Electronic supplementary materials *Mendeleev Commun.*, 2023, **33**, 160–163

Features of doxorubicin adsorption on Fe_3O_4 magnetic nanoparticles coated with SiO_2 or SiO_2/aminopropylsilane

Alexander M. Demin, Alexander V. Vakhrushev, Marina S. Valova, Marina A. Korolyova, Mikhail A. Uimin, Artem S. Minin, Konstantin A. Chistyakov, Victor P. Krasnov and Valery N. Charushin

Experimental procedures

All reagents are commercially available.

Synthesis of starting nanoparticles (MNPs and MNPs–PMIDA).

A saturated solution of NH_4OH (10 mL) was added to 100 mL of an aqueous solution of $FeCl_3 \times 6H_2O$ (2.335 g, 8.64 mmol) and $FeSO_4 \times 7H_2O$ (1.200 g, 4.32 mmol) under sonification at 40 °C (as described in ref.[S1,S2]). After 10 min, nanoparticles were deposited with a magnet, washed with water (3×50 mL), and suspended in water (100 mL) to afford a suspension of MNPs. Then MNPs were modified with PMIDA (as described in ref.[S3,S4]): a solution of PMIDA (0.265 g, 1.17 mmol) in water (30 mL) was added to 100 ml of a suspension of MNPs (1.08 g, 4.66 mmol) at 40 °C under sonification and stirring. The reaction mixture was stirred for 20 h to afford **MNPs–PMIDA** solution (10.88 mg/mL).

Synthesis of nanocomposites with SiO_2 (MNPs–SiO_2-1 and MNPs–SiO_2-2) and SiO_2/APS shell (MNPs–SiO_2–APS-1 and MNPs–SiO_2–APS-2).

EtOH (80 mL) was added to a suspension of MNPs or **MNPs–PMIDA** (0.435 g) in water (40 mL); the reaction mixture was heated to 40 °C, then a solution of TEOS (0.55 μL, 2.82 mmol) in EtOH (20 mL) was added under ultrasound stirring, and a saturated solution of NH_4OH (6 ml) was added dropwise for 10 min. Stirring was continued for 20 h. The resulting **MNPs–SiO_2-1** and **MNPs–SiO_2-2** were functionalized with APTMS. A solution of APTMS (3 mol per 1 g of the starting nanoparticles) in EtOH (20 mL) was added to an aqueous suspension of **MNPs–SiO_2** (80 mL) under ultrasonic stirring at 40 °C. Stirring was continued for 20 h. Modified MNPs were precipitated with a magnet, washed with EtOH (50 mL), water (2×50 mL), and dispersed in water (40 mL) to afford suspensions **MNPs–SiO_2–APS-1** and **MNPs–SiO_2–APS-2**.

Doxorubicin sorption.

A solution of Dox (11.5 mg) in water (1 mL) was added to 9 mL of an aqueous suspension of corresponding nanocomposite (10 mg); the reaction mixture was stirred at room temperature for 24 h. MNPs were precipitated by centrifugation, the precipitate was washed with water (2×5 mL), and then dispersed in water (2 mL). The amount of Dox in supernatant was determined by UV spectrometry as described in ref.[S5].

The Dox loading efficiency (LE, wt.%) and loading content (LC, wt.%) were calculated by formulas (1) and (2), respectively:

$$LE = (m_{\text{Dox load}} - m_{\text{Dox}}) \times 100\% / m_{\text{Dox load}} \quad (1),$$

$$LC = (m_{\text{Dox load}} - m_{\text{Dox}}) \times 100\% / m_{\text{nanocomposite}} \quad (2),$$

where $m_{\text{Dox load}}$ is the mass (mg) of Dox loaded in the reaction, m_{Dox} is the amount (mg) of Dox in supernatant, $m_{\text{nanocomposite}}$ is the mass (mg) of Dox-containing nanocomposite.

Doxorubicin release. To prepare a phosphate buffer solution (pH = 5.8), $Na_2HPO_4 \times 2H_2O$ (1.19 g) and KH_2PO_4 (8.25 g) were dissolved in water (1000 mL). To prepare a phosphate buffer solution (pH = 7.4), $Na_2HPO_4 \times 2H_2O$ (2.38 g) and KH_2PO_4 (0.19 g) were dissolved in water (1000 mL). Aliquots (500 μL) were taken from an aqueous suspension of the corresponding nanocomposite and precipitated by centrifugation (10 min, 10000 rpm); 3 mL of a phosphate buffer solution (pH = 5.8 or 7.4) was added to the precipitate; the reaction mixture was sonicated. The resulting solutions were stirred at 37 °C for 24 h. To determine the amount of Dox desorbed, the samples were centrifuged (10 min, 10000 rpm) and analyzed by UV spectrometry.

Characterization of nanocomposite materials

TEM images of MNPs were obtained on a Tecnai G2 30 Twin transmission electron microscope (TEM) (Thermo Fisher Scientific). The EDX spectra and fractions of Fe, Si, and P were determined on an EDX-7000 X-ray fluorescence spectrometer (Shimadzu, Japan). Mass fractions of C, H and N were determined using a CHN EuroEA 3000 automatic analyzer (EuroVector Instruments, USA). The IR spectra were recorded on a Perkin Elmer Spectrum Two FTIR-spectrometer (Perkin Elmer, USA) by the attenuated total reflection (ATR) on the diamond crystal and the diffuse reflectance infrared Fourier transform spectroscopy (DRIFT) accessories. The amount of Dox in aqueous solutions was measured using a UV 2600 spectrometer (Shimadzu, Japan). DLS characterization of aqueous solutions was carried out on a Malvern Zetasizer Nano ZS instrument (Malvern Instruments). The magnetic properties were studied on a magnetic vibromagnetometer with fields up to 25 kOe.

Computational details

Optimization of the geometry of Dox base complexes with a small cluster SiO_2[S6] and its functional derivatives, APS and PMIDA conjugates, as well as calculation of their total electronic energies were performed using the ORCA 4.0.1 program.[S7] We used the Becke's hybrid three-parameter nonlocal exchange functional combined with the Lee–Yang–Parr correlation functional B3LYP[S8] and the def2-SVP Alrichs' basis set[S9] for all atoms. Dispersion effects were corrected using the semiempirical pairwise correction scheme by Grimme (D3).[S10] At each optimization step, the total electron energies *E* were calculated using both D3 and the geometrical counterpoise (gCP) correction of basis set superposition error.[S11] Before the DFT calculation, we simulated all the complexes using the VEGA ZZ program,[S12] by orienting the Dox molecule (the xyz structure was taken from the PubMed open databank) at different positions relative to the SiO_2 cluster and its APS or PMIDA conjugates at a distance of 1.8–2 Å. The energy (E_b) of doxorubicin binding to clusters in the gaseous phase was determined as described, for example, in ref.[S13], using the formula:

$E_b = E_c - (E_{Dox} + E_{cl})$, where E_c, E_{Dox} and E_{cl} are the total electronic energies of the complexes, the starting doxorubicin, and the cluster, respectively.

Energy parameters

Table S1 Total energies (*E*) of the best optimized complexes of Dox and corresponding sums of energies of Dox–SiO_2 conjugates

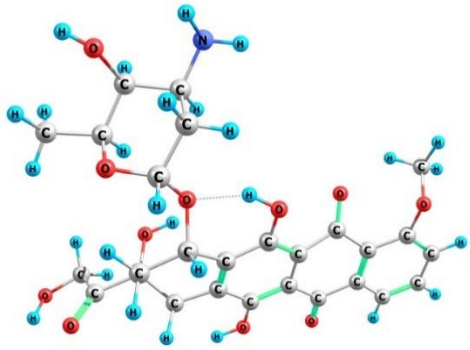
Structure	Energy Type	Energy/Hartrees
Dox+SiO_2-cluster		-7011.145172381
Dox+1APS-SiO_2-cluster	$E_{Dox} + E_{cl}$	-7108.998694492
Dox+2APS-SiO_2-cluster		-7206.858523516
Dox+PMIDA-SiO_2-cluster		-7976.637961575
Dox-SiO_2-complex	E_c	-7011.207488811
Dox-1APS-SiO_2-complex		-7109.003616256
Dox-2APS-SiO_2-complex		-7206.872846610
Dox-PMIDA-SiO_2-complex		-7976.678403700
Dox-PMIDA (free OH)-SiO_2 salt (**1**)		-8053.058920439
Dox-PMIDA (free OH)-SiO_2 salt (**2**)		-8053.0925333042

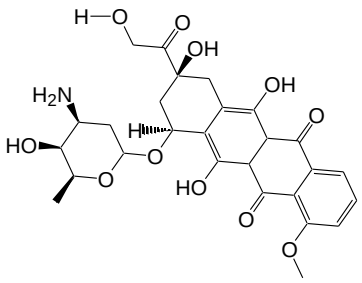
Table S2 Binding energies E_b for the best optimized complexes of Dox

Structure	E_b, kJ/mol
Dox-SiO_2-complex	-163.61
Dox-1APS-SiO_2-complex	-12.92
Dox-2APS-SiO_2-complex	-37.60
Dox-PMIDA-SiO_2-complex	-106.18
Dox-PMIDA (free OH)-SiO_2 salt (**1**)	-229.95
Dox-PMIDA (free OH)-SiO_2 salt (**2**)	-318.20

Cartesian coordinates of Dox, conjugates of SiO_2-cluster with APS and PMIDA, and their best complexes with Dox at B3LYP-D3-gCP/def2-SVP level of theory (*E* is total electronic energy in Hartrees)

Dox

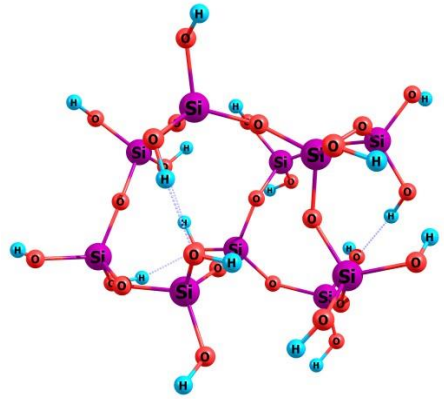




E = -1925.918434992

O	2.089384000	0.642445000	-0.745919000	C	-5.543047000	0.569943000	0.090503000
O	4.341994000	1.191721000	-1.188280000	C	-5.873492000	-2.109997000	0.875552000
O	2.929056000	-1.453652000	1.590500000	C	-6.827033000	0.037603000	0.296241000
O	5.165420000	4.052444000	-0.808629000	C	-6.991858000	-1.292859000	0.693892000
O	-0.516405000	0.941007000	-1.031041000	C	-5.531673000	2.918106000	0.547377000
O	-1.049674000	-4.127055000	1.101611000	H	1.551869000	-0.742008000	-2.191466000
O	4.556507000	-3.969256000	-0.220654000	H	2.927481000	-2.486446000	-1.641170000
O	5.729303000	-4.410450000	2.142899000	H	3.907487000	-1.154485000	-0.999667000
O	-2.791630000	1.502928000	0.225371000	H	1.492564000	-3.690419000	1.541615000
O	-3.623329000	-3.659834000	1.303217000	H	1.696415000	-4.068512000	-0.187152000
O	-5.437065000	1.842594000	-0.394707000	H	2.957668000	0.905733000	-2.620819000
N	2.559638000	4.970177000	-0.272298000	H	1.546836000	2.935744000	-1.945002000
C	1.781961000	-0.731709000	-1.103237000	H	3.209614000	3.316545000	-2.435892000
C	2.891403000	-2.380974000	0.508037000	H	2.260074000	3.047611000	0.484258000
C	2.958188000	-1.697914000	-0.869450000	H	4.498744000	3.679387000	1.138359000
C	1.594284000	-3.235046000	0.536496000	H	4.072705000	1.311020000	0.877026000
C	0.486993000	-1.140062000	-0.393866000	H	2.140163000	-0.884787000	1.569358000
C	0.368490000	-2.386122000	0.236607000	H	6.339069000	0.408693000	0.320688000
C	3.009833000	1.351576000	-1.607592000	H	6.780542000	1.958825000	-0.457264000
C	2.607442000	2.832316000	-1.644719000	H	6.474698000	1.895169000	1.310134000
C	2.876727000	3.538928000	-0.294243000	H	1.597990000	5.115494000	-0.597893000
C	4.349541000	3.309759000	0.101437000	H	3.156742000	5.449970000	-0.954260000
C	4.680596000	1.796422000	0.085738000	H	3.894965000	-3.670274000	2.813710000
C	-0.642032000	-0.274676000	-0.460982000	H	5.087382000	-2.432993000	2.386990000
C	4.101503000	-3.317704000	0.702856000	H	6.013294000	4.248482000	-0.379378000
C	-0.915475000	-2.865756000	0.626315000	H	0.438739000	1.180118000	-0.996075000
C	-1.891074000	-0.692713000	0.042942000	H	-0.196493000	-4.592547000	1.075541000
C	-2.054088000	-2.030813000	0.517595000	H	-5.985254000	-3.154251000	1.182752000
C	6.155700000	1.497913000	0.328725000	H	5.834760000	-4.750999000	1.232383000
C	4.712735000	-3.439343000	2.094849000	H	-7.695517000	0.682344000	0.115585000
C	-3.010792000	0.300210000	0.169302000	H	-7.999129000	-1.696740000	0.853310000
C	-3.416830000	-2.527141000	0.881738000	H	-6.497520000	2.897958000	1.091937000
C	-4.397985000	-0.244389000	0.299084000	H	-5.465388000	3.852971000	-0.034832000
C	-4.582157000	-1.596562000	0.672489000	H	-4.699298000	2.883681000	1.274122000

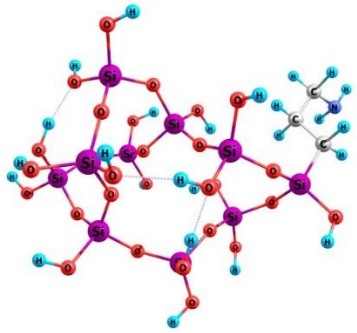
SiO_2-cluster ($Si_{10}H_{18}O_{29}$)

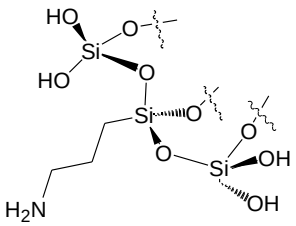


E = -5085.226737389

Si	-0.225174000	-0.998140000	4.053390000
O	-0.622950000	-1.896852000	5.387897000
Si	0.107323000	-3.203368000	6.099707000
O	1.734784000	-3.089450000	5.799617000
Si	3.007735000	-2.238302000	6.442924000
O	4.136505000	-1.965450000	5.264547000
Si	3.686953000	-6.217691000	6.014055000
Si	4.498989000	-1.935083000	3.653902000
Si	3.259560000	-4.684278000	3.170553000
O	4.343245000	-3.450305000	3.002137000
O	3.435988000	-5.304445000	4.675467000
O	3.722870000	-7.807832000	5.588161000
Si	3.368566000	-8.618195000	4.173604000
O	1.877684000	-8.088632000	3.692676000
Si	0.537262000	-7.675626000	2.842947000
O	1.723350000	-4.135640000	2.963526000
Si	0.678750000	-3.303350000	1.984019000
O	0.027625000	-2.022468000	2.779155000
O	-0.516607000	-4.564465000	5.438874000
Si	-0.835110000	-6.174857000	5.238595000
O	-0.387543000	-6.599676000	3.696283000
O	3.374001000	-10.204655000	4.617794000
H	3.336862000	-10.859458000	3.899913000
O	-0.350166000	-9.001935000	2.417503000
H	-0.781409000	-9.499120000	3.133564000
O	1.435500000	-2.659497000	0.661091000
H	1.858279000	-3.263238000	0.027899000
O	3.615491000	-5.822241000	2.008593000
H	2.817502000	-6.244854000	1.607045000
O	3.404809000	-0.872185000	2.974064000
H	3.371356000	-0.831572000	2.000798000
O	6.019966000	-1.378002000	3.371051000
H	6.756071000	-1.992022000	3.539614000
O	-0.207994000	-3.244961000	7.724370000
H	0.027966000	-2.457899000	8.244323000
O	3.688797000	-3.095708000	7.687716000
H	4.489544000	-3.615603000	7.481809000
O	1.126920000	-0.088869000	4.361896000
H	1.927299000	-0.261554000	3.808920000
O	-1.555479000	-0.052327000	3.811023000
H	-1.483087000	0.631060000	3.123933000
O	-0.493503000	-4.378355000	1.486340000
H	-0.950249000	-4.855057000	2.204909000
O	2.430445000	-0.834550000	7.100673000
H	1.927299000	-0.261554000	3.808920000
O	-1.555479000	-0.052327000	3.811023000
H	-1.483087000	0.631060000	3.123933000
O	-0.493503000	-4.378355000	1.486340000
H	-0.950249000	-4.855057000	2.204909000
O	2.430445000	-0.834550000	7.100673000
H	1.948787000	-0.273511000	6.459619000
O	-2.465359000	-6.454787000	5.276943000
H	-2.926936000	-6.177614000	6.086563000
O	-0.064795000	-7.102737000	6.357815000
H	0.799771000	-6.786830000	6.708097000
O	2.436582000	-6.061987000	7.114091000
H	2.453042000	-5.243910000	7.647086000
O	5.104234000	-5.654597000	6.669754000
H	5.486820000	-6.171558000	7.400691000
O	1.063681000	-6.946502000	1.434659000
H	0.459576000	-6.272981000	1.060733000
O	4.495350000	-8.360301000	2.993833000
H	4.438212000	-7.490704000	2.541103000

SiO_2-1APS

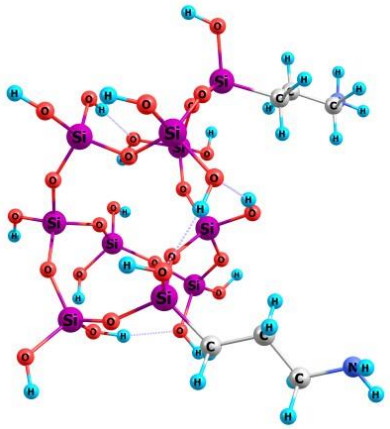


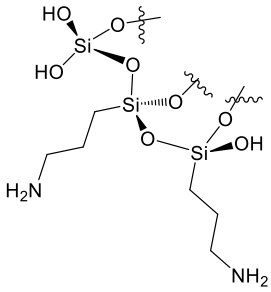


E = -5183.08025950

Si	-0.166235000	-1.300803000	3.995507000
O	-0.529356000	-2.367978000	5.184175000
Si	0.107580000	-3.422294000	6.281017000
O	1.742594000	-3.498287000	5.996344000
Si	3.037810000	-2.587168000	6.427535000
O	4.115415000	-2.414597000	5.192945000
Si	3.720657000	-6.618581000	5.499269000
Si	4.701017000	-2.285401000	3.664936000
Si	3.237639000	-4.803799000	2.890879000
O	4.482642000	-3.696626000	2.839108000
O	3.268031000	-5.531507000	4.355432000
O	3.218140000	-8.126799000	5.116907000
Si	2.799801000	-9.216058000	3.922894000
C	4.168396000	-9.292050000	2.659765000
H	3.921402000	-10.061457000	1.900903000
H	4.177659000	-8.322243000	2.122631000
C	5.555395000	-9.558113000	3.280590000
H	5.791532000	-8.781966000	4.031208000
H	5.542965000	-10.524128000	3.827248000
C	6.691579000	-9.574428000	2.250479000
H	6.459833000	-10.342071000	1.471845000
H	6.703761000	-8.600938000	1.719674000
N	7.990362000	-9.752457000	2.909372000
H	8.049683000	-10.688664000	3.323637000
H	8.748688000	-9.699278000	2.223204000
O	1.352562000	-8.756421000	3.252488000
Si	0.243743000	-7.615509000	2.853128000
O	1.832968000	-3.941907000	2.741456000
Si	0.779668000	-3.219960000	1.691550000
C	1.657899000	-2.403557000	0.259903000
H	0.937044000	-1.700633000	-0.207304000
H	2.441634000	-1.766685000	0.721199000
C	2.284971000	-3.316724000	-0.812922000
H	2.997512000	-4.032988000	-0.361832000
H	1.490190000	-3.930109000	-1.285601000
C	3.017343000	-2.515341000	-1.900711000
H	2.309879000	-1.756032000	-2.320741000
H	3.831993000	-1.931716000	-1.422752000
N	3.618019000	-3.398213000	-2.900851000
H	2.889322000	-3.858102000	-3.455771000
H	4.181916000	-2.858208000	-3.563105000
O	-0.063416000	-2.074749000	2.538268000
O	-0.565019000	-4.894946000	6.090289000
Si	-0.496141000	-6.460017000	5.586401000
O	0.139154000	-6.478328000	4.062863000
O	2.605151000	-10.709614000	4.616964000
H	1.892090000	-10.800711000	5.267128000
O	-1.266123000	-8.245641000	2.608316000
H	-1.866028000	-8.142572000	3.369390000
O	3.440141000	-5.873371000	1.657560000
H	2.624382000	-6.370639000	1.414634000
O	3.852695000	-1.007957000	2.973962000
H	4.310284000	-0.503069000	2.284161000
O	6.298451000	-1.872233000	3.648221000
H	6.935726000	-2.601029000	3.598782000
O	-0.231633000	-2.951726000	7.827595000
H	0.156364000	-2.110128000	8.115169000
O	3.777419000	-3.448264000	7.646502000
H	4.680337000	-3.201092000	7.896899000
O	1.273276000	-0.512800000	4.326919000
H	2.045926000	-0.603109000	3.729364000
O	-1.437056000	-0.249016000	3.981271000
H	-1.388091000	0.507219000	3.379126000
O	-0.340966000	-4.358231000	1.143467000
H	-1.193806000	-4.352841000	1.608865000
O	2.514395000	-1.118723000	6.985518000
H	2.119744000	-0.568263000	6.277799000
O	-2.040462000	-7.066983000	5.402749000
H	-2.552377000	-7.233717000	6.208122000
O	0.327357000	-7.421978000	6.634660000
H	1.209018000	-7.106687000	6.931246000
O	2.989147000	-6.298968000	6.963046000
H	3.178671000	-5.424241000	7.360636000
O	5.377322000	-6.510612000	5.590518000
H	5.829357000	-7.207479000	6.089712000
O	0.813150000	-6.904933000	1.459583000
H	0.302506000	-6.120943000	1.153087000

SiO_2-2APS

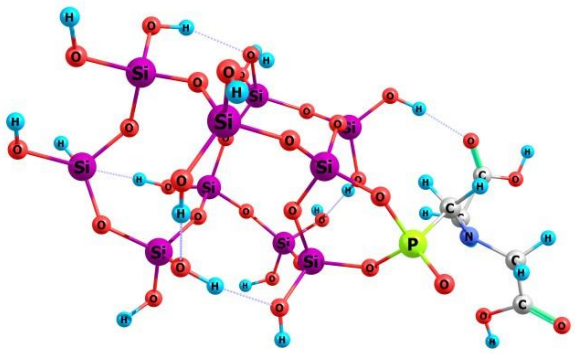


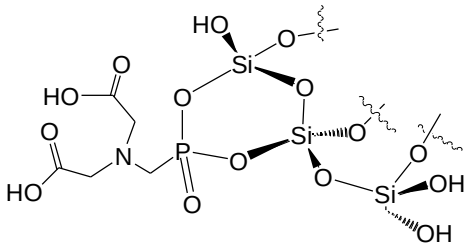


E = -5280.940088524

Si	-0.166235000	-1.300803000	3.995507000
O	-0.529356000	-2.367978000	5.184175000
Si	0.107580000	-3.422294000	6.281017000
O	1.742594000	-3.498287000	5.996344000
Si	3.037810000	-2.587168000	6.427535000
O	4.115415000	-2.414597000	5.192945000
Si	3.720657000	-6.618581000	5.499269000
Si	4.701017000	-2.285401000	3.664936000
Si	3.237639000	-4.803799000	2.890879000
O	4.482642000	-3.696626000	2.839108000
O	3.268031000	-5.531507000	4.355432000
O	3.218140000	-8.126799000	5.116907000
Si	2.799801000	-9.216058000	3.922894000
C	4.168396000	-9.292050000	2.659765000
H	3.921402000	-10.061457000	1.900903000
H	4.177659000	-8.322243000	2.122631000
C	5.555395000	-9.558113000	3.280590000
H	5.791532000	-8.781966000	4.031208000
H	5.542965000	-10.524128000	3.827248000
C	6.691579000	-9.574428000	2.250479000
H	6.459833000	-10.342071000	1.471845000
H	6.703761000	-8.600938000	1.719674000
N	7.990362000	-9.752457000	2.909372000
H	8.049683000	-10.688664000	3.323637000
H	8.748688000	-9.699278000	2.223204000
O	1.352562000	-8.756421000	3.252488000
Si	0.243743000	-7.615509000	2.853128000
O	1.832968000	-3.941907000	2.741456000
Si	0.779668000	-3.219960000	1.691550000
C	1.657899000	-2.403557000	0.259903000
H	0.937044000	-1.700633000	-0.207304000
H	2.441634000	-1.766685000	0.721199000
C	2.284971000	-3.316724000	-0.812922000
H	2.997512000	-4.032988000	-0.361832000
H	1.490190000	-3.930109000	-1.285601000
C	3.017343000	-2.515341000	-1.900711000
H	2.309879000	-1.756032000	-2.320741000
H	3.831993000	-1.931716000	-1.422752000
N	3.618019000	-3.398213000	-2.900851000
H	2.889322000	-3.858102000	-3.455771000
H	4.181916000	-2.858208000	-3.563105000
O	-0.063416000	-2.074749000	2.538268000
O	-0.565019000	-4.894946000	6.090289000
Si	-0.496141000	-6.460017000	5.586401000
O	0.139154000	-6.478328000	4.062863000
O	2.605151000	-10.709614000	4.616964000
H	1.892090000	-10.800711000	5.267128000
O	-1.266123000	-8.245641000	2.608316000
H	-1.866028000	-8.142572000	3.369390000
O	3.440141000	-5.873371000	1.657560000
H	2.624382000	-6.370639000	1.414634000
O	3.852695000	-1.007957000	2.973962000
H	4.310284000	-0.503069000	2.284161000
O	6.298451000	-1.872233000	3.648221000
H	6.935726000	-2.601029000	3.598782000
O	-0.231633000	-2.951726000	7.827595000
H	0.156364000	-2.110128000	8.115169000
O	3.777419000	-3.448264000	7.646502000
H	4.680337000	-3.201092000	7.896899000
O	1.273276000	-0.512800000	4.326919000
H	2.045926000	-0.603109000	3.729364000
O	-1.437056000	-0.249016000	3.981271000
H	-1.388091000	0.507219000	3.379126000
O	-0.340966000	-4.358231000	1.143467000
H	-1.193806000	-4.352841000	1.608865000
O	2.514395000	-1.118723000	6.985518000
H	2.119744000	-0.568263000	6.277799000
O	-2.040462000	-7.066983000	5.402749000
H	-2.552377000	-7.233717000	6.208122000
O	0.327357000	-7.421978000	6.634660000
H	1.209018000	-7.106687000	6.931246000
O	2.989147000	-6.298968000	6.963046000
H	3.178671000	-5.424241000	7.360636000
O	5.377322000	-6.510612000	5.590518000
H	5.829357000	-7.207479000	6.089712000
O	0.813150000	-6.904933000	1.459583000
H	0.302506000	-6.120943000	1.153087000

SiO_2-PMIDA

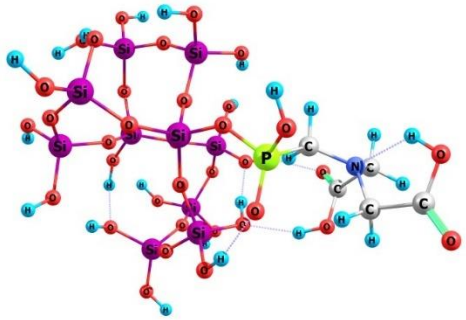


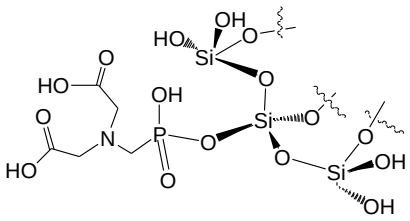


E = -6050.719526583

Si	-0.691694000	-1.640008000	4.492570000
O	-1.323522000	-3.019148000	5.216303000
Si	-0.922161000	-3.913307000	6.543090000
O	0.726630000	-3.936341000	6.721185000
Si	1.681843000	-3.075127000	7.745078000
O	2.877344000	-2.241797000	7.005521000
Si	3.445652000	-6.561050000	6.207335000
Si	3.725546000	-1.759802000	5.674222000
Si	3.186338000	-4.355661000	3.941134000
O	3.652729000	-2.847806000	4.449306000
O	2.974670000	-5.281090000	5.290836000
O	3.464416000	-7.962888000	5.331390000
Si	2.904989000	-8.378631000	3.835006000
O	1.496262000	-7.551838000	3.579474000
Si	-0.100746000	-7.798047000	3.230102000
O	1.752996000	-4.231711000	3.135508000
Si	0.511863000	-3.501966000	2.349989000
O	0.104983000	-2.093499000	3.122281000
O	-1.506354000	-5.416815000	6.414710000
Si	-1.363461000	-7.018097000	5.967814000
O	-1.027544000	-6.994375000	4.342357000
O	2.693268000	-9.999069000	3.655803000
H	1.758332000	-10.281315000	3.652008000
O	-0.253999000	-9.457385000	3.337588000
H	-1.124550000	-9.845924000	3.163521000
O	0.986275000	-3.191446000	0.803602000
H	0.333757000	-2.777498000	0.219288000
O	4.394837000	-4.937544000	3.001619000
H	4.386412000	-5.894967000	2.791497000
O	2.991150000	-0.333783000	5.191695000
H	3.397004000	0.126808000	4.440131000
O	5.286576000	-1.420007000	6.084499000
H	5.943815000	-2.115743000	5.929789000
O	-1.508861000	-3.196005000	7.942973000
P	-0.911285000	-2.041971000	8.947524000
C	-1.561535000	-0.507386000	8.177265000
H	-1.368692000	-0.586358000	7.102015000
H	-2.667493000	-0.543707000	8.303480000
N	-0.949395000	0.711754000	8.683978000
C	-0.524597000	1.660593000	7.657813000
H	0.021358000	2.494542000	8.126788000
H	0.165303000	1.144827000	6.966784000
C	-1.690101000	2.201262000	6.811878000
O	-2.022253000	3.469404000	7.106616000
H	-2.785107000	3.720892000	6.545859000
O	-2.304354000	1.554920000	5.982545000
C	-1.519125000	1.239011000	9.912193000
H	-2.409931000	1.894568000	9.764249000
H	-1.869240000	0.383502000	10.522212000
C	-0.573223000	2.017916000	10.832644000
O	0.726490000	1.958691000	10.467894000
H	1.229580000	2.470659000	11.131703000
O	-0.958846000	2.619496000	11.805430000
O	-1.252313000	-2.222889000	10.380029000
O	2.360719000	-4.216790000	8.756024000
H	3.060846000	-3.931821000	9.363779000
O	0.358109000	-1.015842000	5.612890000
H	1.205770000	-0.599984000	5.334513000
O	-1.877934000	-0.591093000	4.078277000
H	-2.107998000	0.118352000	4.713007000
O	-0.837641000	-4.492407000	2.297996000
H	-1.334194000	-4.603821000	3.128771000
O	0.698726000	-2.054615000	8.629866000
O	-2.823545000	-7.768909000	6.144811000
H	-3.055053000	-8.044066000	7.044196000
O	-0.261601000	-7.822947000	6.870980000
H	0.635448000	-7.473145000	7.073472000
O	2.338271000	-6.787700000	7.429072000
H	2.273278000	-6.029167000	8.050669000
O	4.966949000	-6.210291000	6.771512000
H	5.490456000	-6.960597000	7.091535000
O	-0.519308000	-7.297586000	1.724983000
H	-0.711149000	-6.338384000	1.655488000
O	4.084757000	-7.839007000	2.772170000
H	4.087432000	-8.249131000	1.892815000

SiO_2-PMIDA (with one free P(O)-OH)

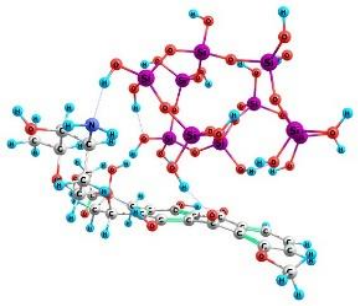


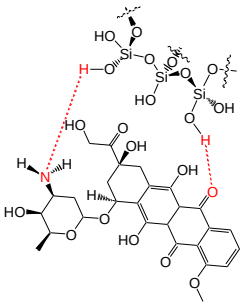


E = -6127.0526988

Si	0.804278000	-1.008312000	3.286038000
O	-0.002431000	-1.958506000	4.371385000
Si	0.326610000	-3.022852000	5.582496000
O	1.912132000	-2.992235000	5.966028000
Si	3.156275000	-2.171401000	6.709254000
O	4.479899000	-2.298838000	5.715046000
Si	3.504240000	-6.488230000	6.550561000
Si	5.247938000	-2.566845000	4.295238000
Si	3.675469000	-5.085439000	3.696170000
O	5.027698000	-4.139159000	3.798944000
O	3.251956000	-5.608960000	5.187559000
O	3.866725000	-8.044438000	6.132619000
Si	3.204733000	-9.021079000	4.948476000
O	1.739970000	-8.325110000	4.579939000
Si	0.618588000	-7.937815000	3.428504000
O	2.400639000	-4.204984000	3.115142000
Si	1.893041000	-3.473596000	1.732015000
O	1.324481000	-1.965238000	2.026483000
O	-0.184481000	-4.520846000	5.208086000
Si	-0.960833000	-5.993441000	5.358480000
O	-0.514679000	-6.936902000	4.074006000
O	2.998566000	-10.515794000	5.604340000
H	3.128048000	-11.278973000	5.023032000
O	-0.083367000	-9.289292000	2.782999000
H	-0.741193000	-9.747443000	3.327406000
O	3.151119000	-3.259991000	0.665211000
H	3.575648000	-4.056138000	0.307554000
O	4.015325000	-6.316252000	2.634540000
H	3.176405000	-6.745775000	2.323712000
O	4.585043000	-1.516593000	3.170593000
H	4.640554000	-1.770872000	2.232556000
O	6.856977000	-2.234119000	4.394493000
H	7.370241000	-2.651295000	5.101540000
O	3.502020000	-2.836935000	8.173674000
H	4.048727000	-3.641373000	8.170110000
O	2.123092000	-0.260497000	3.976363000
H	3.002764000	-0.544211000	3.631817000
O	-0.308338000	0.083466000	2.755039000
H	0.014230000	0.868916000	2.289850000
O	0.721279000	-4.504731000	1.138450000
H	0.062897000	-4.160640000	0.515268000
O	2.723878000	-0.598297000	6.946384000
H	2.458368000	-0.153593000	6.117362000
O	-2.587098000	-5.850818000	5.333384000
H	-2.917930000	-5.136990000	5.923903000
O	-0.446041000	-6.717906000	6.768607000
H	0.535547000	-6.701374000	6.905645000
O	2.109187000	-6.372801000	7.429708000
H	2.026517000	-6.503348000	8.397172000
O	4.749612000	-5.800454000	7.411241000
H	5.533230000	-6.336177000	7.603928000
O	1.419508000	-7.151344000	2.188560000
H	0.945543000	-6.405431000	1.761152000
O	4.182085000	-9.138275000	3.624887000
H	4.473780000	-8.303363000	3.211390000
P	-1.746044000	-2.894130000	7.847375000
C	-0.843134000	-3.717322000	9.214336000
H	-0.280198000	-4.497833000	8.654146000
H	-0.067692000	-3.007129000	9.569200000
N	-1.587877000	-4.260192000	10.357933000
C	-3.033636000	-4.560657000	10.269571000
C	-3.819835000	-3.963472000	11.458223000
O	-3.125787000	-3.072762000	12.190111000
H	-2.233727000	-3.032948000	11.771689000
O	-4.957410000	-4.270969000	11.702422000
H	-3.478735000	-4.155948000	9.344538000
H	-3.248420000	-5.642925000	10.227555000
C	-0.794444000	-5.281234000	11.060441000
C	-0.303541000	-6.374340000	10.087113000
O	-1.305064000	-6.902345000	9.384413000
H	-0.997323000	-7.205234000	8.487263000
O	0.874533000	-6.632636000	9.918576000
H	-1.401946000	-5.725689000	11.869752000
H	0.100168000	-4.822489000	11.520581000
O	-2.774855000	-3.744972000	7.176307000
O	-2.381918000	-1.518870000	8.418372000
H	-1.803406000	-0.739071000	8.359436000
O	-0.510748000	-2.414968000	6.930700000

SiO_2-Dox complex

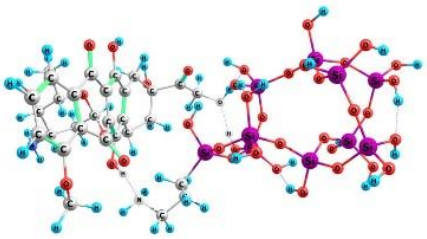


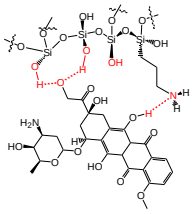


E = -7011.207488811

O	3.218199000	0.362206000	-0.261548000
O	2.558359000	2.633402000	-0.179064000
O	5.611048000	0.964680000	1.876719000
O	-0.239734000	3.236136000	0.889114000
O	3.025452000	-2.036872000	-1.591575000
O	7.761583000	-2.934337000	1.092425000
O	8.130856000	2.543918000	-0.113179000
O	8.662383000	3.818050000	2.176738000
N	-0.967341000	0.573380000	1.062990000
C	4.527568000	0.225492000	-0.874316000
C	6.418448000	1.046792000	0.704022000
C	5.516499000	1.350165000	-0.509354000
C	7.170082000	-0.278717000	0.450618000
C	5.010488000	-1.184484000	-0.539091000
C	6.233088000	-1.414435000	0.097410000
C	2.344992000	1.385160000	-0.779501000
C	0.890569000	0.918188000	-0.611192000
C	0.442631000	0.938984000	0.863084000
C	0.706637000	2.333410000	1.465228000
C	2.176841000	2.759416000	1.210996000
C	4.174055000	-2.278945000	-0.915382000
C	7.459826000	2.186830000	0.837293000
C	6.620736000	-2.750279000	0.395110000
C	4.564057000	-3.599996000	-0.645041000
C	3.648488000	-4.759875000	-0.889671000
O	2.426665000	-4.637247000	-0.890547000
C	4.282538000	-6.105813000	-1.018004000
C	3.617851000	-7.195958000	-1.650038000
O	2.506573000	-6.923017000	-2.358631000
C	1.779065000	-7.964189000	-2.994194000
H	2.394927000	-8.505796000	-3.741251000
H	1.377739000	-8.689929000	-2.259175000
H	0.937383000	-7.477146000	-3.513292000
C	4.162913000	-8.492416000	-1.536081000
H	3.658379000	-9.345317000	-1.998350000
C	5.814802000	-3.837385000	-0.010280000
C	6.270945000	-5.215865000	0.252053000
O	7.301580000	-5.438538000	0.908867000
C	5.510057000	-6.343901000	-0.355806000
C	6.034044000	-7.639543000	-0.242375000
H	6.966073000	-7.790377000	0.309866000
C	5.346449000	-8.706423000	-0.822338000
H	5.739493000	-9.725692000	-0.725829000
C	2.457584000	4.207491000	1.600737000
C	7.639392000	2.865251000	2.193091000
H	4.373754000	0.269210000	-1.975955000
H	6.184112000	1.527997000	-1.371022000
H	4.952931000	2.284612000	-0.350563000
H	7.786761000	-0.548435000	1.325897000
H	7.888313000	-0.120764000	-0.378540000
H	2.581559000	1.536368000	-1.854142000
H	0.752379000	-0.094041000	-1.035432000
H	0.257125000	1.611684000	-1.195274000
H	1.057812000	0.208767000	1.418171000
H	0.557892000	2.266622000	2.564076000
H	2.821078000	2.089032000	1.817466000
H	6.019620000	0.348783000	2.519423000
H	3.519042000	4.456833000	1.425406000
H	1.839886000	4.895110000	0.997135000
H	2.238290000	4.373303000	2.672271000
H	-1.155374000	-0.355280000	0.672405000
H	-1.569351000	1.250236000	0.583903000
H	7.837738000	2.074153000	2.953227000
H	6.655585000	3.303062000	2.482413000
H	-0.443471000	3.932354000	1.530625000
H	2.616788000	-1.246132000	-1.182273000
H	7.878029000	-3.925388000	1.193109000
H	8.985394000	3.863655000	1.255373000
Si	-0.216737000	-0.965051000	4.102851000
O	-0.646073000	-1.842470000	5.446214000
Si	0.045602000	-3.191450000	6.102049000
O	1.682164000	-3.111375000	5.819407000
Si	2.949963000	-2.251972000	6.456700000
O	4.100180000	-2.000811000	5.280226000
Si	3.645663000	-6.197998000	5.995861000
Si	4.518214000	-1.935696000	3.695960000
Si	3.236881000	-4.640970000	3.169155000
O	4.351122000	-3.423888000	2.998756000
O	3.396290000	-5.246953000	4.685245000
O	3.714015000	-7.781079000	5.571121000
Si	3.369667000	-8.637485000	4.183247000
O	1.881428000	-8.095426000	3.708877000
Si	0.539300000	-7.683528000	2.862593000
O	1.724630000	-4.069758000	2.926587000
Si	0.594351000	-3.283570000	1.993693000
O	-0.026105000	-2.017926000	2.831140000
O	-0.551148000	-4.545138000	5.392578000
Si	-0.862681000	-6.162000000	5.238783000
O	-0.392498000	-6.602241000	3.701861000
O	3.368200000	-10.233741000	4.597719000
H	3.764429000	-10.835852000	3.951039000
O	-0.344459000	-9.018142000	2.454842000
H	-0.831667000	-9.457554000	3.167931000
O	1.232105000	-2.642122000	0.622199000
H	1.594180000	-3.259292000	-0.058371000
O	3.612038000	-5.811922000	2.049367000
H	2.817892000	-6.245115000	1.649373000
O	3.527642000	-0.785534000	3.006388000
H	3.822504000	-0.334111000	2.190157000
O	6.097463000	-1.446958000	3.468053000
H	6.723636000	-2.111392000	3.127664000
O	-0.276387000	-3.290781000	7.724537000
H	-0.074292000	-2.504860000	8.255845000
O	3.627020000	-3.143216000	7.681140000
H	4.451368000	-3.619326000	7.472764000
O	1.235362000	-0.203674000	4.440598000
H	2.006797000	-0.344205000	3.845975000
O	-1.387570000	0.126647000	3.784470000
H	-1.379102000	0.405111000	2.823204000
O	-0.561214000	-4.421023000	1.592995000
H	-0.925207000	-4.921927000	2.346483000
O	2.376914000	-0.845799000	7.096010000
H	1.921050000	-0.304937000	6.416568000
O	-2.492182000	-6.452820000	5.256673000
H	-2.950623000	-6.267859000	6.089827000
O	-0.111072000	-7.074700000	6.372791000
H	0.757216000	-6.787846000	6.731418000
O	2.420672000	-6.043635000	7.121098000
H	2.404656000	-5.179702000	7.577527000
O	5.080239000	-5.657475000	6.654307000
H	5.538209000	-6.267677000	7.253269000
O	1.077306000	-6.957348000	1.457306000
H	0.496894000	-6.267113000	1.076979000
O	4.495060000	-8.416767000	2.996104000
H	4.478385000	-7.545272000	2.550711000

SiO_2-1APS-Dox complex

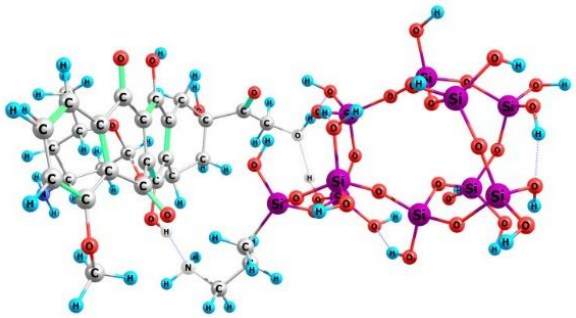


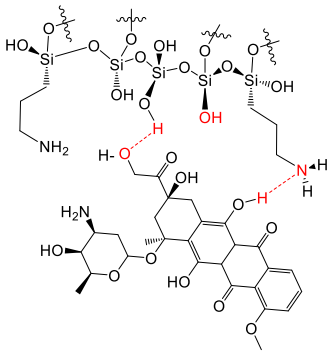


E = -7109.003616256

Si	-2.554132000	-2.462289000	7.717901000
O	-1.085465000	-2.848475000	8.350173000
Si	-0.261838000	-2.667668000	9.774147000
O	-1.312290000	-2.076615000	10.916971000
Si	-2.524200000	-2.604479000	11.893628000
O	-3.760360000	-1.509446000	11.978163000
Si	-0.349919000	0.878513000	13.509346000
Si	-4.592528000	-0.216417000	11.379699000
Si	-2.124392000	1.523338000	10.895602000
O	-3.665085000	1.149240000	11.385340000
O	-1.043788000	1.052137000	12.027984000
O	0.869103000	1.955225000	13.715037000
Si	2.102843000	2.745170000	12.895031000
C	2.440634000	4.448887000	13.578905000
H	1.530114000	4.816656000	14.093149000
H	3.205064000	4.353695000	14.370328000
C	2.860790000	5.454748000	12.478825000
H	3.545605000	4.986836000	11.741232000
H	1.970221000	5.736824000	11.886831000
C	3.527438000	6.732695000	13.011919000
H	3.391005000	7.557747000	12.279329000
H	3.023768000	7.055998000	13.943051000
N	4.960799000	6.510336000	13.315782000
H	5.492153000	6.478746000	12.438750000
H	5.348707000	7.302840000	13.838370000
O	1.561665000	2.941824000	11.329277000
Si	1.687297000	2.580762000	9.734534000
O	-1.808522000	0.641159000	9.512746000
Si	-2.370074000	0.671548000	7.971523000
O	-2.567746000	-0.835563000	7.360136000
O	0.961747000	-1.606780000	9.596611000
Si	2.096285000	-0.542531000	10.120368000
O	1.699508000	0.935929000	9.520421000
O	3.505657000	1.854304000	12.931204000
H	3.408983000	0.917328000	12.664269000
O	3.013012000	3.270626000	9.043915000
H	3.784644000	2.676979000	8.897270000
O	-2.114924000	3.129548000	10.549474000
H	-1.270788000	3.428726000	10.138229000
O	-5.041460000	-0.616974000	9.815783000
H	-5.033167000	0.117485000	9.166037000
O	-5.962839000	0.051762000	12.251998000
H	-5.861828000	0.513907000	13.097530000
O	0.403083000	-4.107246000	10.227380000
H	-0.185971000	-4.874478000	10.284879000
O	-1.798037000	-2.727278000	13.391280000
H	-2.362579000	-2.927429000	14.153800000
O	-3.764109000	-2.836512000	8.800753000
H	-4.345922000	-2.096498000	9.106868000
O	-2.730239000	-3.334408000	6.328192000
H	-3.621783000	-3.651145000	6.124207000
O	-1.300218000	1.590074000	7.078741000
H	-1.184995000	1.372420000	6.141033000
O	-3.096307000	-4.075141000	11.410186000
H	-3.529236000	-4.031193000	10.533266000
O	3.586354000	-0.950699000	9.477612000
H	4.266293000	-1.128889000	10.157809000
O	2.309097000	-0.541132000	11.758144000
H	1.588340000	-0.750578000	12.406208000
O	0.319907000	-0.652419000	13.589108000
H	-0.307800000	-1.408827000	13.610371000
O	-1.539837000	1.058695000	14.648728000
H	-1.247444000	1.343164000	15.528080000
O	0.293148000	3.209775000	9.059224000
H	-0.024245000	2.779435000	8.239677000
O	8.386018000	4.337835000	13.403034000
O	9.886255000	2.622486000	14.095018000
O	8.759049000	1.579068000	10.742848000
O	12.429961000	3.521032000	15.431473000
O	5.452900000	4.545425000	15.319838000
O	7.268124000	-0.684234000	15.234292000
O	5.847518000	-0.120815000	11.099022000
O	5.014049000	1.325581000	8.748719000
O	3.330421000	3.323251000	16.801143000
O	6.129395000	-0.923238000	17.619520000
O	3.222121000	3.966403000	19.753213000
N	11.822370000	6.254600000	15.191963000
C	7.141524000	3.700561000	13.047040000
C	7.547304000	1.567311000	11.525761000
C	7.067765000	3.041215000	11.657522000
C	7.773314000	0.863061000	12.886212000
C	6.627383000	2.763427000	14.124107000
C	6.994251000	1.411450000	14.069359000
C	9.648330000	3.714091000	13.222368000
C	10.710597000	4.805247000	13.415113000
C	10.826798000	5.224107000	14.901093000
C	11.110705000	3.974086000	15.755459000
C	10.031793000	2.893768000	15.498529000
C	5.813790000	3.249089000	15.179619000
C	6.492227000	0.816221000	10.667559000
C	6.738546000	0.565784000	15.175783000
C	5.414054000	2.348881000	16.189242000
C	5.964025000	1.041650000	16.258873000
C	10.343797000	1.551908000	16.163328000
C	6.346616000	1.278749000	9.202037000
C	4.328584000	2.715345000	17.159714000
C	5.766687000	0.236889000	17.503422000
C	4.484169000	2.194242000	18.550051000
C	5.152389000	0.948468000	18.690833000
C	3.887559000	2.786551000	19.697083000
C	5.220529000	0.301154000	19.928687000
C	3.973687000	2.114972000	20.935844000
C	4.630445000	0.891789000	21.051356000
C	3.594798000	5.119694000	19.001795000
H	6.459793000	4.559607000	12.983343000
H	5.995281000	3.091177000	11.384510000
H	7.610409000	3.652814000	10.913738000
H	8.851702000	0.944799000	13.118831000
H	7.516246000	-0.204571000	12.743479000
H	9.714873000	3.265161000	12.212267000
H	10.454433000	5.676816000	12.784035000
H	11.682061000	4.404553000	13.069269000
H	9.838745000	5.609514000	15.222981000
H	11.054945000	4.272533000	16.825213000
H	9.070571000	3.286198000	15.897361000
H	9.206288000	0.721353000	10.838245000
H	9.518193000	0.834229000	16.018407000
H	11.259421000	1.115064000	15.724499000
H	10.495321000	1.671853000	17.252759000
H	11.666577000	7.075743000	14.600131000
H	12.754835000	5.895463000	14.964092000
H	6.970709000	0.580383000	8.596202000
H	6.788934000	2.278556000	9.056297000
H	12.754438000	2.961687000	16.152071000
H	5.383574000	5.090449000	14.488851000
H	7.798841000	-0.850847000	14.440368000
H	5.731037000	-0.665179000	19.985632000
H	4.559670000	0.453212000	8.849091000
H	3.514888000	2.600389000	21.804716000
H	4.693417000	0.397443000	22.028678000
H	4.675652000	5.120662000	18.757927000
H	3.367957000	5.991619000	19.641975000
H	3.027270000	5.187474000	18.058719000
O	-3.902267000	1.349947000	7.933791000
H	-3.957741000	2.294574000	8.154669000

SiO_2-2APS-Dox complex





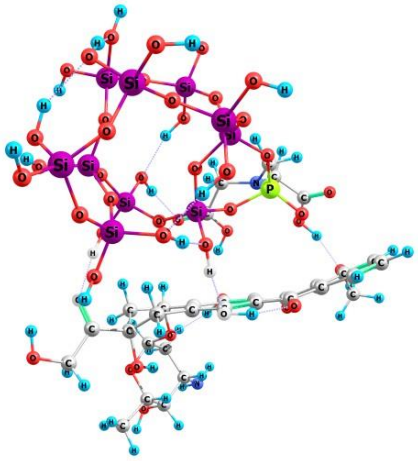
E = -7206.872846100

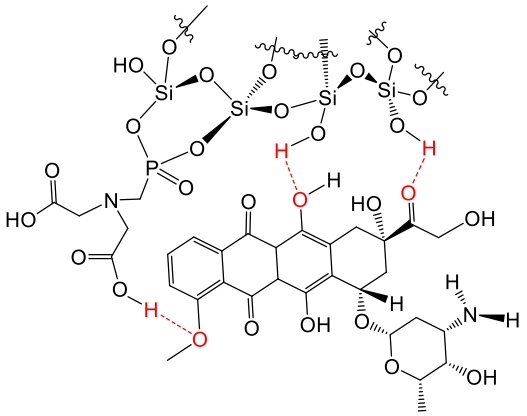
Si	-1.571997000	1.352527000	5.573450000
O	-1.045117000	-0.035941000	6.302694000
Si	-1.178799000	-0.922955000	7.686127000
O	-2.512900000	-0.417481000	8.495474000
Si	-3.952888000	0.227723000	8.915821000
O	-3.803591000	1.791234000	9.411517000
Si	-1.322351000	0.664946000	12.264213000
Si	-3.637851000	3.418468000	9.446576000
Si	-0.775441000	2.963894000	10.149920000
O	-2.212761000	3.801633000	10.180446000
O	-0.965851000	1.515286000	10.907094000
O	0.017472000	0.295523000	13.124913000
Si	1.614779000	-0.011079000	13.478766000
C	1.944322000	0.697617000	15.179152000
H	1.353660000	0.114793000	15.914672000
H	3.002823000	0.551324000	15.461300000
C	1.550591000	2.190629000	15.236976000
H	2.055725000	2.734650000	14.419374000
H	0.468969000	2.282477000	15.019618000
C	1.832358000	2.926334000	16.559561000
H	1.141026000	3.795746000	16.621981000
H	1.579753000	2.268282000	17.415191000
N	3.240710000	3.350059000	16.691901000
H	3.508822000	3.965723000	15.910168000
H	3.355456000	3.907037000	17.545182000
O	2.545246000	0.783333000	12.346861000
Si	3.005455000	0.746962000	10.755912000
O	-0.446314000	2.657392000	8.559735000
Si	0.467528000	2.986306000	7.213413000
C	1.060006000	4.754985000	7.073538000
H	1.387411000	4.897047000	6.022015000
H	0.193912000	5.432873000	7.219460000
C	2.206131000	5.123936000	8.041996000
H	1.838332000	5.080446000	9.083394000
H	3.016836000	4.372866000	7.961750000
C	2.814323000	6.509960000	7.781063000
H	3.110450000	6.572183000	6.706822000
H	2.041367000	7.290581000	7.936726000
N	3.937729000	6.769750000	8.692611000
H	4.634824000	6.010396000	8.651776000
H	4.422868000	7.633100000	8.431078000
O	-0.494930000	2.564882000	5.924039000
O	0.154412000	-0.726009000	8.621505000
Si	1.172340000	-1.610153000	9.605305000
O	2.395660000	-0.608809000	10.031960000
O	1.931218000	-1.646612000	13.443291000
H	1.513887000	-2.116913000	12.688866000
O	4.620884000	0.845386000	10.543472000
H	5.268415000	0.284196000	11.026328000
O	0.358899000	3.909794000	10.870227000
H	1.237627000	3.469669000	10.829672000
O	-3.672627000	3.892899000	7.837458000
H	-3.884260000	4.819969000	7.648660000
O	-4.877394000	4.184717000	10.218913000
H	-2.821622000	-0.843160000	11.351497000
O	-2.350579000	1.612113000	13.164810000
H	-2.536574000	1.311528000	14.066766000
O	2.345063000	2.108929000	10.056714000
H	2.398704000	2.138611000	9.074998000
O	5.755396000	2.526601000	13.553599000
O	4.567972000	4.516507000	14.012704000
O	6.587539000	-0.458549000	11.960447000
O	4.293437000	6.369382000	11.521092000
O	5.673590000	2.462095000	17.569992000
O	10.329549000	0.429007000	15.309999000
O	8.297669000	-1.942068000	14.375171000
O	5.015872000	-2.627985000	13.070157000
O	6.985757000	1.869769000	19.903735000
O	11.468224000	0.966592000	17.738876000
O	8.062080000	4.289478000	21.514515000
N	6.077493000	4.784606000	9.997550000
C	5.642137000	1.623983000	14.662554000
C	6.818813000	-0.302404000	13.375383000
C	5.509564000	0.220101000	14.039400000
C	7.986592000	0.679211000	13.608195000
C	6.845997000	1.634398000	15.595954000
C	8.040580000	1.123848000	15.054342000
C	5.830831000	3.926882000	13.755888000
C	6.463536000	4.500652000	12.481502000
C	5.531605000	4.282935000	11.270726000
C	4.171761000	4.956420000	11.568355000
C	3.601741000	4.476378000	12.928182000
C	6.779627000	2.007265000	16.958887000
C	7.192503000	-1.712062000	13.922475000
C	9.205918000	0.993178000	15.837708000
C	7.966824000	1.926932000	17.731180000
C	9.187611000	1.476031000	17.170631000
C	2.398740000	5.304271000	13.370825000
C	6.147995000	-2.851386000	13.868458000
C	7.919933000	2.223369000	19.203604000
C	10.431466000	1.543769000	18.015152000
C	9.136752000	2.882236000	19.768218000
C	10.377049000	2.452849000	19.225319000
C	9.138958000	3.747224000	20.894926000
C	11.589738000	2.827504000	19.813234000
C	10.376262000	4.130213000	21.458345000
C	11.581366000	3.667434000	20.934229000
C	6.829922000	4.570889000	20.857444000
H	4.715100000	1.845177000	15.219877000
H	5.190693000	-0.462417000	14.847872000
H	4.706408000	0.237927000	13.291207000
H	7.790647000	1.549679000	12.962492000
H	8.935254000	0.228090000	13.277995000
H	6.440759000	4.157948000	14.653745000
H	7.448616000	4.024599000	12.313265000
H	6.626303000	5.585421000	12.629990000
H	5.352060000	3.200457000	11.142535000
H	3.451711000	4.606833000	10.799862000
H	3.300077000	3.417794000	12.786988000

SiO_2-2APS-Dox (continuation)

H	-4.743387000	4.396492000	11.155258000	H	7.427403000	-0.656508000	11.513144000
O	-1.229628000	-2.546228000	7.341603000	H	2.025368000	4.976759000	14.356954000
H	-1.897411000	-2.866606000	6.717613000	H	2.677995000	6.369116000	13.430894000
O	-4.397978000	-0.673031000	10.250694000	H	1.571710000	5.188766000	12.648752000
H	-5.238720000	-0.451002000	10.679420000	H	6.848620000	4.186108000	9.689466000
O	-3.105642000	1.767544000	6.071823000	H	6.480432000	5.716028000	10.148891000
H	-3.241027000	2.597591000	6.584476000	H	5.904806000	-3.095474000	14.926883000
O	-1.583641000	1.001298000	3.960759000	H	6.701264000	-3.733930000	13.483491000
H	-2.057422000	1.614415000	3.380427000	H	4.032974000	6.647242000	10.608455000
O	1.858487000	2.036122000	7.263202000	H	4.843570000	2.536683000	17.023494000
H	1.719038000	1.074786000	7.192316000	H	10.064032000	-0.381163000	14.835930000
O	-5.086611000	0.090947000	7.729214000	H	12.521550000	2.446312000	19.383538000
H	-4.832988000	0.556990000	6.909220000	H	4.226433000	-2.420001000	13.598570000
O	1.848797000	-2.868688000	8.779892000	H	10.349506000	4.808489000	22.318731000
H	1.219092000	-3.459156000	8.336523000	H	12.525148000	3.981922000	21.396963000
O	0.387221000	-2.180302000	10.956613000	H	6.986518000	4.862413000	19.799055000
H	-0.500570000	-1.833758000	11.208621000	H	6.380506000	5.422070000	21.399417000
O	-1.962719000	-0.810187000	11.829578000	H	6.148626000	3.703880000	20.884335000

SiO_2-PMIDA-DOX complex





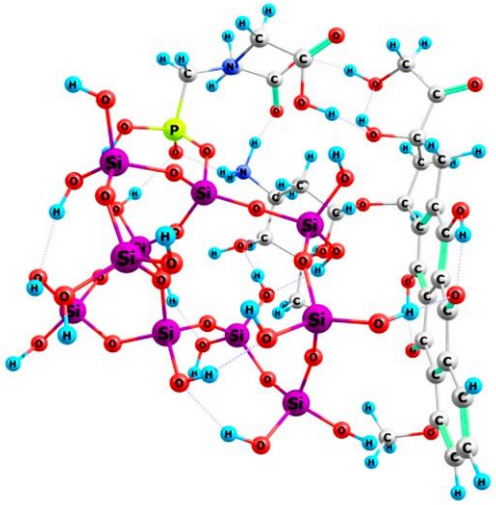
E=-7976.67840370

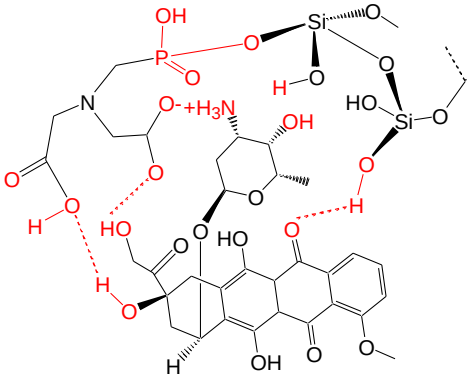
O	3.599113000	-0.586963000	-1.888545000
O	4.564188000	-0.656337000	0.231414000
O	1.914966000	1.364388000	0.040068000
O	7.564597000	-0.583058000	0.427565000
O	3.303850000	-0.812006000	-4.600048000
O	-0.601474000	2.931978000	-3.440144000
O	-1.037709000	-0.387472000	0.923692000
O	-0.519828000	0.726689000	3.280312000
O	3.829666000	0.760075000	-6.803127000
O	-0.344400000	3.839455000	-5.758100000
O	3.218084000	0.737309000	-9.534285000
N	7.976097000	-0.720126000	-2.332057000
C	2.180912000	-0.895738000	-2.050965000
C	0.857419000	0.473219000	-0.303753000
C	1.368324000	-0.917023000	-0.747622000
C	-0.009588000	1.075026000	-1.433844000
C	1.694652000	0.121000000	-3.078017000
C	0.698682000	1.055921000	-2.770404000
C	4.393036000	-1.363224000	-0.967918000
C	5.738787000	-1.705795000	-1.623932000
C	6.648651000	-0.460642000	-1.787973000
C	6.778851000	0.249140000	-0.423930000
C	5.372714000	0.538740000	0.157416000
C	2.342576000	0.130976000	-4.346237000
C	-0.015733000	0.284813000	0.950020000
C	0.333227000	1.999426000	-3.760664000
C	1.958460000	1.043227000	-5.343149000
C	0.921314000	1.969892000	-5.044555000
C	5.390965000	1.139706000	1.559679000
C	0.422348000	0.907918000	2.262573000
C	2.686823000	1.160721000	-6.660808000
C	0.444518000	2.931242000	-6.065948000
C	1.948621000	1.857211000	-7.771092000
C	0.897924000	2.757994000	-7.464710000
C	2.279251000	1.666245000	-9.133365000
C	0.230033000	3.470002000	-8.471089000
C	1.568638000	2.340202000	-10.136062000
C	0.563929000	3.255397000	-9.808027000
C	4.549498000	1.210583000	-9.790653000
H	2.101018000	-1.907943000	-2.502399000
H	0.493205000	-1.564568000	-0.927798000
H	1.955293000	-1.384792000	0.062254000
H	-0.293358000	2.108504000	-1.169173000
H	-0.950180000	0.501596000	-1.518834000
H	3.847483000	-2.289881000	-0.697729000
H	5.568329000	-2.204039000	-2.599652000
H	6.249536000	-2.438091000	-0.970347000
H	6.139605000	0.253211000	-2.467245000
H	7.288942000	1.222663000	-0.598472000
H	4.896394000	1.262957000	-0.541026000
H	2.683267000	1.177981000	-0.523132000
H	4.367180000	1.395506000	1.878311000
H	5.808021000	0.417173000	2.282787000
H	5.999215000	2.063888000	1.583518000
H	7.917016000	-1.209860000	-3.229423000
H	8.500718000	-1.318124000	-1.688714000
H	0.642625000	1.984381000	2.085631000
H	1.414006000	0.453406000	2.508561000
H	7.945307000	-0.041273000	1.135293000
H	3.818938000	-0.927331000	-3.773818000
H	-0.656669000	3.551040000	-4.243998000
H	-0.579400000	4.147779000	-8.186385000
H	-1.214231000	0.140897000	2.929810000
H	1.806586000	2.107844000	-11.180409000
H	0.015527000	3.774788000	-10.601890000
H	4.540311000	2.014818000	-10.554615000
H	5.124277000	0.353400000	-10.179900000
H	5.019863000	1.576738000	-8.859589000
Si	-5.771763000	-3.185232000	-5.931557000
O	-5.920450000	-1.610596000	-6.421355000
Si	-5.408857000	-0.090639000	-6.113542000
O	-4.725244000	-0.053358000	-4.597295000
Si	-3.178642000	0.302014000	-4.156058000
O	-2.630873000	-0.654423000	-2.950265000
Si	-5.405120000	1.783504000	-0.925814000
Si	-2.863546000	-2.149712000	-2.235097000
Si	-5.744093000	-1.357462000	-1.348436000
O	-4.430308000	-2.283953000	-1.747035000
O	-5.314081000	0.225776000	-1.456440000
O	-6.846807000	2.088686000	-0.189408000
Si	-8.425891000	1.626390000	-0.292140000
O	-9.041578000	1.932542000	-1.797996000
Si	-9.557754000	1.027884000	-3.088726000
O	-6.912614000	-1.690902000	-2.479666000
Si	-7.516685000	-3.027947000	-3.220744000
O	-6.608120000	-3.423924000	-4.529376000
O	-6.624014000	0.985082000	-6.246233000
Si	-7.629242000	1.878522000	-5.258072000
O	-8.305808000	0.834300000	-4.166300000
O	-9.219915000	2.517602000	0.844322000
H	-10.175452000	2.623302000	0.737467000
O	-10.818045000	1.787766000	-3.832650000
H	-10.620100000	2.124158000	-4.726893000
O	-7.641761000	-4.326598000	-2.208490000
H	-6.852809000	-4.623385000	-1.732926000

SiO_2-PMIDA-Dox (continuation)

O	-6.223327000	-1.787389000	0.162188000	H	2.433322000	-0.896445000	-9.435757000
H	-7.031680000	-1.311151000	0.441592000	O	0.183033000	-0.785150000	-10.177299000
O	-2.608441000	-3.354729000	-3.353977000	O	-1.861929000	1.448619000	-7.673127000
H	-1.659210000	-3.468743000	-3.601881000	O	-3.121691000	1.894239000	-3.722095000
O	-1.770947000	-2.322760000	-1.025401000	O	-4.195589000	-3.621656000	-5.716301000
H	-1.687052000	-1.634587000	-0.328874000	H	-3.774526000	-3.636767000	-4.827118000
O	-4.178979000	0.330100000	-7.178610000	O	-6.449619000	-4.036752000	-7.174762000
P	-2.542571000	0.252466000	-7.117704000	H	-6.292240000	-4.993336000	-7.183628000
C	-2.192129000	-1.362537000	-7.952696000	O	-9.071001000	-2.645358000	-3.702143000
H	-3.078457000	-2.023210000	-7.825373000	H	-9.483434000	-3.204649000	-4.372626000
H	-2.132614000	-1.078514000	-9.019392000	O	-2.236403000	-0.002162000	-5.521389000
N	-0.941809000	-2.003838000	-7.555934000	O	-8.915479000	2.443926000	-6.162384000
C	-1.044232000	-2.810194000	-6.351561000	H	-8.767723000	3.228288000	-6.712224000
H	-1.885819000	-2.452576000	-5.741832000	O	-6.853857000	3.144846000	-4.573480000
H	-1.275595000	-3.884389000	-6.562125000	H	-6.419224000	3.071953000	-3.692330000
C	0.170408000	-2.787526000	-5.425043000	O	-5.287574000	2.794429000	-2.243775000
O	1.299315000	-2.432552000	-6.021117000	H	-4.487160000	2.633368000	-2.798850000
H	2.039602000	-2.331611000	-5.381444000	O	-4.166015000	1.987664000	0.155661000
O	0.095290000	-3.106101000	-4.245236000	H	-4.228890000	2.754468000	0.743148000
C	-0.203576000	-2.635716000	-8.658986000	O	-10.007005000	-0.417871000	-2.421792000
H	0.464323000	-3.408750000	-8.249127000	H	-9.842269000	-1.240624000	-2.942580000
H	-0.886114000	-3.121947000	-9.392571000	O	-8.495570000	-0.025326000	-0.014228000
C	0.643108000	-1.590468000	-9.395046000	H	-9.090526000	-0.472927000	-0.659615000
O	1.935361000	-1.661616000	-9.052974000	H	-2.240275000	2.293572000	-3.513508000

SiO_2-PMIDA-DOX salt 1, on COOH PMIDA





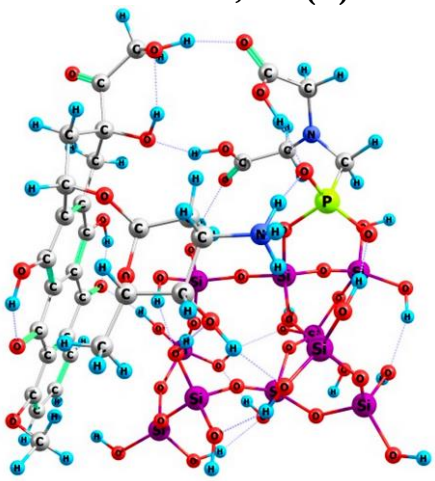
E=-8053.058920439

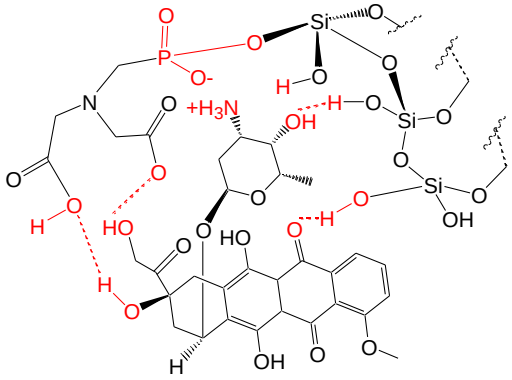
Si	4.228066000	-5.173640000	6.411864000
O	4.435525000	-4.428341000	7.870816000
Si	4.895996000	-3.016137000	8.568616000
O	6.037263000	-2.245206000	7.670626000
Si	6.555883000	-1.293485000	6.419747000
O	7.450033000	-2.218830000	5.400692000
Si	9.276970000	-2.036820000	9.497384000
Si	8.364222000	-3.480604000	4.903402000
Si	8.839265000	-4.656942000	7.687535000
O	9.220375000	-4.141904000	6.165561000
O	8.744256000	-3.377828000	8.695692000
O	10.558275000	-2.477112000	10.421005000
Si	10.943987000	-3.915083000	11.178980000
O	9.513050000	-4.634090000	11.602632000
Si	8.333028000	-5.787136000	11.606915000
O	7.353600000	-5.391115000	7.662153000
Si	6.728513000	-6.774250000	7.024049000
O	5.207280000	-6.533151000	6.473511000
O	5.370898000	-3.247672000	10.093395000
Si	5.870892000	-3.803640000	11.575051000
O	6.858143000	-5.109010000	11.297257000
O	11.833899000	-3.481089000	12.491387000
H	12.010607000	-4.148052000	13.172706000
O	8.344608000	-6.658892000	12.996177000
H	8.105889000	-6.203238000	13.832797000
O	7.631155000	-7.218867000	5.679822000
H	8.500705000	-7.617546000	5.847355000
O	9.984422000	-5.760566000	8.160583000
H	9.665882000	-6.284766000	8.944150000
O	7.340289000	-4.653499000	4.288597000
H	7.549663000	-5.590121000	4.493258000
O	9.399381000	-2.879583000	3.773904000
H	9.900662000	-3.500267000	3.226095000
O	7.452944000	-0.024051000	7.006490000
H	8.360573000	-0.228942000	7.330894000
O	4.647030000	-4.220017000	5.133116000
H	5.521278000	-4.350638000	4.702572000
O	2.652553000	-5.638540000	6.293810000
H	2.229925000	-5.497693000	5.433831000
O	6.824148000	-7.921299000	8.228807000
H	6.215889000	-8.675953000	8.189524000
O	5.269228000	-0.674857000	5.580701000
H	4.717996000	-0.019930000	6.067878000
O	4.566997000	-4.237106000	12.490452000
H	3.989919000	-4.947583000	12.176967000
O	6.636514000	-2.642864000	12.440186000
H	7.238277000	-2.050989000	11.937977000
O	0.781631000	0.910015000	14.173251000
H	0.287721000	0.951462000	13.304829000
O	1.257392000	-1.187936000	16.960532000
O	2.820440000	-0.756215000	13.835605000
H	2.224623000	-0.011932000	13.575252000
C	3.564027000	0.677373000	15.686326000
H	3.576777000	0.719466000	16.793526000
C	3.760636000	-1.842015000	15.740278000
C	5.845404000	-0.400796000	15.405221000
C	5.253936000	-1.646670000	15.582014000
C	5.338981000	0.406577000	12.753021000
C	4.386823000	0.633078000	11.568373000
C	4.732150000	1.888190000	10.763934000
C	6.223940000	1.869431000	10.374261000
C	7.027589000	1.776959000	11.702356000
C	7.275391000	-0.266268000	15.367507000
C	6.082857000	-2.819321000	15.598157000
C	8.097470000	-1.412968000	15.404976000
C	7.486321000	-2.706108000	15.480704000
C	8.542847000	1.847126000	11.526060000
C	9.552427000	-1.254006000	15.328510000
C	8.297617000	-3.901975000	15.366083000
C	10.400660000	-2.481926000	15.393842000
C	9.780040000	-3.763156000	15.394766000
C	11.818317000	-2.421111000	15.508685000
O	8.074635000	-1.402561000	10.405253000
H	7.487487000	-0.657146000	10.116488000
O	9.751448000	-0.883262000	8.371026000
H	10.685841000	-0.869928000	8.110683000
O	8.682534000	-6.822920000	10.332185000
H	7.936414000	-7.315932000	9.936024000
O	11.860325000	-4.875921000	10.203637000
H	11.464557000	-5.191018000	9.367759000
P	2.718460000	-1.177978000	7.501652000
O	3.281947000	0.230644000	7.392136000
C	0.947439000	-1.383576000	7.943165000
H	0.773731000	-2.473834000	7.868982000
H	0.360592000	-0.916700000	7.117118000
N	0.613871000	-0.893480000	9.255307000
C	0.241167000	0.523852000	9.320545000
C	0.548948000	1.142555000	10.711771000
O	1.536634000	1.944442000	10.803999000
O	-0.196130000	0.801093000	11.651117000
H	0.807178000	1.065330000	8.543482000
H	-0.846967000	0.671015000	9.113235000
C	-0.058189000	-1.801838000	10.172524000
C	0.666037000	-2.111858000	11.492411000
O	1.976993000	-1.845794000	11.462243000
H	2.347739000	-1.918646000	12.376631000

SiO_2-PMIDA-Dox salt 1, on COOH PMIDA (continuation)

H	5.465879000	1.679599000	15.739772000
C	2.909651000	-0.662304000	15.259603000
C	1.470498000	-0.716626000	15.864308000
C	0.327123000	-0.146289000	15.002849000
H	-0.471657000	0.180212000	15.701711000
H	-0.076132000	-1.002010000	14.415463000
C	10.543671000	-4.938561000	15.482708000
C	12.558398000	-3.611265000	15.644263000
C	11.932125000	-4.860741000	15.620465000
C	12.856269000	-0.650113000	14.296455000
H	2.956550000	1.528371000	15.332537000
H	3.449859000	-2.755461000	15.203601000
H	3.536389000	-2.029044000	16.809259000
H	5.258467000	-0.641304000	13.071771000
H	4.435474000	-0.252507000	10.909873000
H	3.357363000	0.714888000	11.934594000
H	4.554423000	2.781925000	11.391322000
H	6.503318000	2.803786000	9.841636000
H	6.709975000	2.627867000	12.343070000
H	9.029973000	1.685654000	12.503059000
H	8.914484000	1.079002000	10.828748000
H	8.840955000	2.842075000	11.146302000
H	12.528173000	-5.776194000	15.719284000
H	13.455906000	-1.340823000	13.671649000
O	0.087338000	-2.592212000	12.442621000
H	-0.226274000	-2.781302000	9.680255000
H	-1.057108000	-1.424694000	10.468046000
O	2.761855000	-1.993603000	6.099040000
H	3.583118000	-1.852047000	5.572237000
H	2.709052000	1.978624000	10.028093000
O	3.526226000	-2.038830000	8.594692000
O	5.026249000	1.299784000	13.798979000
O	6.703065000	0.547845000	12.350521000
O	6.501967000	0.725581000	9.554893000
O	7.775780000	0.967595000	15.306923000
H	8.774169000	0.865022000	15.271231000
O	5.467567000	-3.996744000	15.696736000
H	6.156991000	-4.702702000	15.560004000
O	10.060993000	-0.119276000	15.226009000
O	7.776920000	-5.044177000	15.274962000
O	12.519348000	-1.258652000	15.550993000
N	3.786508000	2.005706000	9.608721000
H	3.860933000	1.233503000	8.910592000
C	5.004592000	0.846594000	15.178899000
H	3.913669000	2.886098000	9.093808000
H	6.774723000	0.933287000	8.639180000
H	10.034674000	-5.906240000	15.467012000
H	13.644728000	-3.522987000	15.760556000
H	13.452262000	0.245962000	14.536904000
H	11.954442000	-0.346589000	13.736379000

SiO_2-PMIDA-DOX salt 2, on P(O)OH PMIDA





***E*=-8053.092533304**

Si	0.169128000	-7.685294000	5.632167000
O	0.704819000	-6.478366000	6.592920000
Si	1.431685000	-5.377533000	7.552740000
O	2.664261000	-4.619490000	6.761286000
Si	3.092471000	-3.585018000	5.534858000
O	3.417000000	-4.545087000	4.217546000
Si	6.054741000	-4.764487000	8.423428000
Si	4.144537000	-5.965686000	3.805465000
Si	5.009812000	-7.168427000	6.528349000
O	5.126045000	-6.554799000	5.001522000
O	5.301925000	-5.981639000	7.607208000
O	7.290732000	-5.374883000	9.305367000
Si	7.906377000	-6.911364000	9.594373000
O	6.710224000	-7.763990000	10.354097000
Si	5.207792000	-8.449980000	10.359304000
O	3.493890000	-7.801139000	6.760617000
Si	2.754453000	-9.195338000	6.274592000
O	1.163549000	-8.991235000	5.967474000
O	1.962347000	-6.046942000	8.929432000
Si	2.689590000	-6.441191000	10.368513000
O	4.072874000	-7.293773000	10.068636000
O	9.235292000	-6.774857000	10.555062000
H	9.083046000	-6.761820000	11.513192000
O	4.921784000	-9.261584000	11.757627000
H	4.587375000	-8.741879000	12.517136000
O	3.449290000	-9.708491000	4.838346000
H	4.363415000	-10.034831000	4.887363000
O	6.115814000	-8.403853000	6.689638000
H	5.936825000	-8.951034000	7.500809000
O	2.924878000	-7.073130000	3.502297000
H	3.181964000	-8.016397000	3.565164000
O	5.131933000	-5.748543000	2.502263000
H	4.785406000	-5.219847000	1.768434000
O	4.435315000	-2.683324000	5.930270000
H	5.298962000	-3.095795000	6.157379000
O	0.154411000	-7.335591000	4.030798000
H	1.023094000	-7.110648000	3.633971000
O	-1.379716000	-8.033772000	6.106557000
H	-1.984349000	-8.337874000	5.413313000
O	2.982998000	-10.304515000	7.502554000
H	2.297248000	-10.979158000	7.628574000
O	1.943905000	-2.436547000	5.292319000
H	0.991580000	-2.787420000	5.237050000
O	1.707977000	-7.387306000	11.276957000
H	0.753578000	-7.164890000	11.299852000
O	3.076622000	-5.050064000	11.175029000
H	3.807760000	-4.533277000	10.773671000
O	-2.917355000	-1.552024000	13.029376000
H	-3.544511000	-1.776132000	12.295179000
O	-1.814468000	-2.974244000	16.034977000
O	-0.645029000	-2.890714000	12.660703000
H	-1.327203000	-2.218419000	12.415867000
C	0.305075000	-1.426933000	14.378409000
H	0.393828000	-1.326962000	15.477396000
C	0.418372000	-3.957106000	14.513940000
C	2.525955000	-2.605394000	14.028866000
C	1.902243000	-3.827448000	14.255302000
C	2.029057000	-1.939810000	11.373837000
C	1.207419000	-1.790790000	10.077480000
C	1.669995000	-0.637339000	9.172518000
C	3.211008000	-0.621657000	9.031983000
C	3.826490000	-0.624979000	10.452055000
C	3.957033000	-2.528632000	13.957509000
C	2.677583000	-5.033887000	14.250470000
C	4.728819000	-3.712494000	13.938286000
C	4.073725000	-4.979177000	14.056129000
C	5.351999000	-0.558606000	10.450946000
C	6.178347000	-3.614169000	13.731626000
C	4.829985000	-6.213709000	13.915208000
C	6.972946000	-4.876407000	13.658168000
C	6.314802000	-6.130811000	13.810715000
C	8.393814000	-4.875512000	13.549701000
O	5.010225000	-3.961418000	9.403819000
H	4.476271000	-3.200141000	9.066528000
O	6.647683000	-3.676392000	7.281863000
H	7.567762000	-3.803852000	7.001533000
O	5.245315000	-9.528964000	9.078199000
H	4.398038000	-9.940034000	8.804402000
O	8.440629000	-7.576309000	8.191204000
H	7.796311000	-7.872508000	7.518706000
P	-0.901591000	-3.530267000	6.984125000
C	-2.418822000	-4.577637000	7.109990000
H	-2.179786000	-5.547622000	6.631628000
H	-3.165147000	-4.083811000	6.454126000
N	-2.959619000	-4.781178000	8.436759000
C	-4.046201000	-3.971095000	8.942919000
C	-3.733449000	-2.846652000	9.972172000
O	-2.831849000	-1.930887000	9.678806000
H	-2.259907000	-2.105272000	8.859377000
O	-4.377452000	-2.772380000	11.011310000
H	-4.558851000	-3.478931000	8.089393000
H	-4.800890000	-4.610046000	9.444417000
C	-2.523381000	-5.933311000	9.192699000
C	-1.562697000	-5.678240000	10.364039000
O	-1.520695000	-4.401500000	10.703262000
H	-0.995352000	-4.185350000	11.521105000
O	-0.967892000	-6.574559000	10.934550000

SiO_2-PMIDA-Dox salt 2, on P(O)OH PMIDA (continuation)

H	0.139279000	-1.687456000	10.324382000
H	1.338839000	0.330595000	9.591674000
H	3.537234000	0.290847000	8.488485000
H	3.425334000	0.252894000	11.003469000
H	5.724061000	-0.625325000	11.485651000
H	5.791521000	-1.391097000	9.876788000
H	5.697470000	0.396361000	10.013550000
H	0.941294000	0.142316000	7.331642000
H	4.011889000	-1.668044000	7.444630000
H	6.503823000	-8.273288000	14.003569000
H	10.198732000	-6.032213000	13.669700000
H	9.008821000	-8.228925000	13.985371000
H	9.420847000	-3.995286000	11.271194000
H	9.873004000	-2.405457000	12.000082000
H	8.141267000	-2.809279000	11.741748000
H	-2.039451000	-6.670763000	8.525559000
H	-3.395746000	-6.463114000	9.640683000
O	-0.420018000	-3.469342000	5.543096000
O	-1.189397000	-2.169789000	7.689718000
H	0.038042000	-1.253889000	7.820443000
O	0.237348000	-4.263453000	7.936274000
O	1.616281000	-1.007226000	12.345355000
O	3.425282000	-1.827997000	11.105618000
O	3.615673000	-1.796757000	8.336236000
O	4.509399000	-1.315040000	13.909022000
H	5.500547000	-1.462064000	13.834202000
O	2.011947000	-6.180697000	14.387982000
H	2.649548000	-6.923310000	14.200736000
O	6.729735000	-2.497808000	13.649043000
O	4.264923000	-7.332280000	13.893681000
O	9.142123000	-3.764383000	13.337391000
N	1.028615000	-0.764508000	7.807793000
H	1.590672000	-1.373001000	7.174214000
C	1.710845000	-1.345243000	13.764432000
H	2.235520000	-0.487484000	14.221719000
C	-0.427600000	-2.756223000	14.068624000
C	-1.785328000	-2.760794000	14.842398000
C	-3.084276000	-2.512028000	14.060041000
H	-3.852790000	-2.206605000	14.800034000
H	-3.399974000	-3.499823000	13.652203000
C	7.041439000	-7.327289000	13.901412000
C	9.104145000	-6.083318000	13.705167000
C	8.437673000	-7.298795000	13.880700000
C	9.131018000	-3.221003000	12.008010000
H	-0.295654000	-0.570797000	14.019794000
H	0.030970000	-4.874253000	14.035649000
H	0.273983000	-4.101231000	15.602882000
H	1.904963000	-2.974514000	11.723480000
H	1.314426000	-2.740276000	9.528261000

References

S1 A. M. Demin, A. I. Maksimovskikh, A. V. Mekhaev, D. K. Kuznetsov, A. S. Minin, A. G. Pershina, M. A. Uimin, V. Y. Shur and V. P. Krasnov, *Ceram. Int.*, 2021, **47**, 23078.

S2 A. M. Demin, A. V. Mekhaev, O. F. Kandarakov, V. I. Popenko, O. G. Leonova, A. M. Murzakaev, D. K. Kuznetsov, M. A. Uimin, A. S. Minin, V. Ya. Shur, A. V. and V. P. Krasnov, *Colloids Surf., B*, 2020, **190**, 110879.

S3 A. M. Demin, A. G. Pershina, A. S. Minin, A. V. Mekhaev, V. V. Ivanov, S. P. Lezhava, A. A. Zakharova, I. V. Byzov, M. A. Uimin, V. P. Krasnov and L. M. Ogorodova, *Langmuir*, 2018, **34**, 3449.

S4 A. M. Demin, A. V. Mekhaev, A. A. Esin, D. K. Kuznetsov, P. S. Zelenovskiy, V. Y. Shur and V. P. Krasnov, *Appl. Surf. Sci.*, 2018, **440**, 1196.

S5 A. M. Demin, A. V. Vakhrushev, M. S. Valova, A. S. Minin, D. K. Kuznetsov, M. A. Uimin, V. Ya. Shur, V. P. Krasnov and V. N. Charushin, *Russ. Chem. Bull.*, 2021, **70**, 987.

S6 M. Najafi, A. Morsali and M.R. Bozorgmehr, *Struct. Chem.*, 2019, **30**, 715.

S7 F. Neese, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2012, **2**, 73.

S8 A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 1372.

S9 F. Weigend and R. Ahlichs, *J. Phys. Chem. Chem. Phys.*, 2005, **7**, 3297.

S10 S. Grimme, A. Hansen, J. G. Brandenburg and C. Bannwarth, *Chem. Rev.*, 2016, **116**, 5105.

S11 H. Kruse and S. Grimme, *J. Chem. Phys.*, 2012, **126**, 154101.

S12 A. Pedretti, L. Villa and G. Vistoli, *J. Mol. Graph.*, 2002, **21**, 47.

S13 M. Kaviani and C. Di Valentin, *Nanoscale*, 2019, **33**, 15576.