Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information

Theoretical study on the formation of iodine oxides aggregates and monohydrates.

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Table S1. Components for CCSD(T)//MP2/aug-cc-pVTZ level of theory of the Atomization Energies (kJ mol^{-1}).

Molecule	**ΔE_{ele}**	**ΔE_{ZPE}**	**ΔE_{SO}**	**ΣD_0 (0 K)** [a]
IO	232.22	3.85	-13.86	214.51
OIO	491.37	11.93	-22.71	456.72
IOI	381.38	7.35	-34.60	339.44
IIO	327.88	7.50	-40.03	280.35
IIO_2	595.84	16.34	-42.17	537.32
IOIO	581.18	14.13	-36.10	530.96
IOOI	557.98	14.64	-36.17	507.17
OIIO	474.77	13.71	-38.19	422.87
I_2O_3	892.70	23.35	-39.54	829.81
I_2O_4	1086.40	29.72	-40.94	1015.74
I_2O_5	1386.18	38.79	-44.80	1302.59
$I_2O_3\cdots IO$	1142.47	29.06	-61.38	1052.03
$I_2O_3\cdots OIO$	1411.95	45.63	-64.86	1301.46
$I_2O_4\cdots IO$	1384.68	37.65	-62.11	1284.91
$I_2O_4\cdots OIO$	1655.08	45.03	-65.08	1544.97
$I_2O_5\cdots OIO$	1918.68	60.33	-67.97	1790.38
$I_2O_3\cdots I_2O_3$	1845.47	48.91	-78.29	1718.27
$I_2O_4\cdots I_2O_4$	2320.17	65.47	-80.67	2174.02
$I_2O_5\cdots I_2O_5$ [b]	2863.59	78.26	-88.93	2696.40
$I_2O_3\cdots I_2O_4$ [b]	2062.29	54.07	-79.58	1928.64
$I_2O_3\cdots I_2O_5$	2367.35	65.03	-83.61	2218.72
$I_2O_4\cdots I_2O_5$ [b]	2583.06	69.07	-85.31	2428.67

[a] Total Atomization Energy at 0 K: ΣD_0 (0 K) = ΔE_{ele} - ΔE_{ZPE} + ΔE_{SO}.

[b] Optimized geometries and ZPE corrections calculated at B3LYP level.

Table S2. Dimerisation energy $\Delta E_{dim} = (E_{complex} - E_{monomers})$ calculated at the B3LYP/aug-cc-pVTZ level of theory for dimer structures of iodine oxides. Zero point energy correction included (values in kJ mol^{-1}).

Complex	Structure [a]	ΔE_r
$(I_2O_3)_2$	**C1**	-38
$(I_2O_4)_2$	**C1**	-109
	C2	-58
	C3	-38
$(I_2O_5)_2$	**C1**	-63
$I_2O_3 \cdots I_2O_4$	**C1**	-58
	C2	-33
	C3	-25
$I_2O_3 \cdots I_2O_5$	**C1**	-58
	C2	-46
	C3	-38
$I_2O_4 \cdots I_2O_5$	**C1**	-67
	C2	-58
	C3	-58
	C4	-54
	C5	-54
	C6	-46

[a] Structure labeling refers to Figures S1 and S2

Table S3. Bond lengths (r_e) and topological descriptors of critical points of the electron density in the lowest lying structure of the I_2O_4 dimer.

BCP [a]	Bond	r_e [b]	ρ_C [c]	$\nabla^2\rho_C$	ε	G_C	V_C	H_C
1	I1O1	1.965	0.1380	0.2534	0.0914	0.1386	-0.2139	-0.0753
10	I4O6	1.965	0.1379	0.2532	0.0914	0.1385	-0.2138	-0.0753
2	I2O1	2.016	0.1230	0.2129	0.1346	0.1160	-0.1788	-0.0628
9	I3O6	2.015	0.1230	0.2129	0.1347	0.1160	-0.1788	-0.0628
4	I1O3	1.761	0.2073	0.7490	0.0309	0.3256	-0.4640	-0.1384
12	I4O8	1.760	0.2073	0.7490	0.0309	0.3256	-0.4640	-0.1384
5	I1O4	1.753	0.2102	0.7771	0.0315	0.3354	-0.4766	-0.1412
11	I4O7	1.754	0.2102	0.7771	0.0315	0.3354	-0.4766	-0.1412
3	I2O2	1.930	0.1498	0.2754	0.2030	0.1549	-0.2409	-0.0860
8	I3O5	1.929	0.1498	0.2753	0.2031	0.1548	-0.2408	-0.0860
6	I2···O5	2.130	0.1020	0.1279	0.2070	0.0801	-0.1282	-0.0481
7	I3···O2	2.130	0.1020	0.1279	0.2070	0.0801	-0.1282	-0.0481
RCP	-	-	0.0415	0.1750	-	0.0443	-0.0447	-0.0004

[a] BCP are bond critical points, RCP is the ring critical point. BCP and atom numbering refer to Fig. 8. [b] r_e is given in Å. [c] The topological descriptors (in a.u.) are the following variables at the critical points: electron density ρ_C, Laplacian of the electron density $\nabla^2\rho_C$, ellipticity ε, kinetic energy density G_C, potential energy density V_C, and total energy density $H_C = G_C + V_C$.

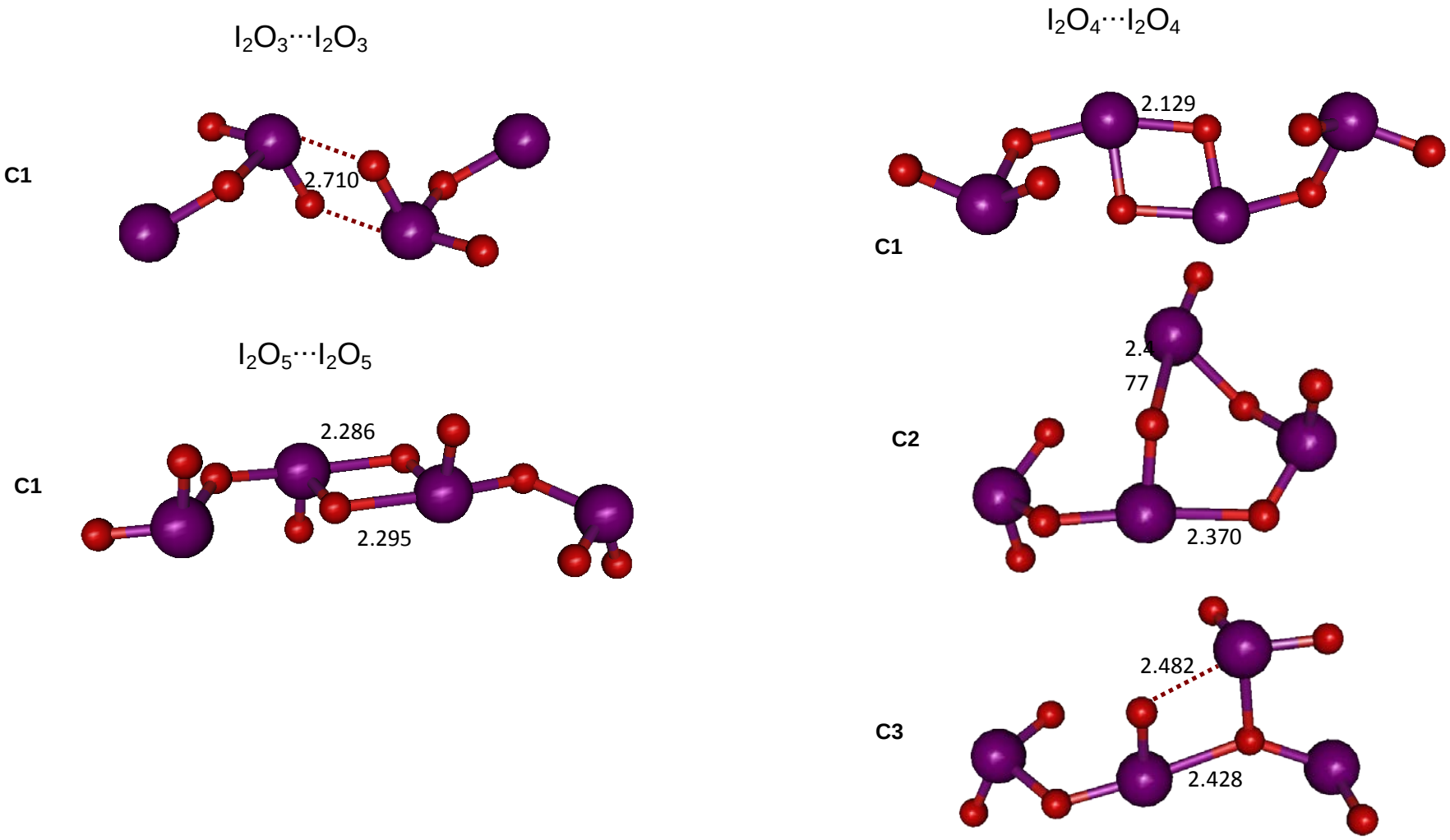

Figure S1. MP2 optimized geometries of several structures of homodimers of I_2O_y (y = 3-5) iodine oxides. C1 denotes the lowest-lying structure in all cases. Bond distances in Å.

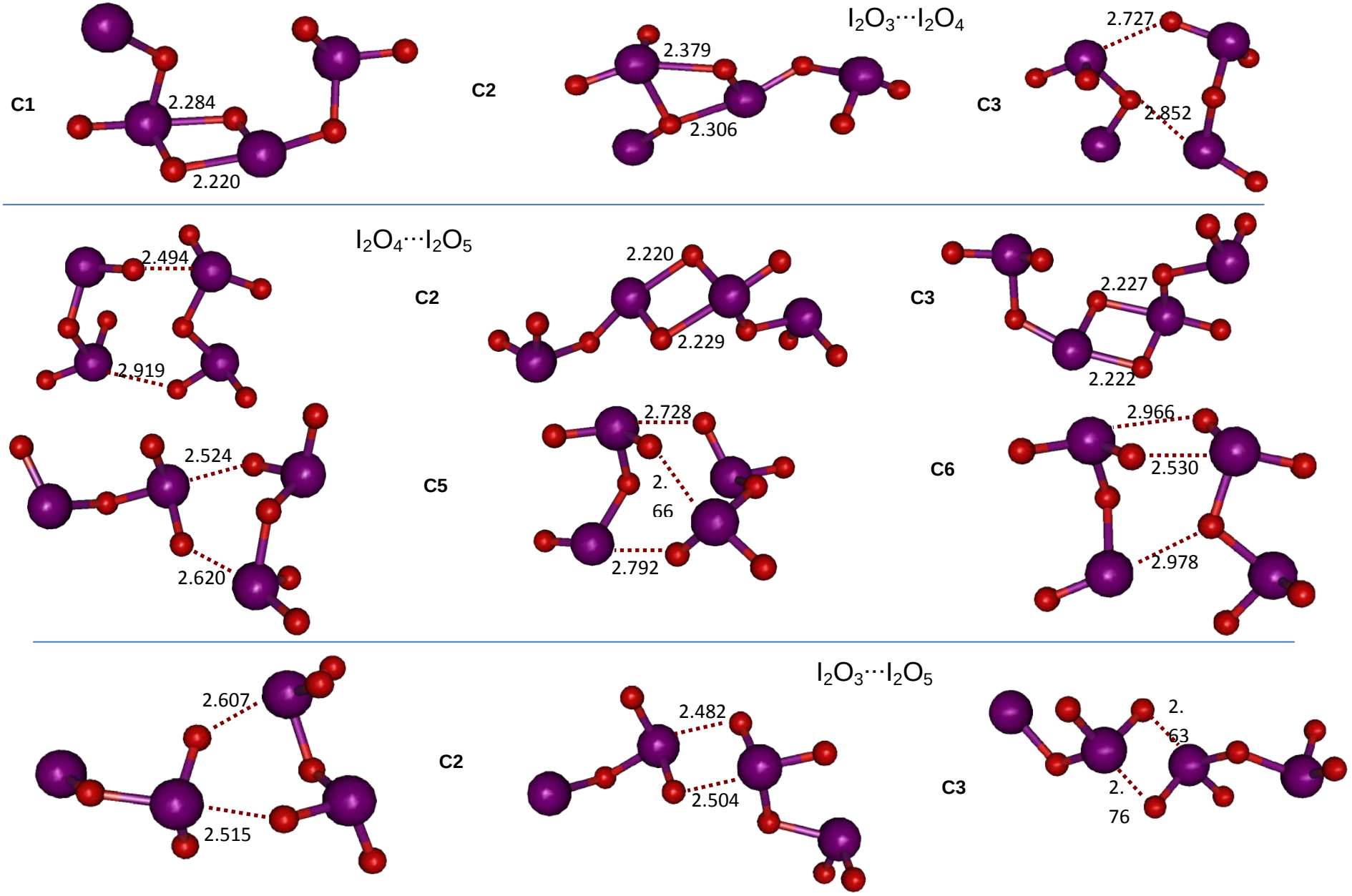

Figure S2. MP2 optimized geometries of several structures of heterodimers of I_2O_y (y = 3-5) iodine oxides. C1 denotes the lowest-lying structure in all cases. Bond distances in Å.

Table S3. Atomic coordinates (Å) of all species shown in Figure S1 and S2.

C1- I_2O_3···I_2O_3

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	-4.122068	-0.578990	-0.068894
2	8	-2.390575	-0.278766	0.882869
3	53	-1.299600	1.211924	0.189245
4	8	-2.550493	2.271180	-0.444287
5	8	-0.586379	0.427000	-1.237491
6	53	1.299557	-1.211861	-0.189218
7	8	0.586437	-0.426893	1.237544
8	8	2.550397	-2.271212	0.444260
9	8	2.390606	0.278752	-0.882893
10	53	4.122112	0.578917	0.068867

C1- I_2O_4···I_2O_4

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	3.770821	0.383966	0.601048
2	8	3.070648	-0.768959	-0.827554
3	53	1.075050	-1.048947	-0.842872
4	8	1.001683	0.877687	-0.909298
5	8	2.600896	0.036004	1.869648
6	8	5.265178	-0.473011	0.927537
7	8	-1.002596	-0.649372	-1.082841
8	53	-1.075826	1.213074	-0.584804
9	8	-3.071366	0.936306	-0.632091
10	53	-3.769748	-0.510537	0.499182
11	8	-5.265652	0.248319	1.009595
12	8	-2.600763	-0.455780	1.814332

C2- I_2O_4···I_2O_4

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	-2.881023	-0.995288	0.464452
2	8	-1.918933	0.486007	1.090732
3	53	-1.133943	2.006332	-0.267918
4	8	-2.038401	3.425783	0.401140
5	8	-3.464450	-0.542094	-1.123116
6	8	-1.538491	-2.189094	0.240958

7	8	-0.215451	-0.061605	-1.274966
8	53	0.614303	-1.422317	-0.386123
9	8	2.509437	-0.997565	-0.972028
10	53	3.491334	0.283179	0.121186
11	8	3.868471	-0.672446	1.545227
12	8	2.197120	1.399635	0.545226

C3- I_2O_4···I_2O_4

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	-1.805364	1.791876	-0.228148
2	8	-1.564961	-0.337898	0.089138
3	53	-3.201702	-1.376351	0.479924
4	8	-3.735319	-2.003073	-1.108953
5	8	-3.564629	1.674032	-0.018664
6	8	-1.150835	2.327814	1.309958
7	8	0.414349	0.998209	-1.004311
8	53	0.784712	-0.697254	-0.404747
9	8	2.658225	-0.749606	-1.026610
10	53	4.043918	0.116973	0.121347
11	8	5.070005	-1.269597	0.432697
12	8	3.055308	0.451626	1.536253

C1- I_2O_5···I_2O_5

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	4.659756	-0.431513	-0.070705
2	8	3.141455	0.693297	0.370346
3	53	1.274247	-0.080668	0.200563
4	8	1.247922	-0.893820	1.749086
5	8	3.716652	-1.816554	-0.658755
6	8	5.338014	0.408018	-1.459770
7	8	0.660519	1.621767	0.525235
8	8	-0.994223	-0.260016	-0.096306
9	53	-1.600605	1.463157	0.226415
10	8	-1.571894	2.247675	-1.338061
11	8	-3.444799	0.807644	0.202845
12	53	-4.080446	-1.010423	-0.334369
13	8	-4.013981	-1.834907	1.219305
14	8	-5.755473	-0.579274	-0.659037

C1- I_2O_3···I_2O_4

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	3.037319	0.862321	-0.511049
2	8	2.872976	-0.825349	0.506548
3	53	0.981424	-1.319456	0.932485
4	8	0.556253	-1.001694	-0.876907
5	8	1.915537	1.870012	0.394125
6	8	4.683995	1.247756	-0.046039
7	8	-1.178563	-1.816792	0.816120
8	53	-1.722393	-1.147803	-0.814910
9	8	-3.466281	-1.189539	-0.543700
10	8	-1.404861	0.763872	-0.456330
11	53	-2.896962	1.748596	0.424596

C2- $I_2O_3\cdots I_2O_4$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	2.965371	-1.724797	-0.047459
2	8	1.559565	-0.442449	-0.619526
3	53	2.041596	1.685157	-0.118387
4	8	3.766252	1.413481	-0.443587
5	8	1.870698	1.545625	1.627504
6	53	-0.575454	-0.477557	0.250455
7	8	-0.285721	1.249683	-0.354524
8	8	-2.332988	-0.054601	1.080209
9	53	-3.895390	0.175310	-0.113019
10	8	-4.947067	-1.074507	0.523580
11	8	-3.182554	-0.372228	-1.625443

C3- $I_2O_3\cdots I_2O_4$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	2.423415	1.394989	-0.597623
2	8	0.959449	0.050732	-0.475516
3	53	1.529015	-1.764190	0.306076
4	8	1.021028	-1.525457	1.968506
5	8	3.272707	-1.506641	0.229536
6	53	-1.039838	1.851254	0.469910
7	8	-2.311341	3.068696	0.806104
8	8	-1.953989	0.067786	1.004481
9	53	-2.509222	-1.161161	-0.362682
10	8	-1.039566	-2.143043	-0.528283
11	8	-2.620609	-0.137982	-1.783713

C1- I_2O_4···I_2O_5

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	-1.828451	1.681512	-0.040590
2	8	-0.935537	-0.078868	-0.332453
3	53	-2.050133	-1.674567	0.093652
4	8	-2.838197	-1.953140	-1.451616
5	8	-3.342788	0.830560	0.393113
6	8	-1.151973	2.194730	1.503023
7	8	-0.635768	-2.754740	0.129994
8	53	1.947875	1.920025	-0.053905
9	8	0.402657	2.282317	-0.978973
10	8	2.521149	0.263272	-0.852950
11	53	2.026240	-1.563611	-0.003714
12	8	1.700507	-0.939960	1.613529
13	8	3.647048	-2.251426	0.006517

C2- I_2O_4···I_2O_5

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	-1.499088	1.342171	-0.304516
2	8	-2.146646	-0.477460	-0.373588
3	53	-4.110670	-0.832369	0.053048
4	8	-4.796728	-0.616254	-1.552880
5	8	-3.058170	2.031545	0.200460
6	8	-0.635531	1.302202	1.299250
7	8	-3.915802	-2.558009	0.342923
8	53	1.352138	0.091248	0.892099
9	8	0.609912	0.308016	-0.804255
10	8	2.798261	-1.131386	0.274181
11	53	4.454271	-0.473847	-0.577269
12	8	5.645003	-0.970377	0.623800
13	8	4.196891	1.269009	-0.429659

C3- I_2O_4···I_2O_5

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	-1.697564	-1.448322	0.438328
2	8	-1.808693	0.473034	0.275481
3	53	-3.596298	1.297062	-0.269427

4	8	-4.388307	1.328396	1.301950
5	8	-3.345717	-1.744686	-0.157551
6	8	-0.738301	-1.840094	-1.057675
7	8	-2.958341	2.904112	-0.596574
8	53	1.499782	-1.235323	-0.539272
9	8	0.593239	-0.994317	1.071900
10	8	3.280764	-0.786879	0.219689
11	53	3.950574	1.069381	0.382291
12	8	2.824458	1.884275	-0.708652
13	8	5.504128	0.877618	-0.427546

C4- $I_2O_4\cdots I_2O_5$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	2.345892	1.829067	-0.089665
2	8	2.676683	0.075343	-0.996529
3	53	2.831543	-1.536404	0.103501
4	8	1.114597	-1.812788	0.503786
5	8	2.536665	1.164546	1.544339
6	8	3.857953	2.640558	-0.477534
7	8	3.241588	-2.659400	-1.181233
8	53	-1.168559	-0.489785	0.363211
9	8	-0.246370	0.981576	-0.045157
10	8	-1.672903	-1.195354	-1.167435
11	8	-2.855573	0.423838	0.856460
12	53	-4.496850	0.408923	-0.280034
13	8	-5.419811	-1.021496	0.320584

C5- $I_2O_4\cdots I_2O_5$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	-1.124037	-2.034657	0.136746
2	8	-1.150155	-0.065163	0.197168
3	53	-2.834555	0.950438	-0.151649
4	8	-3.591089	0.879124	1.433871
5	8	-2.801448	-2.175396	-0.424607
6	8	-0.116851	-2.301925	-1.292280
7	8	-1.984445	2.494546	-0.288524
8	53	2.571559	-1.168730	-0.093365
9	8	1.267400	-1.368247	1.120050
10	8	4.004782	-0.777069	0.847027
11	8	2.065109	0.502721	-0.924999
12	53	1.321069	2.183652	-0.019784
13	8	2.743715	3.270506	0.180642

C6- I_2O_4···I_2O_5

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	-1.742394	-1.650448	0.030426
2	8	-1.645821	0.273445	0.297784
3	53	-3.230925	1.451373	-0.133133
4	8	-4.144651	1.272134	1.360118
5	8	-3.350851	-1.665448	-0.713795
6	8	-0.598330	-1.846549	-1.312977
7	8	-2.352696	2.975448	-0.063860
8	53	2.009720	-1.542583	-0.027949
9	8	0.759468	-1.588502	1.245039
10	8	3.550043	-1.533733	0.830210
11	8	1.892609	0.354499	-0.544311
12	53	3.177919	1.736916	0.134253
13	8	4.470356	1.790126	-1.122036

C1- I_2O_3···I_2O_5

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	1.865022	1.926420	-0.038199
2	8	2.366840	0.248463	-1.010280
3	53	2.794338	-1.344852	0.039643
4	8	1.151728	-1.868814	0.500610
5	8	2.232681	1.255671	1.563020
6	8	3.239722	2.930447	-0.482876
7	8	3.302744	-2.373414	-1.288643
8	53	-1.287142	-0.860775	0.411051
9	8	-0.577030	0.747850	0.102970
10	8	-1.644887	-1.531311	-1.173102
11	8	-3.075697	-0.309671	0.987770
12	53	-4.428233	0.415174	-0.291660

C2- I_2O_3···I_2O_5

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	-1.365940	1.168606	-0.579024
2	8	-2.070999	-0.572958	-0.114916
3	53	-4.066788	-0.809117	0.199913
4	8	-4.585295	-1.117288	-1.452447

5	8	-2.912305	2.030430	-0.506011
6	8	-0.561319	1.588421	0.961806
7	8	-3.937647	-2.349912	1.039877
8	53	1.815435	0.439961	0.842958
9	8	1.006739	-0.107989	-0.658146
10	8	2.643218	1.930308	0.410604
11	8	3.294837	-0.829592	0.880103
12	53	4.692429	-0.885702	-0.548507

C3- I_2O_3···I_2O_5

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	1.083494	-1.147848	0.170898
2	8	2.194135	0.375113	-0.312457
3	53	4.203070	0.276977	-0.085713
4	8	4.633828	-0.508986	-1.600183
5	8	2.398784	-2.148204	0.813463
6	8	0.253159	-0.485229	1.592317
7	8	4.493671	2.004884	-0.253751
8	53	-1.815267	1.239584	0.398039
9	8	-0.929932	0.421429	-0.916296
10	8	-2.808792	2.450511	-0.404688
11	8	-3.141039	-0.117941	0.868170
12	53	-4.542062	-0.669329	-0.451010

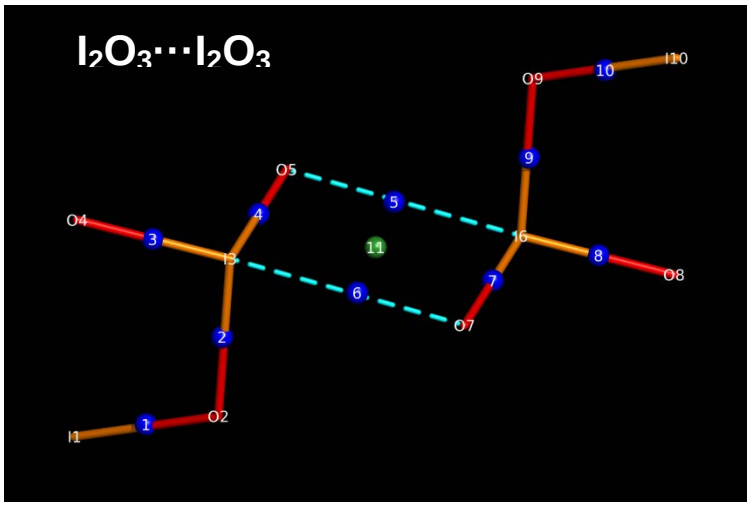

Table S4. Bond distances (*Dist*) and topological descriptors of critical points of the electron density in the lowest-lying structure of the $(I_2O_3)_2$ dimer

BCP	Bond	*Dist*	*Rho*	*Lap*	*Ellip*	*Kin*	*Pot*	*Tot*
1	I1O2	1.998	0.1232	0.2340	0.0051	0.1191	-0.1797	-0.0606
2	I3O2	1.974	0.1371	0.2321	0.0853	0.1331	-0.2082	-0.0751
3	I3O4	1.756	0.2086	0.7637	0.0401	0.3307	-0.4704	-0.1398
4	I3O5	1.777	0.2006	0.6793	0.0466	0.3017	-0.4336	-0.1319
5	I6··O5	2.710	0.0319	0.0843	0.1274	0.0235	-0.0259	-0.0024
6	I3··O7	2.710	0.0319	0.0843	0.1274	0.0235	-0.0259	-0.0024
7	I6O7	1.778	0.2006	0.6793	0.0466	0.3017	-0.4336	-0.1319
8	I6O8	1.756	0.2086	0.7637	0.0401	0.3307	-0.4704	-0.1398
9	I6O9	1.974	0.1371	0.2321	0.0853	0.1331	-0.2082	-0.0751
10	I10O9	1.998	0.1232	0.2340	0.0051	0.1191	-0.1797	-0.0606
RCP								
11	ring[1]		0.0208	0.0825		0.0182	-0.0157	0.0024
	ring[1] = [I6-O7-I3-O5-I6]							

Electron density obtained in MP2/TZVPP all-electron calculations. BCP are bond critical points, RCP is the ring critical point. BCP, RCP, and atom numbering refers to the scheme displayed above. *Dist* is given in Å. The topological descriptors are the following values (in a.u.) at the critical points: electron density *Rho*, Laplacian of the electron density *Lap*, ellipticity *Ellip*, kinetic energy density *Kin*, potential energy density *Pot*, and total energy density *Tot* = *Kin* + *Pot*

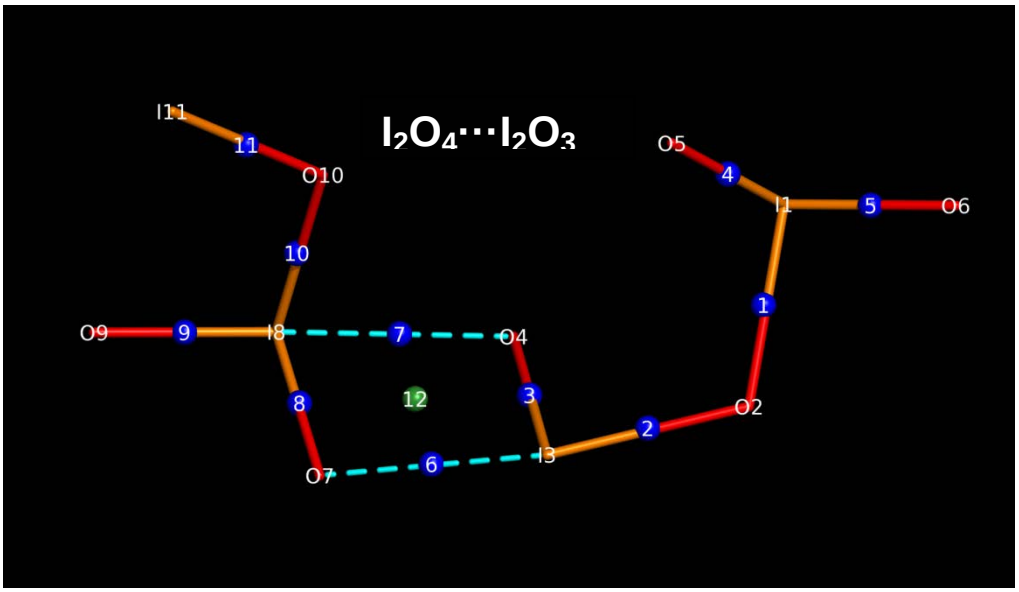

Table S5. Bond distances (*Dist*) and topological descriptors of critical points of the electron density in the lowest-lying structure of the ($I_2O_4\cdots I_2O_3$) dimer

BCP	Bond	*Dist*	*Rho*	*Lap*	*Ellip*	*Kin*	*Pot*	*Tot*
1	I1O2	1.977	0.1346	0.2367	0.0951	0.1319	-0.2046	-0.0727
2	I3O2	2.001	0.1271	0.2223	0.1407	0.1220	-0.1884	-0.0664
3	I3O4	1.885	0.1629	0.3418	0.1447	0.1825	-0.2796	-0.0971
4	I1O5	1.758	0.2079	0.7579	0.0311	0.3283	-0.4671	-0.1388
5	I1O6	1.754	0.2099	0.7751	0.0329	0.3347	-0.4756	-0.1409
6	I3··O7	2.366	0.0831	0.1182	0.0619	0.0627	-0.0758	-0.0131
7	I8··O4	2.515	0.0776	0.1040	0.0541	0.0549	-0.0638	-0.0089
8	I8O7	1.845	0.1764	0.4728	0.1238	0.2273	-0.3364	-0.1091
9	I8O9	1.765	0.2054	0.7522	0.0395	0.3246	-0.4611	-0.1365
10	I8O10	1.971	0.1385	0.2240	0.1327	0.1327	-0.2095	-0.0767
11	I11O10	1.993	0.1247	0.2425	0.0087	0.1224	-0.1841	-0.0618
RCP								
12	ring[1]		0.0383	0.1619		0.0401	-0.0398	0.0003
	ring[1] = [I3-O4-I8-O7-I3]							

Electron density obtained in MP2/TZVPP all-electron calculations. BCP are bond critical points, RCP is the ring critical point. BCP, RCP, and atom numbering refers to the scheme displayed above. *Dist* is given in Å. The topological descriptors are the following values (in a.u.) at the critical points: electron density *Rho*, Laplacian of the electron density *Lap*, ellipticity *Ellip*, kinetic energy density *Kin*, potential energy density *Pot*, and total energy density *Tot* = *Kin* + *Pot*

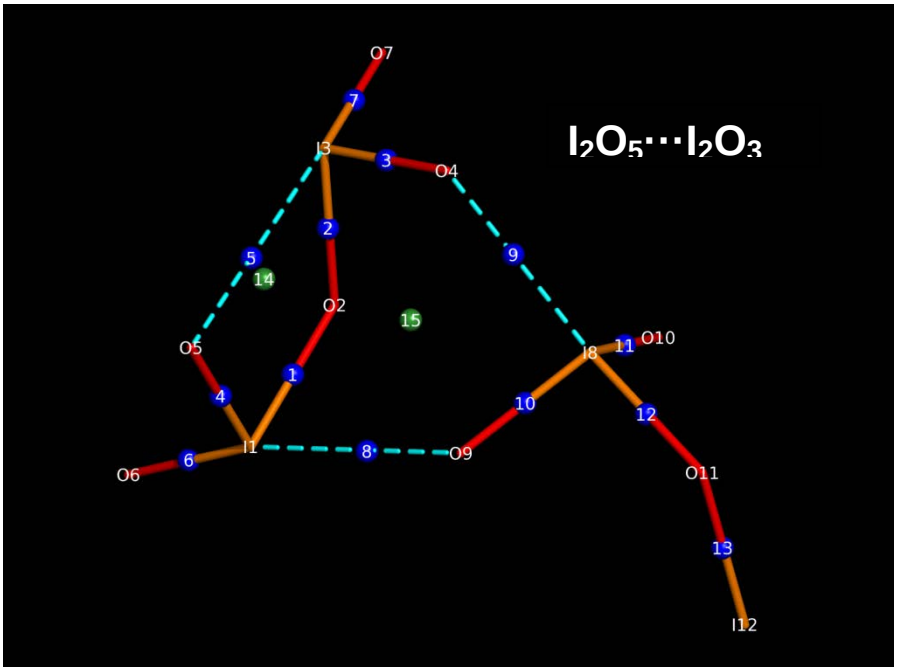

Table S6. Bond distances (*Dist*) and topological descriptors of critical points of the electron density in the lowest-lying structure of the ($I_2O_5\cdots I_2O_3$) dimer

BCP	Bond	*Dist*	*Rho*	*Lap*	*Ellip*	*Kin*	*Pot*	*Tot*
1	I1O2	2.015	0.1258	0.1936	0.0650	0.1147	-0.1810	-0.0663
2	I3O2	1.958	0.1397	0.2554	0.0728	0.1408	-0.2178	-0.0770
3	I3O4	1.786	0.1964	0.6591	0.0084	0.2915	-0.4183	-0.1268
4	I1O5	1.773	0.2030	0.6937	0.0213	0.3081	-0.4427	-0.1346
5	I3··O5	2.862	0.0241	0.0742	0.5254	0.0184	-0.0183	0.0001
6	I1O6	1.757	0.2084	0.7906	0.0474	0.3363	-0.4749	-0.1386
7	I3O7	1.748	0.2126	0.7909	0.0295	0.3418	-0.4858	-0.1440
8	I1··O9	2.607	0.0368	0.1016	0.0488	0.0286	-0.0317	-0.0032
9	I8··O4	2.515	0.0435	0.1026	0.0379	0.0319	-0.0381	-0.0062
10	I8O9	1.781	0.1985	0.6623	0.0187	0.2950	-0.4245	-0.1295
11	I8O10	1.748	0.2128	0.7827	0.0324	0.3401	-0.4846	-0.1445
12	I8O11	1.961	0.1390	0.2613	0.0506	0.1417	-0.2180	-0.0764
13	I12O11	1.998	0.1233	0.2340	0.0013	0.1190	-0.1795	-0.0605
RCP								
14	ring[1]		0.0229	0.0852		0.0197	-0.0180	0.0016
15	ring[2]		0.0070	0.0281		0.0055	-0.0040	0.0015
	ring[1] = [I1-O2-I3-O5-I1]							
	ring[2] = [I1-O9-I8-O4-I3-O2-I1]							

Electron density obtained in MP2/TZVPP all-electron calculations. BCP are bond critical points, RCP are ring critical points. BCP, RCP, and atom numbering refers to the scheme displayed above. *Dist* is given in Å. The topological descriptors are the following values (in a.u.) at the critical points: electron density *Rho*, Laplacian of the electron density *Lap*, ellipticity *Ellip*, kinetic energy density *Kin*, potential energy density *Pot*, and total energy density *Tot* = *Kin* + *Pot*

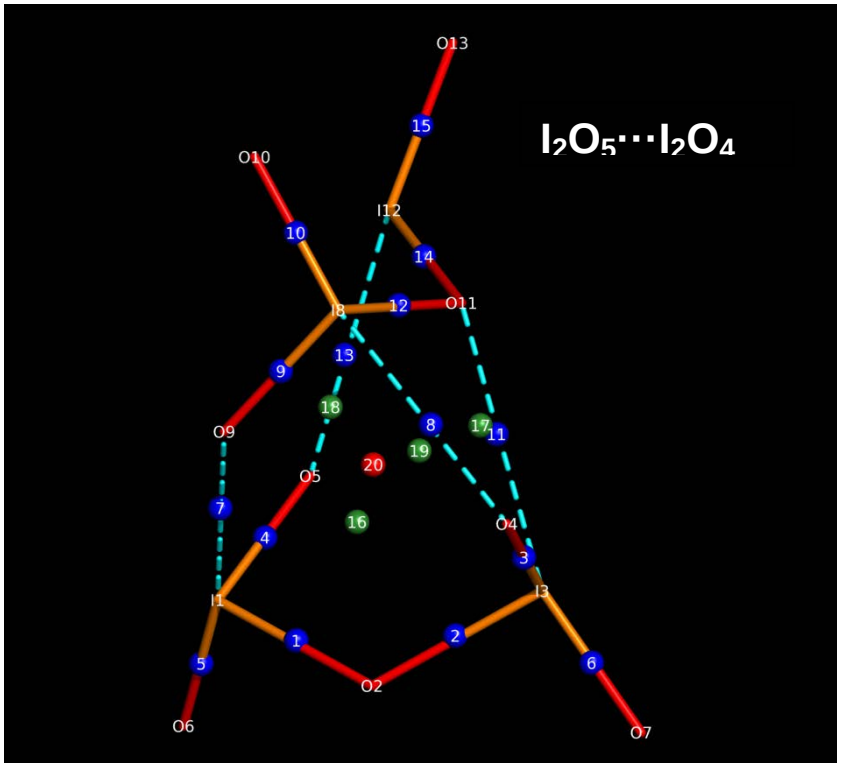

Table S7. Bond distances (*Dist*) and topological descriptors of critical points of the electron density in the lowest-lying structure of the ($I_2O_5\cdots I_2O_4$) dimer

BCP	Bond	*Dist*	*Rho*	*Lap*	*Ellip*	*Kin*	*Pot*	*Tot*
1	I1O2	1.984	0.1313	0.2353	0.0719	0.1282	-0.1975	-0.0693
2	I3O2	1.977	0.1323	0.2431	0.0425	0.1305	-0.2003	-0.0697
3	I3O4	1.774	0.2021	0.7033	0.0384	0.3087	-0.4415	-0.1329
4	I1O5	1.776	0.2006	0.6835	0.0321	0.3025	-0.4340	-0.1316
5	I1O6	1.752	0.2106	0.7968	0.0401	0.3406	-0.4819	-0.1414
6	I3O7	1.747	0.2126	0.7927	0.0340	0.3420	-0.4859	-0.1438
7	I1··O9	2.494	0.0331	0.0945	0.0276	0.0257	-0.0279	-0.0021
8	I8··O4	2.728	0.0298	0.0821	0.0618	0.0222	-0.0238	-0.0016
9	I8O9	1.780	0.1988	0.6692	0.0284	0.2969	-0.4265	-0.1296
10	I8O10	1.756	0.2093	0.7698	0.0356	0.3329	-0.4733	-0.1404
11	I3··O11	2.919	0.0180	0.0589	0.3515	0.0139	-0.0131	0.0008
12	I8O11	1.965	0.1398	0.2355	0.0506	0.1365	-0.2140	-0.0776
13	I12··O5	2.792	0.0238	0.0791	0.2102	0.0196	-0.0193	0.0002
14	I12O11	2.070	0.1090	0.1746	0.1630	0.0937	-0.1438	-0.0501
15	I12O13	1.792	0.1911	0.6394	0.0599	0.2789	-0.3979	-0.1190
RCP								
16	ring[1]		0.0069	0.0253		0.0051	-0.0038	0.0013
17	ring[2]		0.0159	0.0687		0.0145	-0.0119	0.0026
18	ring[3]		0.0065	0.0248		0.0050	-0.0037	0.0012
19	ring[4]		0.0063	0.0228		0.0046	-0.0035	0.0011
	ring[1] = [I1-O9-I8-O4-I3-O2-I1],				ring[2] = [I3-O4-I8-O11-I3]			
	ring[3] = [I1-O5-I12-O11-I8-O9-I1],				ring[4] = [I1-O2-I3-O11-I12-O5-I1]			
CCP								
20			0.0052	0.0187		0.0038	-0.0029	0.0009

Electron density obtained in MP2/TZVPP all-electron calculations. BCP are bond critical points, RCPs are ring critical points, CCP is the cage critical point. BCP, RCP, CCP and atom numbering refers to the scheme displayed above. *Dist* is given in Å. The topological descriptors are the following values (in a.u.) at the critical points: electron density *Rho*, Laplacian of the electron density *Lap*, ellipticity *Ellip*, kinetic energy density *Kin*, potential energy density *Pot*, and total energy density *Tot* = *Kin* + *Pot*