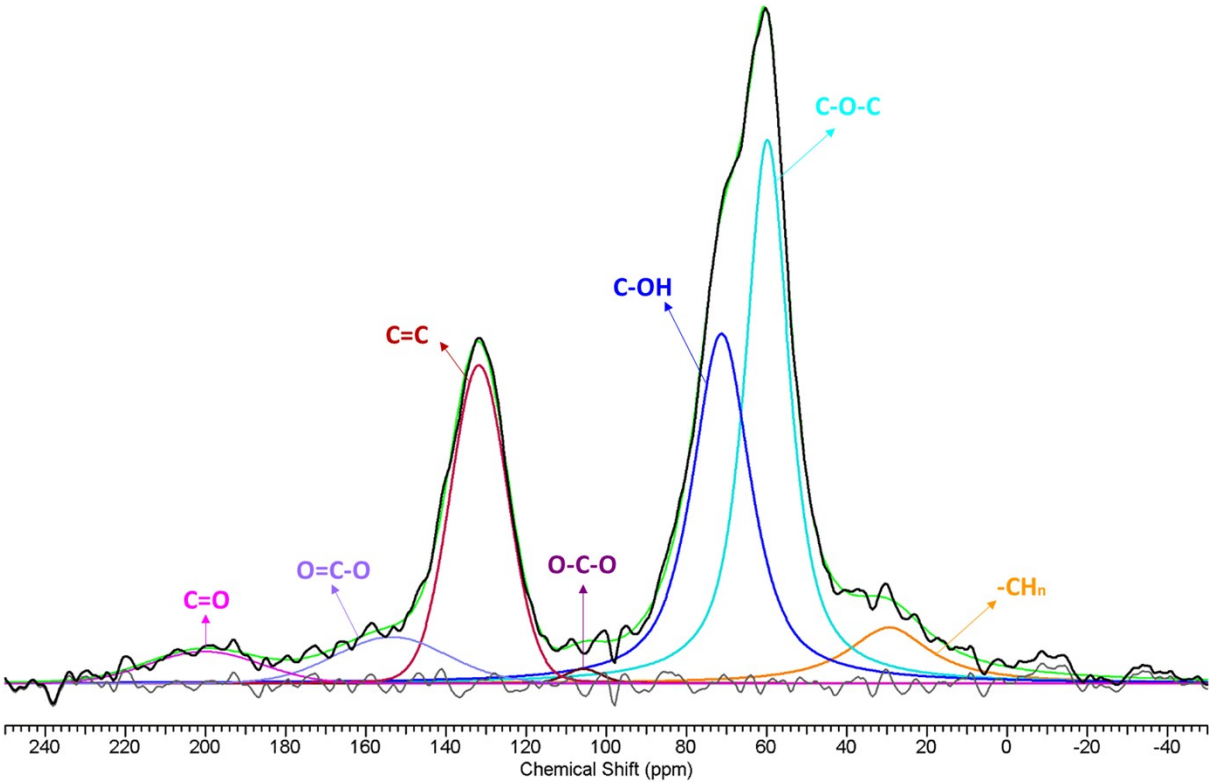


Figure S5. Solid-state ^{13}C NMR spectrum obtained for the GO 50:90 hybrid. The black line is the experimental spectrum, the green line is the fitted spectrum, the gray line indicates the residual (difference between experimental and fitted spectra) and the other colored lines correspond to the components used in the spectral deconvolution, associated with the indicated groups.

Solid-state ^{31}P NMR results

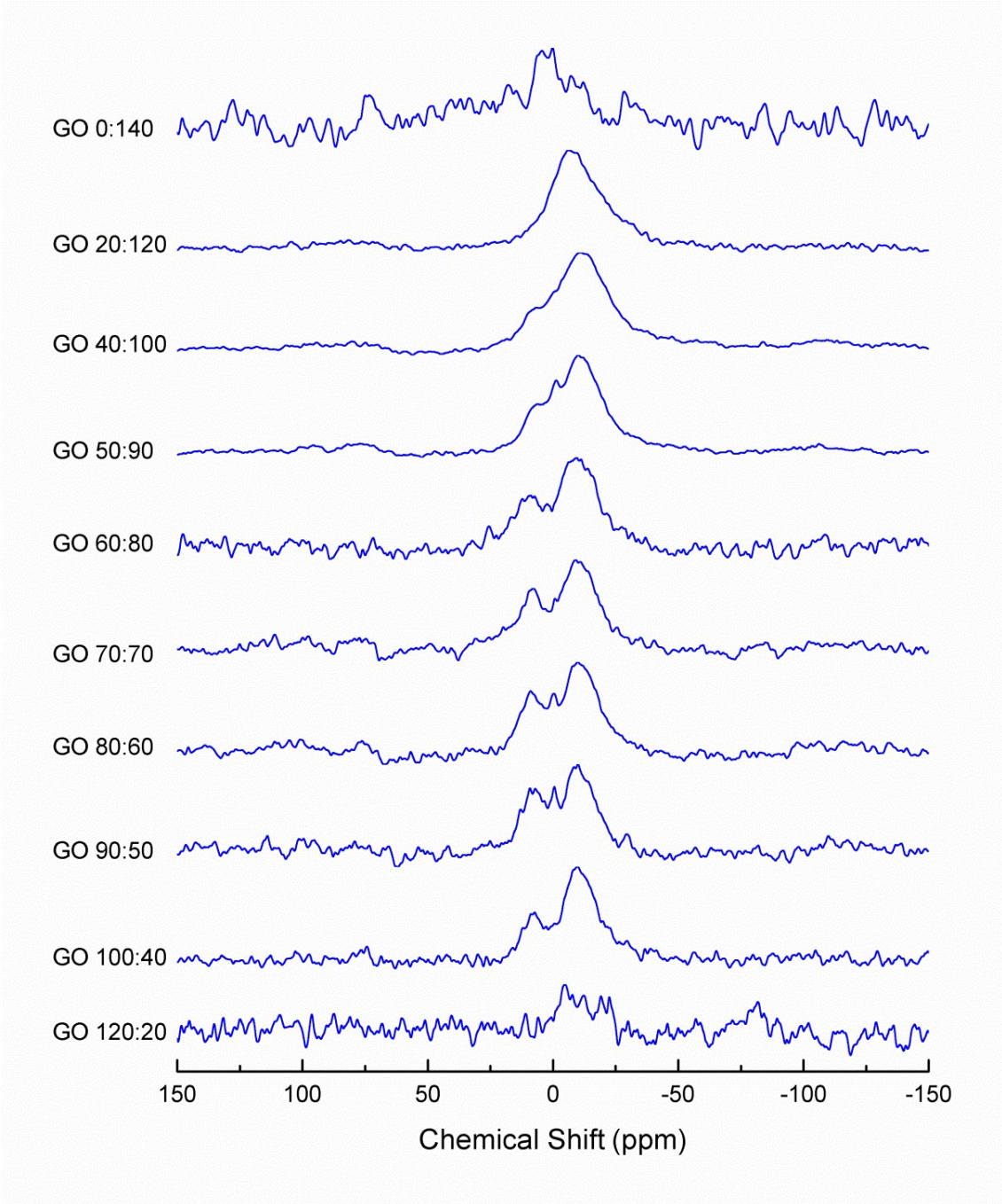


Figure S6. Solid-state ^{31}P NMR spectra of the whole set of synthesized P/GO hybrids.

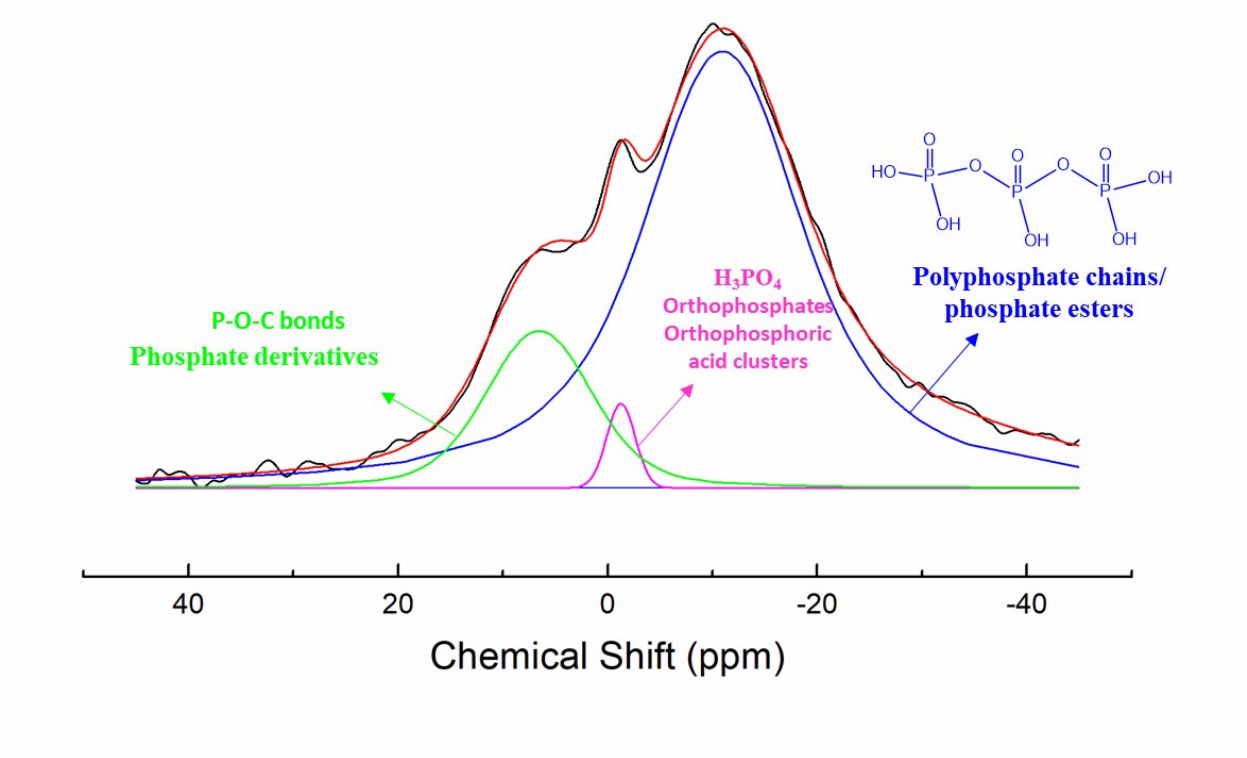


Figure S7. Solid-state ^{31}P NMR spectrum obtained for the GO 50:90 hybrid. The black line is the experimental spectrum, the red line is the fitted spectrum and the other colored lines correspond to the components used in the spectral deconvolution, associated with the indicated groups.

Supplementary DFT calculations

Systems GO-Epoxy-Epoxy-H_3PO_4 and GO-OH-OH-H_3PO_4

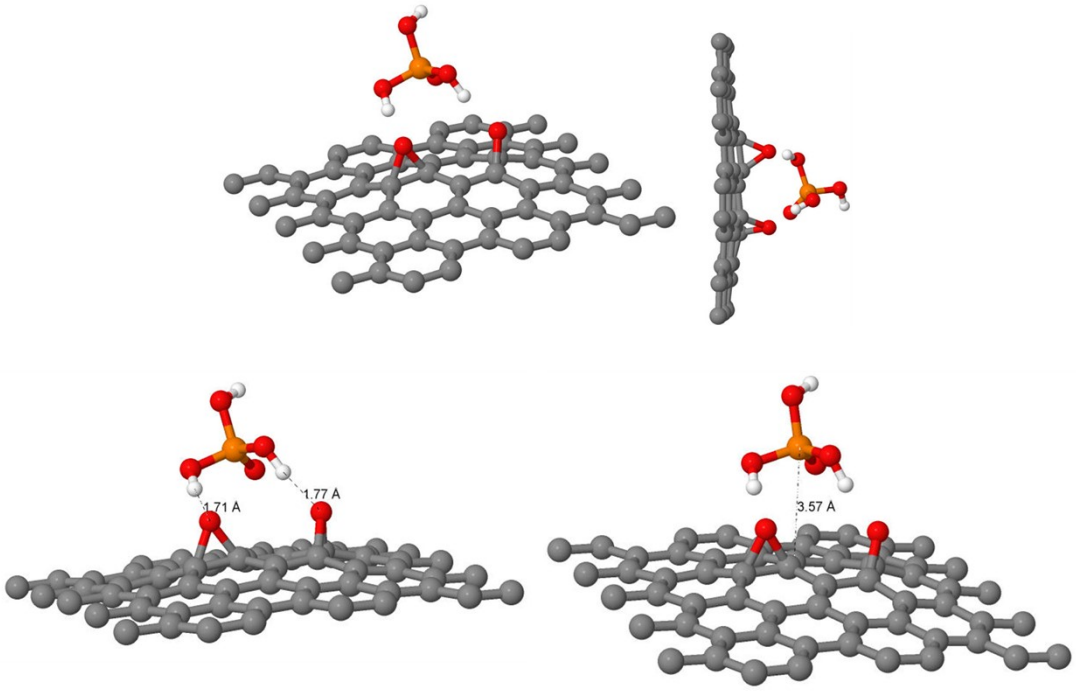


Figure S8. Model system used in the DFT calculations involving the adsorption of H_3PO_4 on a GO sheet containing two neighboring epoxy groups (system GO-Epoxy-Epoxy-H_3PO_4), with indication of the formation of hydrogen bonds.

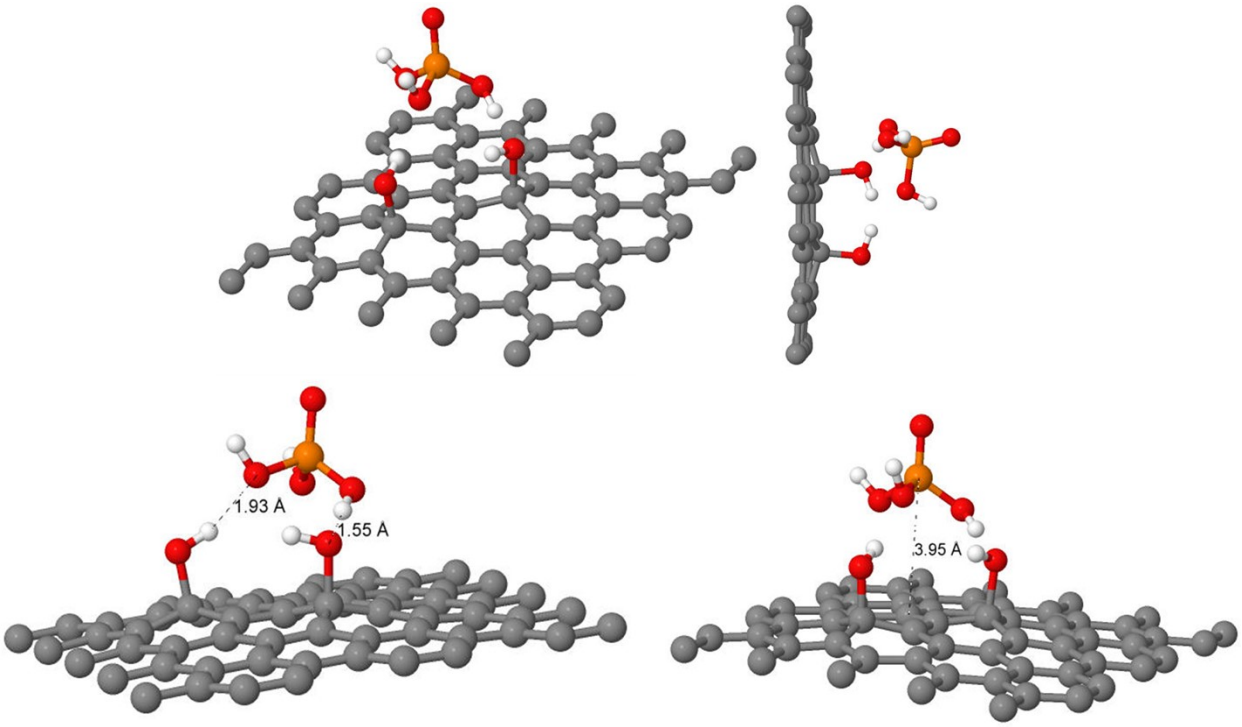


Figure S9. Model system used in the DFT calculations involving the adsorption of H_3PO_4 on a GO sheet containing two neighboring hydroxyl groups (system GO-OH-OH-H_3PO_4), with indication of the formation of hydrogen bonds.

Table S3. Calculated adsorption energies, bond lengths and interatomic distances for the systems GO-Epoxy-Epoxy-H_3PO_4 and GO-OH-OH-H_3PO_4.

System	Energy (eV)	Distances (Å)
GO-Epoxy-Epoxy-H_3PO_4		
	-0.91	*d*: 3.57 Å
		H bond = 1.71 Å /1.77 Å
GO-OH-OH-H_3PO_4		
	-1.14	*d*: 3.95 Å
		H bond = 1.55 Å / 1.93 Å

Table S4. NMR chemical shifts calculated for the ^{13}C and ^{31}P nuclei in the systems GO-Epoxy-Epoxy-H_3PO_4 and GO-OH-OH-H_3PO_4.

System	$\delta^{13}C$ ppm	$\delta^{31}P$ ppm
GO-Epoxy-Epoxy-H_3PO_4		
C=C	116-133	-
C-O	83	-
C-O	78	-
C-O	80	-
C-O	75	-
H_3PO_4	-	5.5
GO-OH-OH-H_3PO_4		
C=C	102-145	-
C-OH	79	-
C-OH	68	-
H_3PO_4	-	-1.4

Predicted NMR parameters

Table S5. Calculated shielding and chemical shift values (in ppm) for all ^{13}C and ^{31}P nuclei in the G-H_3PO_4 system.

Nucleus	σ_{iso}	δ_{calc}
C1	38.84	126.86
C2	38.88	126.82
C3	38.68	127.02
C4	38.11	127.59
C5	38.56	127.14
C6	38.72	126.98
C7	39.89	125.81
C8	38.70	127.00
C9	38.77	126.93
C10	38.50	127.20
C11	37.94	127.76
C12	37.21	128.49
C13	39.30	126.40
C14	38.49	127.21
C15	38.86	126.84
C16	38.78	126.92
C17	38.09	127.61
C18	36.67	129.03
C19	38.80	126.90
C20	38.79	126.91
C21	38.71	126.99
C22	38.39	127.31
C23	38.23	127.47
C24	38.33	127.37
C25	39.37	126.33
C26	38.86	126.84
C27	38.55	127.15
C28	38.94	126.76
C29	38.96	126.74
C30	39.04	126.66
C31	38.72	126.98
C32	38.36	127.34
C33	38.96	126.74

C34	38.72	126.98
C35	38.43	127.27
C36	39.16	126.54
C37	42.13	123.57
C38	38.84	126.86
C39	38.46	127.24
C40	38.56	127.14
C41	36.65	129.05
C42	38.21	127.49
C43	38.57	127.13
C44	38.37	127.33
C45	38.69	127.01
C46	38.45	127.25
C47	37.29	128.41
C48	41.22	124.48
C49	38.82	126.88
C50	38.47	127.23
C51	38.96	126.74
C52	38.82	126.88
C53	38.48	127.22
C54	38.77	126.93
C55	38.69	127.01
C56	38.65	127.05
C57	38.35	127.35
C58	38.63	127.07
C59	38.55	127.15
C60	38.70	127.00
P	277.08	3.94

Table S6. Calculated shielding and chemical shift values (in ppm) for all ^{13}C and ^{31}P nuclei in the GO-Epoxy-H_3PO_4 system.

Nucleus	σ_{iso}	δ_{calc}
C1	44.03	121.67
C2	40.08	125.62
C3	42.8	122.9
C4	42.88	122.82
C5	40.10	125.6
C6	36.27	129.43
C7	35.15	130.55
C8	39.15	126.55
C9	41.20	124.50
C10	43.97	121.73
C11	42.33	123.37
C12	36.28	129.42
C13	86.70	79.00
C14	39.28	126.42
C15	44.68	121.02
C16	45.96	119.74
C17	45.68	120.02
C18	42.50	123.20
C19	40.56	125.14
C20	38.89	126.81
C21	38.23	127.47
C22	45.60	120.10
C23	45.77	119.93
C24	43.49	122.21
C25	40.76	124.94
C26	44.33	121.37
C27	43.24	122.46
C28	44.53	121.17
C29	46.19	119.51
C30	46.10	119.60
C31	43.65	122.05
C32	39.70	126.00
C33	44.45	121.25
C34	41.38	124.32
C35	38.68	127.02

C36	36.73	128.97
C37	38.70	127.00
C38	38.72	126.98
C39	42.92	122.78
C40	43.39	122.31
C41	43.91	121.79
C42	40.98	124.72
C43	81.66	84.04
C44	37.52	128.18
C45	42.99	122.71
C46	45.63	120.07
C47	45.98	119.72
C48	41.21	124.49
C49	39.34	126.36
C50	37.59	128.11
C51	36.68	129.02
C52	45.89	119.81
C53	44.66	121.04
C54	43.15	122.55
C55	42.87	122.83
C56	42.89	122.81
C57	42.95	122.75
C58	46.32	119.38
C59	45.99	119.71
C60	45.96	119.74
P	282.19	-1.17

Table S7. Calculated shielding and chemical shift values (in ppm) for all ^{13}C and ^{31}P nuclei in the GO-OH-H_3PO_4 system.

Nucleus	σ_{iso}	δ_{calc}
C1	40.40	125.30
C2	39.20	126.50
C3	47.81	117.89
C4	42.68	123.02
C5	27.41	138.29
C6	44.30	121.40
C7	45.84	119.86
C8	34.13	131.57
C9	47.62	118.08
C10	44.64	121.06
C11	49.42	116.28
C12	55.71	109.99
C13	7.91	157.79
C14	43.15	122.55
C15	47.76	117.94
C16	41.57	124.13
C17	52.48	113.22
C18	53.83	111.87
C19	17.26	148.44
C20	22.52	143.18
C21	39.15	126.55
C22	59.92	105.78
C23	45.34	120.36
C24	42.25	123.45
C25	51.14	114.56
C26	42.90	122.80
C27	55.10	110.60
C28	46.51	119.19
C29	51.66	114.04
C30	64.37	101.33
C31	56.74	108.96
C32	42.35	123.35
C33	49.76	115.94
C34	45.14	120.56
C35	46.93	118.77
C36	35.71	129.99

C37	36.76	128.94
C38	53.95	111.75
C39	57.23	108.47
C40	48.90	116.80
C41	50.19	115.51
C42	99.74	65.96
C43	8.87	156.83
C44	41.99	123.71
C45	43.57	122.13
C46	61.39	104.31
C47	51.58	114.12
C48	43.68	122.02
C49	36.47	129.23
C50	44.20	121.50
C51	29.66	136.04
C52	44.89	120.81
C53	49.95	115.75
C54	51.59	114.11
C55	44.93	120.77
C56	40.92	124.78
C57	45.66	120.04
C58	61.76	103.94
C59	45.39	120.31
C60	39.60	126.10
P	280.14	0.88

Table S8. Calculated shielding and chemical shift values (in ppm) for all ^{13}C and ^{31}P nuclei in the GO-P-O-C system.

Nucleus	σ_{iso}	δ_{calc}
C1	45.30	120.40
C2	45.44	120.26
C3	48.97	116.73
C4	43.36	122.34
C5	29.22	136.48
C6	39.52	126.18
C7	46.66	119.04
C8	35.92	129.78
C9	44.35	121.35
C10	46.24	119.46
C11	35.57	130.13
C12	26.40	139.30
C14	16.44	149.26
C15	40.60	125.01
C16	43.10	122.60
C17	46.16	119.54
C18	46.42	119.28
C19	40.75	124.95
C20	10.11	155.59
C22	31.05	134.65
C23	35.53	130.17
C24	54.09	111.61
C25	40.54	125.16
C26	38.96	126.74
C27	48.03	117.67
C28	36.73	128.97
C29	44.41	121.29
C30	42.26	123.44
C31	44.12	121.58
C32	48.17	117.53
C33	51.60	114.10
C34	43.40	122.30
C35	41.46	124.24
C36	43.52	122.18
C37	33.69	132.01

C38	28.03	137.67
C39	33.51	132.19
C40	47.09	118.61
C41	47.13	118.57
C42	43.44	122.26
C43	37.13	128.57
C44	45.53	120.17
C45	40.22	125.48
C46	46.04	119.66
C47	51.06	114.64
C48	42.10	123.60
C49	29.01	136.69
C50	37.52	128.18
C51	36.54	129.16
C52	39.11	126.59
C53	42.56	123.14
C54	43.04	122.66
C55	42.78	122.92
C56	39.75	125.95
C57	38.91	126.79
C58	42.36	123.34
C59	47.17	118.53
C60	45.97	119.73
C61	43.99	121.71
P	276.44	4.58

Table S9. Calculated shielding and chemical shift values (in ppm) for all ^{13}C and ^{31}P nuclei in the GO-P-C system.

Nucleus	σ_{iso}	δ_{calc}
C1	43.67	122.03
C2	44.37	121.33
C3	47.06	118.64
C4	42.87	122.83
C5	28.62	137.08
C6	34.36	131.34
C7	40.57	125.13
C8	36.98	128.72
C9	44.22	121.48
C10	44.22	121.48
C11	34.36	131.34
C12	24.90	140.80
C13	13.86	151.84
C14	50.52	115.18
C15	39.08	126.62
C16	42.69	123.01
C17	44.30	121.40
C18	45.40	120.30
C19	37.81	127.89
C20	-1.14	166.84
C21	7.75	157.95
C22	16.87	148.83
C23	33.24	132.46
C24	50.76	114.94
C25	40.57	125.13
C26	40.06	125.64
C27	43.84	121.86
C28	34.08	131.62
C29	43.04	122.66
C30	42.36	123.34
C31	43.32	122.38
C32	46.63	119.07
C33	49.50	116.20
C34	39.55	126.15
C35	41.27	124.43
C36	41.83	123.87

C37	31.06	134.64
C38	24.14	141.56
C39	23.09	142.61
C40	43.19	122.51
C41	45.78	119.92
C42	41.35	124.35
C43	32.94	132.76
C44	35.21	130.49
C45	41.02	124.68
C46	45.10	120.60
C47	49.40	116.30
C48	40.93	124.77
C49	25.26	140.44
C50	30.93	134.77
C51	32.29	133.41
C52	35.87	129.83
C53	40.77	124.93
C54	43.94	121.76
C55	40.83	124.87
C56	36.51	129.19
C57	37.76	127.94
C58	40.22	125.48
C59	45.25	120.45
C60	44.40	121.30
C61	42.03	123.67
P	263.75	17.27

Table S10. Calculated shielding and chemical shift values (in ppm) for all ^{13}C and ^{31}P nuclei in the GO-Epoxy-Epoxy-H_3PO_4 system.

Nucleus	σ_{iso}	δ_{calc}
C1	47.98	117.72
C2	43.52	122.18
C3	46.08	119.62
C4	44.87	120.83
C5	37.16	128.54
C6	37.08	128.62
C7	41.03	124.67
C8	40.79	124.91
C9	47.55	118.15
C10	41.66	124.04
C11	37.44	128.26
C12	82.43	83.27
C13	33.92	131.78
C14	42.63	123.07
C15	43.39	122.31
C16	43.63	122.07
C17	46.99	118.71
C18	32.25	133.45
C19	87.91	77.79
C20	36.28	129.42
C21	41.72	123.98
C22	46.56	119.14
C23	41.35	124.35
C24	41.21	124.49
C25	38.38	127.32
C26	33.63	132.07
C27	41.39	124.31
C28	41.94	123.76
C29	44.72	120.98

C30	45.33	120.37
C31	45.43	120.27
C32	48.15	117.55
C33	49.29	116.41
C34	41.19	124.51
C35	34.10	131.60
C36	39.62	126.08
C37	44.58	121.12
C38	47.63	118.07
C39	42.08	123.62
C40	35.17	130.53
C41	86.09	79.61
C42	46.91	118.79
C43	34.29	131.41
C44	42.28	123.42
C45	48.87	116.83
C46	46.77	118.93
C47	41.06	124.64
C48	37.08	128.62
C49	91.01	74.69
C50	33.86	131.84
C51	36.62	129.08
C52	47.27	118.43
C53	41.91	123.79
C54	39.15	126.55
C55	35.46	130.24
C56	37.36	128.34
C57	43.95	121.75
C58	45.40	120.30
C59	41.93	123.77
C60	47.74	117.96
P	275.56	5.46

Table S11. Calculated shielding and chemical shift values (in ppm) for all ^{13}C and ^{31}P nuclei in the GO-OH-OH-H_3PO_4 system.

Nucleus	σ_{iso}	δ_{calc}
C1	52.22	113.48
C2	45.87	119.83
C3	56.84	108.86
C4	44.88	120.82
C5	38.49	127.21
C6	26.41	139.29
C7	37.97	127.73
C8	54.63	111.07
C9	45.68	120.02
C10	45.65	120.05
C11	38.58	127.12
C12	20.46	145.24
C13	27.42	138.28
C14	45.39	120.31
C15	63.07	102.63
C16	62.68	103.02
C17	49.06	116.64
C18	43.07	122.63
C19	87.08	78.62
C20	37.43	128.27
C21	30.29	135.41
C22	52.17	113.53
C23	54.83	110.87
C24	40.47	125.23
C25	49.11	116.59
C26	41.99	123.71
C27	49.69	116.01
C28	58.77	106.93
C29	49.37	116.33

C30	59.57	106.13
C31	58.89	106.81
C32	49.23	116.47
C33	40.47	125.23
C34	54.95	110.75
C35	40.71	124.99
C36	97.63	68.07
C37	43.87	121.83
C38	47.09	118.61
C39	63.12	102.58
C40	50.07	115.63
C41	31.26	134.44
C42	31.59	134.11
C43	37.09	128.61
C44	44.78	120.92
C45	49.01	116.69
C46	47.02	118.68
C47	55.68	110.02
C48	50.24	115.46
C49	26.48	139.22
C50	38.45	127.25
C51	41.23	124.47
C52	50.64	115.06
C53	45.28	120.42
C54	60.47	105.23
C55	47.67	118.03
C56	33.26	132.44
C57	53.74	111.96
C58	53.37	112.33
C59	65.32	100.38
C60	61.60	104.10
P	282.43	-1.41

Table S12. Calculated shielding and chemical shift values (in ppm) for all ^{13}C and ^{31}P nuclei in the GO-Epoxy-OH-H_3PO_4 system.

Nucleus	σ_{iso}	δ_{calc}
C1	55.92	109.78
C2	51.88	113.82
C3	50.05	115.65
C4	49.79	115.91
C5	43.37	122.33
C6	40.41	125.29
C7	45.56	120.14
C8	43.48	122.22
C9	54.77	110.93
C10	50.82	114.88
C11	33.50	132.20
C12	77.19	88.51
C13	32.35	133.35
C14	54.89	110.81
C15	56.23	109.47
C16	54.70	111.00
C17	48.07	117.63
C18	38.88	126.82
C19	87.38	78.32
C20	46.83	118.87
C21	49.34	116.36
C22	54.73	110.97
C23	51.39	114.31
C24	53.34	112.36
C25	50.66	115.04
C26	45.11	120.59
C27	53.71	111.99
C28	55.24	110.46
C29	58.71	106.99

C30	63.58	102.12
C31	53.62	112.08
C32	48.20	117.50
C33	52.89	112.81
C34	49.63	116.07
C35	34.62	131.08
C36	42.78	122.92
C37	39.08	126.62
C38	51.50	114.20
C39	59.62	106.08
C40	36.17	129.53
C41	66.37	99.33
C42	40.13	125.57
C43	47.34	118.36
C44	50.74	114.96
C45	56.96	108.74
C46	53.39	112.31
C47	52.19	113.51
C48	32.39	133.31
C49	43.30	122.40
C50	45.74	119.96
C51	45.45	120.25
C52	48.95	116.75
C53	51.96	113.74
C54	56.71	108.99
C55	49.09	116.61
C56	43.62	122.08
C57	50.24	115.46
C58	62.83	102.87
C59	55.76	109.94
C60	54.07	111.63
P	278.08	2.94

Table S13. Cartesian coordinates (in Å) of the atoms in all studied systems.

G-H_3PO_4

C	1.028744287	0.826608081	4.466196178
C	3.489048182	0.826916789	4.444926162
C	2.258792000	2.956270082	4.445651634
C	1.028386804	5.086611191	4.445234994
C	5.949131315	0.827328484	4.427883766
C	4.719526873	2.956039945	4.413495631
C	3.489213345	5.085057334	4.409801375
C	2.257208025	7.217920633	4.431453366
C	1.028500563	9.346869395	4.455434787
C	8.408894245	0.827589536	4.441154836
C	7.179110081	2.958108548	4.407212243
C	5.950312489	5.085489422	4.371259193
C	4.720721768	7.217695122	4.380961374
C	3.489009963	9.347095001	4.423516201
C	2.258965530	11.476774300	4.455726577
C	10.868668330	0.827242682	4.463521047
C	9.638382327	2.957404175	4.437178032
C	8.408315800	5.086250682	4.398402617
C	7.180272321	7.214852666	4.381617094
C	5.947815495	9.347816144	4.401800608
C	4.718855177	11.477161535	4.431167628
C	12.098607693	2.956915755	4.457914115
C	10.867823549	5.086783304	4.439602600
C	9.638071727	7.215603629	4.423934666

C	8.410203746	9.347201759	4.428616313
C	7.178968184	11.477371556	4.432402615
C	12.097942474	7.216750313	4.448975940
C	10.868783158	9.346611774	4.454897962
C	9.638990462	11.477216659	4.455935456
C	12.098788079	11.476809720	4.469460183
C	1.028585449	2.246384765	4.460151113
C	3.489343849	2.246481929	4.436341763
C	2.257982047	4.375519122	4.436253261
C	1.028116549	6.506846389	4.443857035
C	5.949524547	2.246944320	4.414596076
C	4.720852341	4.375531270	4.392740802
C	3.488448485	6.506931740	4.406152108
C	2.258576616	8.637012671	4.437283365
C	1.028808947	10.766614872	4.462990466
C	8.408653463	2.247331988	4.428947945
C	7.179738152	4.376481530	4.386062239
C	4.718675260	8.637879763	4.396540985
C	3.489071410	10.766647514	4.437586357
C	2.258953209	12.896497660	4.458533521
C	10.868301256	2.246914884	4.455937513
C	9.637678284	4.377047010	4.425172689
C	8.409413807	6.504744732	4.397470761
C	7.179133902	8.635789868	4.402371035
C	5.948772226	10.767240436	4.421147243
C	4.719159405	12.896975565	4.435205669
C	12.098057056	4.376623011	4.450652550
C	10.868243314	6.506113841	4.439091040

C	9.639172169	8.635755459	4.436439846
C	8.409160964	10.766958022	4.440390070
C	7.179062980	12.896912756	4.434352617
C	12.098729908	8.636375646	4.455451519
C	10.868709365	10.766346105	4.463028444
C	9.638696428	12.897074644	4.455898934
C	12.098633312	12.896572761	4.470180839
C	5.949889870	6.505023748	4.366182214
P	5.974742751	6.467755837	7.906319438
O	5.957020392	6.495478023	9.515418274
H	5.140691459	6.923950942	9.874532158
O	4.456315939	5.989619003	7.610271112
H	4.215239662	6.080297952	6.649962234
O	5.972812407	8.029775603	7.445869424
H	6.706270289	8.183551146	6.795245570
O	7.086678542	5.668641260	7.349176582

GO-Epoxy-H_3PO_4

C	0.83377	0.57611	14.34851
C	3.29242	0.57937	14.46926
C	2.05908	2.70362	14.49213
C	0.83015	4.83348	14.53344
C	5.75046	0.57249	14.61061
C	4.50975	2.70434	14.76117
C	3.28058	4.82771	14.73403
C	2.07045	6.95753	14.62714
C	0.84208	9.08912	14.48496
C	8.21223	0.56698	14.52504
C	6.98984	2.66009	14.84500
C	5.69284	4.82041	15.27380
C	4.53465	6.95867	14.91270
C	3.30032	9.09810	14.60661
C	2.06345	11.22452	14.40549
C	10.66892	0.57219	14.38185
C	9.44599	2.70110	14.59736
C	8.25063	4.83621	14.98319
C	6.98694	6.95117	15.37359
C	5.72650	9.12448	14.87051
C	4.52106	11.22994	14.54278
C	11.89899	2.70831	14.42819
C	10.67096	4.83349	14.62688
C	9.44752	6.95667	14.86949
C	8.24129	9.12067	14.83800
C	6.98286	11.22442	14.63260

C	11.90287	6.96528	14.59519
C	10.67229	9.08981	14.57737
C	9.44796	11.21943	14.47724
C	11.90399	11.22193	14.37330
C	0.82947	1.99644	14.39432
C	3.28777	1.99416	14.55248
C	2.05417	4.12293	14.56433
C	0.83314	6.25521	14.57378
C	5.75833	1.98333	14.76176
C	4.47898	4.09799	14.89985
C	3.28661	6.24924	14.75948
C	2.06627	8.38722	14.56735
C	0.83545	10.51494	14.40389
C	8.20691	1.98338	14.63431
C	7.01996	4.07248	15.22862
C	5.70689	6.26850	15.14722
C	4.52818	8.40674	14.80501
C	3.29398	10.51583	14.50566
C	2.06129	12.64790	14.38171
C	10.66269	1.99868	14.44610
C	9.44948	4.12348	14.71338
C	8.24651	6.22536	15.07843
C	6.98968	8.45167	15.20630
C	5.74597	10.52058	14.67354
C	4.52158	12.64845	14.52628
C	11.89829	4.12393	14.50380
C	10.66814	6.25653	14.69515
C	9.44416	8.39412	14.77896

C	8.21789	10.50942	14.63110
C	6.98213	12.63487	14.57913
C	11.90212	8.38147	14.54730
C	10.67040	10.50979	14.46011
C	9.44090	12.64112	14.43422
C	11.89664	12.64233	14.33853
O	7.02653	7.83228	16.58588
P	6.20640	6.26209	18.78360
O	7.22957	7.21406	19.10046
H	7.05471	8.34134	19.42444
O	6.75949	6.56145	17.52231
H	7.68181	6.26236	17.49447
O	5.45491	5.66215	17.88010
H	4.66916	4.76763	18.16223
O	5.69855	6.01596	20.12093

GO-Epoxy-Epoxy-H_3PO_4

C	0.5184953131	0.6169175664	14.3973477469
C	2.9759438346	0.6199435590	14.5281629474
C	1.7423985157	2.7438420386	14.5551875975
C	0.5130549781	4.8730408144	14.5677867326
C	5.4346519274	0.6128327684	14.6447872869
C	4.1946209497	2.7451547503	14.8122424340
C	2.9636184604	4.8680255498	14.7925329964
C	1.7520191017	6.9973281987	14.6603006340
C	0.5257871911	9.1284107033	14.5006966736
C	7.8967744279	0.6078804220	14.5344410717
C	6.6765053364	2.7000888606	14.8539972319
C	5.3901449591	4.8633809501	15.2827769158
C	4.2178251045	6.9970682393	14.9300260443
C	2.9829140765	9.1372345752	14.6317046443
C	1.7470272710	11.2652434971	14.4473304489
C	10.3540923250	0.6134706289	14.3987941597
C	9.1305330629	2.7432634700	14.5889093140
C	7.9345523301	4.8775349629	14.9440860845
C	6.6764803730	6.9961490035	15.3224596951
C	5.4111451642	9.1640155775	14.8645432780
C	4.2040227051	11.2706101550	14.5762698531
C	11.5838187961	2.7489046879	14.4541668868
C	10.3529559486	4.8736602010	14.5970905319
C	9.1304077064	6.9953929084	14.8023512021
C	7.9262130222	9.1592536720	14.7959471470
C	6.6674389073	11.2656046007	14.6387750123

C	11.5854629735	7.0042996832	14.5824848992
C	10.3565846523	9.1293327220	14.5483296758
C	9.1327389389	11.2612035996	14.4714287997
C	11.5890100277	11.2629392025	14.3896161337
C	0.5137811807	2.0370853524	14.4449860412
C	2.9712519470	2.0346202577	14.6158883728
C	1.7368478356	4.1628731858	14.6235836615
C	0.5157198915	6.2953902177	14.5959259056
C	5.4441389403	2.0236108980	14.7940690106
C	4.1647014213	4.1399374725	14.9498868207
C	2.9681032690	6.2898596826	14.8009802057
C	1.7487858587	8.4266036818	14.5931326375
C	0.5196271134	10.5553009759	14.4294051991
C	7.8919754189	2.0243969089	14.6378796109
C	6.7082362818	4.1176428357	15.2174633735
C	5.3953790693	6.3076552957	15.1447978143
C	4.2122204211	8.4459162742	14.8145951912
C	2.9775174595	10.5559236717	14.5405246216
C	1.7453845336	12.6884920752	14.4361128668
C	10.3478653095	2.0395788957	14.4577025485
C	9.1328712796	4.1648697019	14.6794721736
C	7.9300832685	6.2665944774	15.0187899544
C	6.6788637254	8.4854429518	15.1645546424
C	5.4309242653	10.5614808171	14.6854139107
C	4.2049984362	12.6893344708	14.5717942832
C	11.5816016652	4.1643826414	14.5139258500
C	10.3502576836	6.2953739433	14.6510946970
C	9.1272706903	8.4319913966	14.7233355410

C	7.9019016080	10.5513318002	14.6178033576
C	6.6667704864	12.6762941738	14.5967913160
C	11.5854809443	8.4202819178	14.5369318302
C	10.3545657881	10.5503655560	14.4521029779
C	9.1256639686	12.6826470492	14.4404917498
C	11.5817205929	12.6831782781	14.3674470072
O	6.7234528161	7.8769435398	16.5762024566
O	6.0774898833	4.3761795346	16.5768969077
P	9.0244972423	5.9867970528	18.4046517128
O	9.5860341346	6.1513567595	19.9138782309
H	10.0983253555	5.3381256749	20.1457934291
O	9.0525093300	7.5174573287	17.9251242285
H	8.1997117554	7.7493340752	17.4259424295
O	7.4699918778	5.6259600177	18.6230283488
H	7.0437836097	5.1953699670	17.8165517347
O	9.7932352580	5.0174416230	17.5729232635

GO-OH-H_3PO_4

C 0.84151 0.62801 14.40090

C 3.29955 0.62838 14.46376

C 2.07004 2.74799 14.41870

C 0.84077 4.86367 14.59463

C 5.76147 0.62819 14.45781

C 4.52982 2.75609 14.44975

C 3.29403 4.86463 14.65330

C 2.06665 6.96363 14.92271

C 0.83841 9.10100 14.82703

C 8.21957 0.62705 14.38925

C 6.99057 2.74716 14.40770

C 5.76374 4.86174 14.66558

C 4.52368 6.92540 15.22443

C 3.26904 9.12681 15.01530

C 2.06479 11.21542 14.64482

C 10.68082 0.62576 14.36359

C 9.45083 2.74988 14.36293

C 8.21874 4.86416 14.58113

C 6.99236 6.96419 14.92365

C 5.78827 9.12537 15.01922

C 4.53022 11.21934 14.72376

C 11.90981 2.74970 14.37171

C 10.67993 4.86103 14.54820

C 9.45180 6.97732 14.75620

C 8.22035 9.09994 14.81453

C 6.99542 11.21359 14.63382

C 11.90742 6.97665 14.76712

C 10.67991 9.09507 14.74290

C 9.45307 11.21282 14.56175

C 11.90777 11.21351 14.56892

C 0.84184 2.04335 14.37018

C 3.29994 2.04380 14.42036

C 2.06629 4.16258 14.53142

C 0.83946 6.27099 14.76453

C 5.76039 2.04362 14.41515

C 4.52820 4.15938 14.58002

C 3.27102 6.24818 14.90589

C 2.06644 8.40653 14.96912

C 0.83936 10.51186 14.68819

C 8.21886 2.04282 14.35710

C 6.99361 4.16152 14.52681

C 5.78495 6.24652 14.92620

C 4.52653 8.43584 15.29431

C 3.29262 10.51599 14.79833

C 2.06919 12.62567 14.48790

C 10.68068 2.04424 14.33499

C 9.45196 4.16152 14.47538

C 8.21920 6.27259 14.75197

C 6.99183 8.40638 14.96506

C 5.76708 10.51380 14.79528

C 4.53050 12.61820 14.53967

C 11.90821 4.16118 14.48595

C 10.67940 6.27678 14.68934

C 9.45146 8.39288 14.78563

C	8.22086	10.51053	14.67572
C	6.99185	12.62441	14.47679
C	11.90755	8.39319	14.79526
C	10.68059	10.51329	14.63084
C	9.45167	12.62175	14.41960
C	11.90961	12.62216	14.42622
O	4.80006	3.20335	18.20509
O	3.36257	5.16090	18.33527
O	5.89951	5.50591	18.64455
O	4.63118	4.35527	20.54793
P	4.66696	4.56610	19.08546
H	5.04698	2.47940	18.82851
H	3.32011	6.15237	18.36278
H	5.84053	5.78353	17.69288
O	5.78549	6.85168	16.59237
H	6.34313	7.77233	16.97433

GO-OH-OH-H_3PO_4

C	1.10421	0.28689	14.58087
C	3.56220	0.28546	14.64171
C	2.32208	2.41604	14.75299
C	1.09998	4.55257	14.67183
C	6.01575	0.29590	14.68325
C	4.78086	2.38696	14.92601
C	3.52983	4.56011	14.93454
C	2.32661	6.67606	14.69119
C	1.10300	8.80393	14.58452
C	8.47189	0.30731	14.64903
C	7.24971	2.44123	14.86956
C	6.03383	4.57282	15.08073
C	4.78336	6.68127	14.93694
C	3.56416	8.80124	14.67520
C	2.32774	10.93290	14.56453
C	10.93525	0.29698	14.57900
C	9.70988	2.42993	14.68402
C	8.48879	4.56573	14.88152
C	7.27046	6.70612	15.31395
C	6.03383	8.81101	14.79167
C	4.79182	10.93235	14.62105
C	12.16790	2.42881	14.62140
C	10.93825	4.55588	14.67325
C	9.71205	6.68050	14.79981
C	8.47694	8.82490	14.77560
C	7.25064	10.94772	14.64113

C	12.16797	6.68538	14.63308
C	10.93189	8.81049	14.64576
C	9.71237	10.94985	14.59681
C	12.16762	10.94479	14.55075
C	1.10971	1.71837	14.64024
C	3.56571	1.70150	14.77157
C	2.32764	3.85014	14.78414
C	1.10141	5.97336	14.65207
C	6.00379	1.71261	14.82850
C	4.76255	3.82345	15.35795
C	3.55049	5.96173	14.84595
C	2.33096	8.09777	14.63753
C	1.10571	10.23087	14.55739
C	8.47540	1.72500	14.72855
C	7.25624	3.84828	14.97808
C	6.00690	5.95747	15.06243
C	4.78924	8.08384	14.81668
C	3.56853	10.21752	14.61013
C	2.32926	12.35742	14.57919
C	10.93799	1.72476	14.61225
C	9.71290	3.85228	14.73056
C	8.50784	5.97038	14.95183
C	7.25775	8.13796	14.90813
C	6.02398	10.22822	14.66287
C	4.79013	12.35666	14.63623
C	12.17148	3.84389	14.63842
C	10.93952	5.97734	14.68571
C	9.71888	8.11272	14.76364

C	8.47952	10.24098	14.65257
C	7.24848	12.37252	14.64426
C	12.17270	8.10022	14.61295
C	10.93753	10.24117	14.58772
C	9.71278	12.37391	14.59231
C	12.17364	12.36300	14.55393
O	4.70363	3.69022	16.87460
H	4.61258	4.62075	17.23102
O	7.33429	6.84626	16.92887
H	7.14316	5.92830	17.26202
P	4.34588	7.67861	18.72894
O	5.45701	8.38063	17.86893
H	6.22093	7.75636	17.51132
O	4.67605	6.06573	18.51549
H	4.55771	5.62380	19.39385
O	3.01320	7.94341	17.83153
H	2.23793	8.01390	18.44250
O	4.17341	8.01635	20.16228

GO-Epoxy-OH-H_3PO_4

C	1.0981476925	0.5761819606	14.5879398421
C	3.5580861253	0.5799262209	14.6844160393
C	2.3256052649	2.7042703756	14.6756944000
C	1.0965252155	4.8346554503	14.6474253652
C	6.0174539232	0.5804839080	14.8075302100
C	4.7757225989	2.7129858277	14.9304211184
C	3.5489981691	4.8326701794	14.8112963237
C	2.3374006344	6.9566841194	14.6747524742
C	1.1058592306	9.0892579427	14.6201830766
C	8.4736932958	0.5764305751	14.7448665038
C	7.2529572439	2.6715253999	15.0403447630
C	5.9625091361	4.8477141742	15.3526546090
C	4.7994220992	6.9616232531	14.9040130416
C	3.5690363815	9.0943491062	14.6982656175
C	2.3311837749	11.2256467822	14.6039199192
C	10.9340006636	0.5741049324	14.6311259664
C	9.7100467076	2.7089095019	14.8057171198
C	8.5050755677	4.8536955133	15.0957640078
C	7.2488361593	6.9993797185	15.4882282111
C	6.0237748987	9.1056446668	14.8841166362
C	4.7914156680	11.2313067288	14.6993399851
C	12.1630636885	2.7077396239	14.6340544609
C	10.9360010316	4.8347462394	14.7552886328
C	9.7102857608	6.9623595730	14.9124063312
C	8.4684372720	9.1019000855	14.8945696350
C	7.2485295539	11.2284206010	14.7584241769

C	12.1676979839	6.9636860078	14.6844017126
C	10.9337249964	9.0866457227	14.7230183046
C	9.7065608865	11.2249985777	14.6794107124
C	12.1639240293	11.2240259043	14.5963390041
C	1.0952078966	1.9940538827	14.6117386023
C	3.5536339821	1.9966082301	14.7477606469
C	2.3224562541	4.1243517968	14.6895465721
C	1.1005218305	6.2524257157	14.6539883932
C	6.0223290956	1.9921291745	14.9553944993
C	4.7465833570	4.1125963330	15.0137350135
C	3.5553850737	6.2511967309	14.7770393656
C	2.3305922521	8.3835684066	14.6526547282
C	1.1003625025	10.5142336572	14.5951514459
C	8.4713743379	1.9929965833	14.8528113353
C	7.2729667777	4.0987378480	15.3670846225
C	5.9800195161	6.2845548564	15.1678407653
C	4.7881981304	8.3955505648	14.8314007272
C	3.5616050627	10.5183732224	14.6574788295
C	2.3274213323	12.6479634896	14.6080810128
C	10.9295773272	2.0013714553	14.6758131293
C	9.7129139636	4.1295142213	14.8699586092
C	8.4980701299	6.2432027784	15.1173278410
C	7.2487900642	8.4231334325	15.0405120522
C	6.0196272344	10.5218760497	14.7672719429
C	4.7886047267	12.6499062199	14.7221889901
C	12.1642252020	4.1243792410	14.6582628411
C	10.9347410650	6.2571656970	14.7744026992
C	9.7118154460	8.3841812901	14.8656331660

C	8.4727471138	10.5172645202	14.7579290049
C	7.2472164475	12.6508852903	14.7650997125
C	12.1662100451	8.3797585439	14.6680922614
C	10.9341247354	10.5151517967	14.6580426785
C	9.7050447845	12.6444239858	14.6676326319
C	12.1604903328	12.6439584508	14.5853238241
O	7.3127742604	7.1165579814	17.0584679808
H	7.2511397784	6.1553056350	17.3442294021
O	6.6141468970	4.4121406686	16.7126403480
P	4.2355337011	6.6808606910	18.6189759069
O	5.3857233113	5.6112218889	19.0668461429
H	5.4144288865	4.8618042029	18.4153999439
O	3.2037678590	6.0845708371	17.7247239677
O	5.0299099420	7.9578863577	18.1087558244
H	5.9376876894	7.6965960486	17.6858024756
O	3.6646440553	7.2457581780	20.0237971841
H	2.8410119464	6.7500153728	20.2561346778

GO-P-O-C

C	0.74553	0.36553	14.73214
C	3.20387	0.35575	14.87683
C	1.97238	2.48567	14.65993
C	0.73908	4.62645	14.52975
C	5.66879	0.35634	14.82550
C	4.42911	2.46488	14.65784
C	3.20454	4.60840	14.63198
C	1.98018	6.75376	14.68808
C	0.75133	8.88483	14.72147
C	8.12571	0.36837	14.70699
C	6.88243	2.48027	14.43742
C	5.57477	4.43529	13.86403
H	5.44349	5.33419	13.27454
C	4.29264	6.75965	15.39261
C	3.20825	8.87350	14.94741
C	1.98089	11.00876	14.85504
C	10.58510	0.37616	14.64704
C	9.34186	2.49778	14.40412
C	8.09269	4.62925	14.09967
C	6.95975	6.85522	14.38154
H	6.00847	6.40045	14.23554
C	5.68172	8.86560	15.05429
C	4.44228	11.00712	15.01525
C	11.81131	2.49641	14.51524
C	10.57470	4.63176	14.33246
C	9.36145	6.76682	14.39214

C 8.15287 8.90286 14.75480

C 6.90579 11.01019 14.92017

C 11.82434 6.76108 14.47435

C 10.59652 8.89094 14.63110

C 9.36716 11.02626 14.78245

C 11.82183 11.02003 14.74230

C 0.74092 1.78454 14.63613

C 3.19802 1.77167 14.78230

C 1.97334 3.91237 14.60589

C 0.75403 6.04848 14.51916

C 5.66345 1.76384 14.63481

C 4.41542 3.85890 14.39749

C 3.19692 6.02598 14.87884

C 1.98055 8.17140 14.79510

C 0.75085 10.30503 14.77610

C 8.11930 1.78375 14.52651

C 6.85274 3.86787 14.08285

C 4.43253 8.15351 15.16447

C 3.21223 10.29666 14.94378

C 1.97493 12.43054 14.83840

C 10.57718 1.79265 14.51495

C 9.32524 3.92628 14.25111

C 8.11790 6.07986 14.23476

C 6.92452 8.19089 14.76381

C 5.67588 10.28239 15.02592

C 4.44088 12.42464 14.93713

C 11.80612 3.92233 14.45023

C 10.59063 6.05457 14.36922

C	9.36444	8.18265	14.58112
C	8.14485	10.31544	14.85295
C	6.89946	12.42712	14.83075
C	11.82523	8.18034	14.59147
C	10.59353	10.30961	14.72605
C	9.35847	12.44571	14.72187
C	11.81563	12.44181	14.71537
O	6.43785	5.26181	18.18979
O	3.99274	5.90479	18.35114
O	5.23907	6.02675	16.17916
O	5.78870	7.80388	18.08200
P	5.40152	6.41540	17.74564
H	7.34446	5.65014	18.27113
H	3.75304	6.46134	19.13366

GO-P-C

C	0.81754	0.38953	14.52334
C	3.27474	0.38358	14.69383
C	2.04590	2.51805	14.51158
C	0.81281	4.65309	14.42767
C	5.73423	0.38167	14.69965
C	4.50105	2.50718	14.56563
C	3.27074	4.65544	14.62282
C	2.04519	6.77987	14.63921
C	0.82001	8.91119	14.58110
C	8.19087	0.38437	14.57290
C	6.95443	2.51047	14.41185
C	5.68183	4.54613	14.00363
H	5.61499	5.54094	13.57489
C	4.32282	6.78501	15.54122
C	3.27321	8.90226	14.89080
C	2.05104	11.03510	14.67365
C	10.65281	0.39209	14.46146
C	9.41423	2.51659	14.33064
C	8.17589	4.65507	14.26246
C	7.07630	6.79896	14.88898
H	6.19348	6.23423	15.12397
C	5.73441	8.88752	15.16279
C	4.50772	11.03197	14.89896
C	11.88373	2.51952	14.37324
C	10.65082	4.65518	14.29374
C	9.44005	6.78765	14.42734

C 8.20560 8.91314 14.74128

C 6.96531 11.02855 14.82995

C 11.89680 6.78614 14.36883

C 10.65963 8.91505 14.50458

C 9.42661 11.04208 14.61051

C 11.88998 11.04333 14.53680

C 0.81526 1.81036 14.45856

C 3.27093 1.80243 14.62687

C 2.04545 3.94556 14.50941

C 0.82579 6.07415 14.42508

C 5.73065 1.79594 14.54724

C 4.49620 3.92173 14.40756

C 3.24624 6.06065 14.91395

C 2.04353 8.20014 14.71507

C 0.81966 10.33191 14.59336

C 8.18835 1.80444 14.44731

C 6.93400 3.92125 14.18744

C 4.46913 8.18816 15.23275

C 3.27836 10.32385 14.81823

C 2.04621 12.45637 14.63498

C 10.64890 1.81025 14.37210

C 9.40545 3.94707 14.26701

C 8.20756 6.08178 14.49072

C 6.99507 8.18727 14.97686

C 5.73658 10.30232 14.98692

C 4.50730 12.44898 14.78433

C 11.88143 3.94522 14.34960

C 10.66420 6.07734 14.31769

C	9.42709	8.20440	14.54964
C	8.20243	10.33066	14.74106
C	6.96228	12.44584	14.70868
C	11.89125	8.20526	14.46235
C	10.65783	10.33329	14.54798
C	9.42292	12.46100	14.54780
C	11.88610	12.46311	14.50362
O	5.51530	4.77539	16.99880
O	3.55324	5.95872	18.00235
O	5.80902	7.26830	17.84169
P	4.93032	6.27898	17.16559
H	5.84466	4.44150	17.87146
H	3.32350	6.75586	18.54294

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