Electronic Supplementary Material (ESI) for Dalton Transactions.
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Supporting materials

Table Cartesian coordinates of optimized structure of Type 1a – 3b (in unit of Å)

Type 1a (E = −975.256926 hartree)

Atomic Symbol	x	y	z
C	−5.011060	−0.412317	−0.209613
O(3)	−6.011798	−0.036255	−0.781216
C(2)	−4.161127	0.496373	0.664184
H	−4.462202	1.536814	0.531660
H	−4.350679	0.203198	1.708425
C(1)	−2.662317	0.318595	0.422116
O(2)	−2.241263	−0.880387	0.398331
O(1)	−1.985612	1.378481	0.273682
C	5.011060	0.412317	0.209613
O(6)	6.011798	0.036255	0.781216
C(4)	4.161127	−0.496373	−0.664184
H	4.350679	−0.203198	−1.708425
H	4.462202	−1.536814	−0.531660
C(3)	2.662317	−0.318595	−0.422116
O(4)	2.241263	0.880387	−0.398331
O(5)	1.985612	−1.378481	−0.273682
Ag(2)	−0.157075	−1.405778	0.080625
Ag(1)	0.157075	1.405778	−0.080625
H	−4.664865	−1.461259	−0.287449
H	4.664865	1.461259	0.287449

Type 1b (E = −975.2545361 hartree)

Atomic Symbol	x	y	z
C	−1.604991	4.699197	0.000000
O(6)	−2.579330	3.980921	0.000000
C(4)	−0.161273	4.227517	0.000000
H	0.327428	4.652354	0.886433
C(3)	−0.038742	2.707133	0.000000
O(4)	0.000000	2.152999	1.139126
O(5)	0.000000	2.152999	1.139126
C	1.604991	4.699197	0.000000
O(3)	2.579330	3.980921	0.000000
C(2)	0.161273	4.227517	0.000000
H	−0.327428	4.652354	0.886433
C(1)	0.038742	2.707133	0.000000
O(2)	0.000000	2.152999	1.139126
O(1)	0.000000	2.152999	1.139126
Ag(1)	0.000000	0.000000	1.415649
Ag(2)	0.000000	0.000000	1.415649
H	−1.719036	5.804918	0.000000
H	1.719036	5.804918	0.000000
H	−0.327428	4.652354	0.886433
H	0.327428	4.652354	0.886433

Type 2 (E = −975.2480072 hartree)			
Atomic Symbol	x	y	z
Ag(1)	−0.138546	1.724453	0.095754
Ag(2)	−0.368066	−1.207268	−0.431589
O(5)	−2.196226	0.045359	−1.152322
C(3)	−2.725816	0.529287	−0.113268
O(4)	−2.278556	1.501668	0.571666
C(4)	−3.940448	−0.209990	0.437172
O(2)	1.832290	−0.961278	−0.362503
C(1)	2.457473	0.139350	−0.291062
O(1)	1.973651	1.301366	−0.150342
C(2)	3.983331	0.052062	−0.391103
H	4.451284	1.015522	−0.181938
H	4.216216	−0.236455	−1.427891
C	4.570144	−1.022971	0.506856
H	−4.679674	−0.391499	−0.356515
H	−4.443452	0.344912	1.238713
C	−3.536475	−1.568296	0.976800
O(3)	5.569485	−0.860643	1.175216
O(6)	−2.434425	−2.082297	0.887226
H	4.029174	−1.989261	0.510161
H	−4.341812	−2.120988	1.497837

Type 3a (E = −975.2399128 hartree)

Atomic Symbol	x	y	z
C	−0.076686	3.750626	1.104416
O(6)	0.945880	3.088851	1.084661
C(4)	−1.391907	3.404217	0.438145
H	−2.196108	3.543843	1.171267
H	−1.543885	4.150086	−0.356610
C(3)	−1.394659	1.996422	−0.155742
O(4)	−0.580010	1.779269	−1.098892
O(5)	−2.163537	1.141174	0.375285
C	0.076686	−3.750626	1.104416
O(3)	−0.945880	−3.088851	1.084661
C(2)	1.391907	−3.404217	0.438145
H	2.196108	−3.543843	1.171267
H	1.543885	−4.150086	−0.356610
C(1)	1.394659	−1.996422	−0.155742
O(1)	2.163537	−1.141174	0.375285
O(2)	0.580010	−1.779269	−1.098892
Ag(1)	1.394659	0.879267	−0.291110
Ag(2)	−1.394659	−0.879267	−0.291110
H	−0.081034	4.710866	1.658180
H	0.081034	−4.710866	1.658180

Type 3b (E = −975.2426494 hartree)

Atomic Symbol	x	y	z
C	−3.839857	0.244079	0.387713
O(6)	−3.273773	−0.823133	0.568836
C(4)	−3.265328	1.506421	−0.206983
H	−3.761763	1.631852	−1.182511
H	−3.586016	2.349325	0.417987
C(3)	−1.746341	1.496215	−0.405130
O(4)	−1.270696	0.608162	−1.166358
O(5)	−1.073611	2.357903	0.232823
C	3.839857	−0.244079	−0.387713
O(3)	3.273773	0.823133	−0.568836
C(2)	3.265328	−1.506421	0.206983
H	3.586016	−2.349325	−0.417987
H	3.761763	−1.631852	1.182511
C(1)	1.746341	−1.496215	0.405130
O(1)	1.073611	−2.357903	−0.232823
O(2)	1.270696	−0.608162	1.166358
Ag(1)	−1.036889	−1.513193	−0.004783
Ag(2)	1.036889	1.513193	0.004783
H	−4.904063	0.322450	0.684165
H	4.904063	−0.322450	−0.684165