

Supporting Information for:

Shedding light on the Bonding Situation of Triangular and Square Heterometallic Clusters: A Computational Insight

Daniel F. Coimbra, Alexandre O. Ortolan, Renato P. Orenha, Vanessa B. da
Silva, Renato L. T. Parreira, and Giovanni F. Caramori

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Table S1. Geometrical parameters for complexes **1a-3e**.

	Bond Lengths (Å)											
	M1-M2	M2-M3	M3-M4	My-M1	M1-Mo _a	M1-Mo _b	M2-Mo _a	M2-Mo _b	M3-Mo _a	M3-Mo _b	M4-Mo _a	M4-Mo _b
1a	2.576	2.537		2.675	2.64	2.634	2.624	2.660	2.618	2.648		
1b	2.515	2.529		2.517	2.638	2.626	2.637	2.626	2.647	2.634		
2a	2.870	2.989		2.859	2.866	2.784	2.817	2.830	2.844	2.866		
2b	2.868	2.881		2.869	2.798	2.872	2.793	2.862	2.792	2.861		
3a	3.011	2.890		3.142	2.800	2.770	2.787	2.807	2.779	2.826		
3b	2.914	2.947		2.907	2.837	2.770	2.829	2.767	2.840	2.770		
1c	2.504	2.509	2.569	2.564	2.636	2.594	2.669	2.677	2.597	2.641	2.632	2.635
1d	2.484	2.484	2.484	2.484	2.719	2.719	2.645	2.645	2.720	2.720	2.645	2.645
1e	2.541	2.564	2.559	2.548	2.640	2.635	2.626	2.627	2.628	2.623	2.645	2.637
2c	2.783	2.787	2.845	2.864	2.848	2.769	2.873	2.880	2.773	2.845	2.848	2.853
2d	2.796	2.796	2.796	2.796	2.865	2.865	2.843	2.843	2.865	2.865	2.843	2.843
2e	2.791	2.791	2.791	2.790	2.821	2.882	2.820	2.882	2.821	2.882	2.821	2.882
3c	2.773	2.773	2.815	2.831	2.848	2.771	2.829	2.825	2.774	2.839	2.815	2.820
3d	2.790	2.791	2.790	2.791	2.824	2.824	2.822	2.822	2.824	2.823	2.822	2.822
3e	2.799	2.800	2.800	2.800	2.783	2.835	2.783	2.835	2.783	2.835	2.783	2.835

Table S1. (cont)

	Angles (°)				Dihedrals (°)					
	M-M-M	M-M-M	M-M-M	M-M-M	Mo-M-Mo	Mo-M-Mo	Mo-M-Mo	Mo-M-Mo	$\Theta(\text{Mo-Mo-Mo-M1})$	$\Theta(\text{M-M-Mo-M})$
1a	63.1	59.2	57.8		169.0	174.7	176.2		6.3	
1b	59.9	59.8	60.3		176.6	177.1	177.1		1.1	
2a	62.9	58.7	58.4		177.1	174.9	177.3		0.6	
2b	59.9	59.8	60.3		179.1	178.6	178.8		0.5	
3a	64.3	59.7	56.0		169.1	178.6	173.5		1.2	
3b	59.5	59.7	60.8		177.7	176.4	176.5		1.0	
1c	98.5	83.0	95.4	83.1	160.2	146.1	159.7	157.5		58.6
1d	68.8	111.2	68.8	111.2	150.3	178.7	150.3	178.7		45.2
1e	90.0	89.6	90.0	90.3	151.4	151.7	152.3	152.1		35.7
2c	102.1	79.7	98.7	79.4	166.4	144.5	158.3	162.8		38.3
2d	67.0	113.0	67.0	113.0	151.9	173.3	151.9	173.2		44.3
2e	89.4	89.5	89.4	89.5	168.3	168.5	168.3	168.2		60.2
3c	94.7	86.6	92.5	86.2	157.9	148.2	154.9	167.6		140.5
3d	81.7	98.3	81.7	98.3	162.6	175.8	162.6	175.8		55.0
3e	89.5	89.5	89.5	89.5	156.7	156.7	156.8	156.8		38.8

Figures S1-S15 below are respective to the FSI fragmentation scheme.

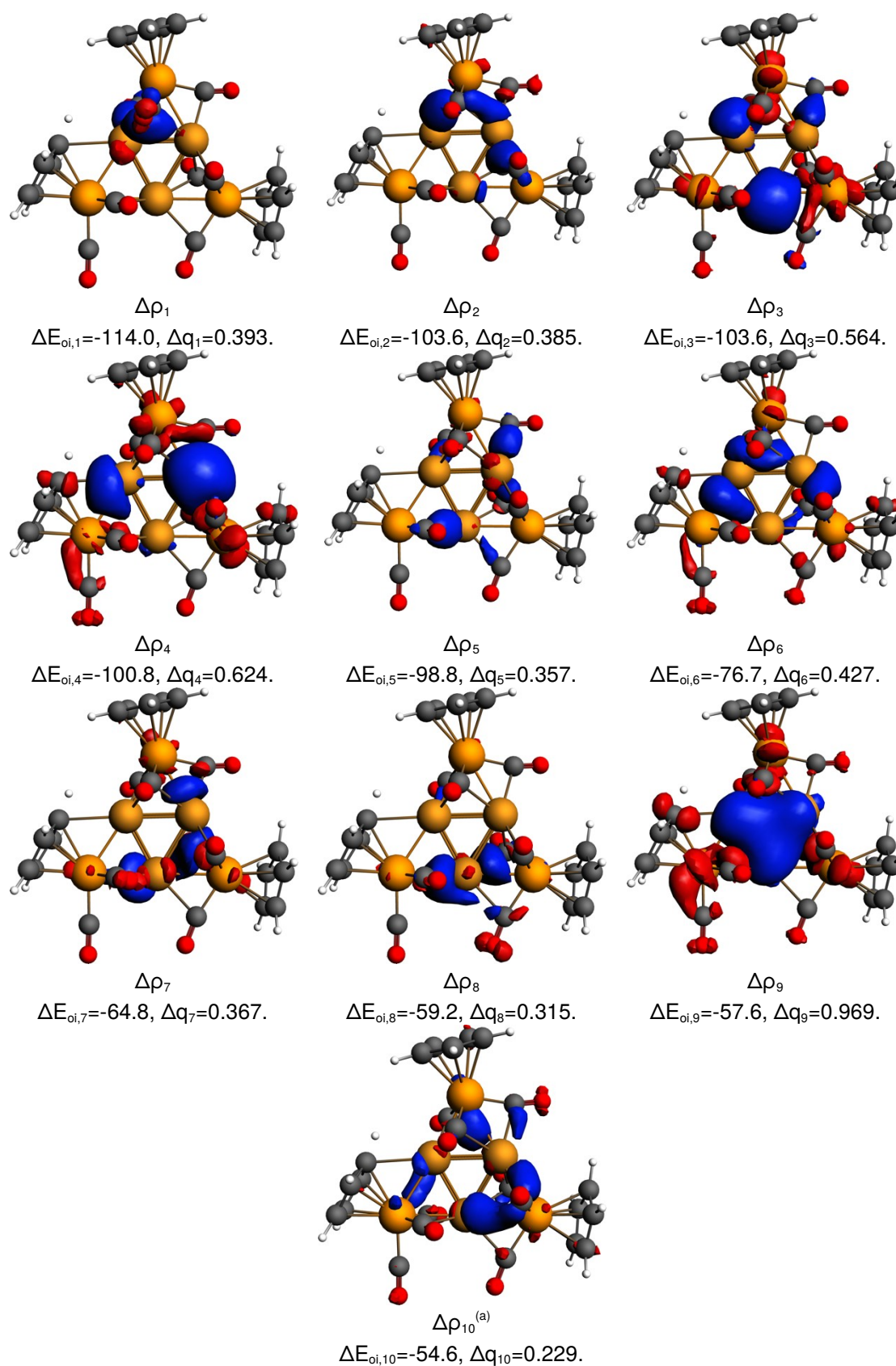


Figure S1: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **1a** in FSI scheme, with their energy, $\Delta E_{oi,j}$ (kcal mol⁻¹) and charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

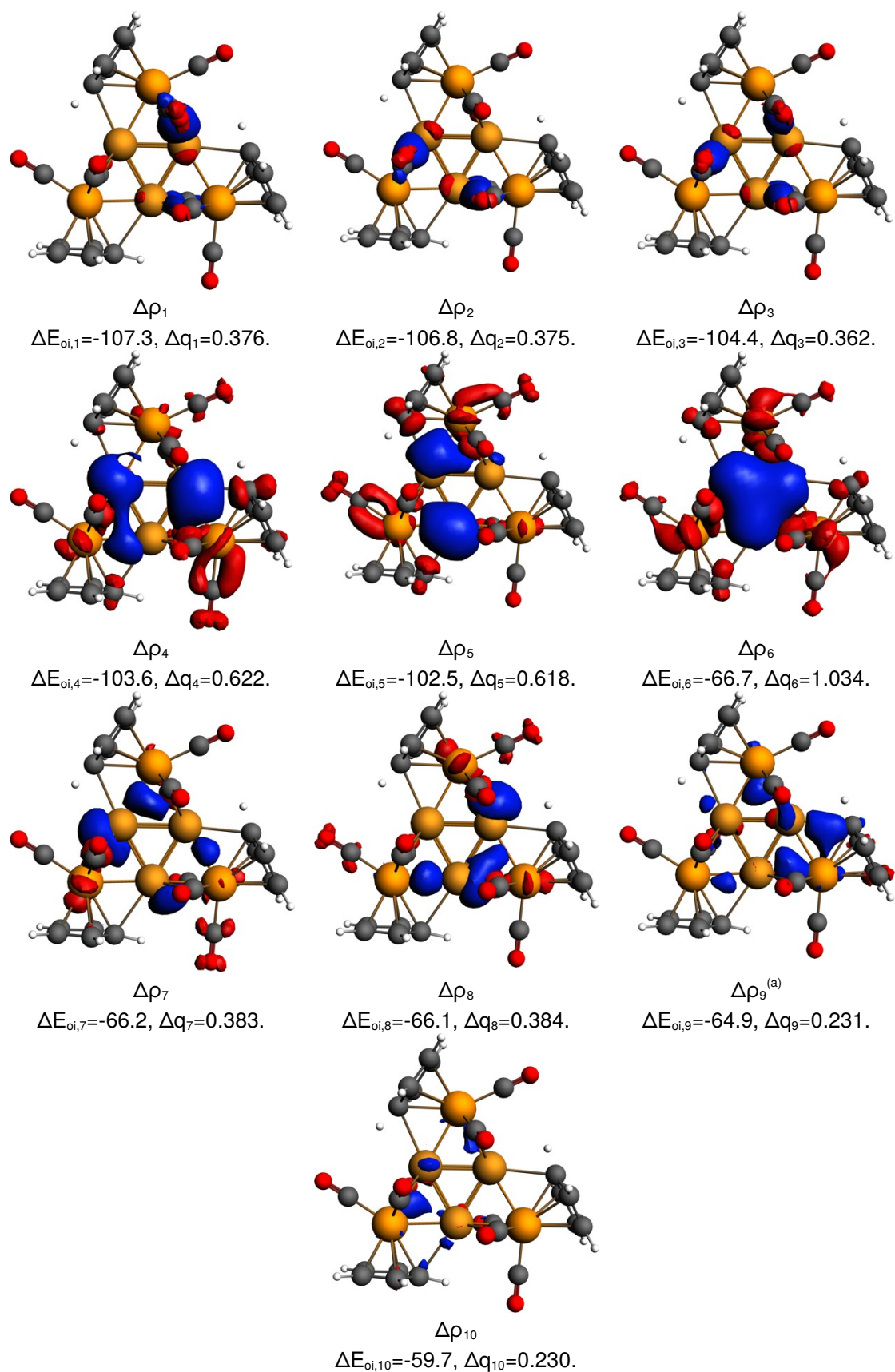


Figure S2: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **1b** in FSI scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

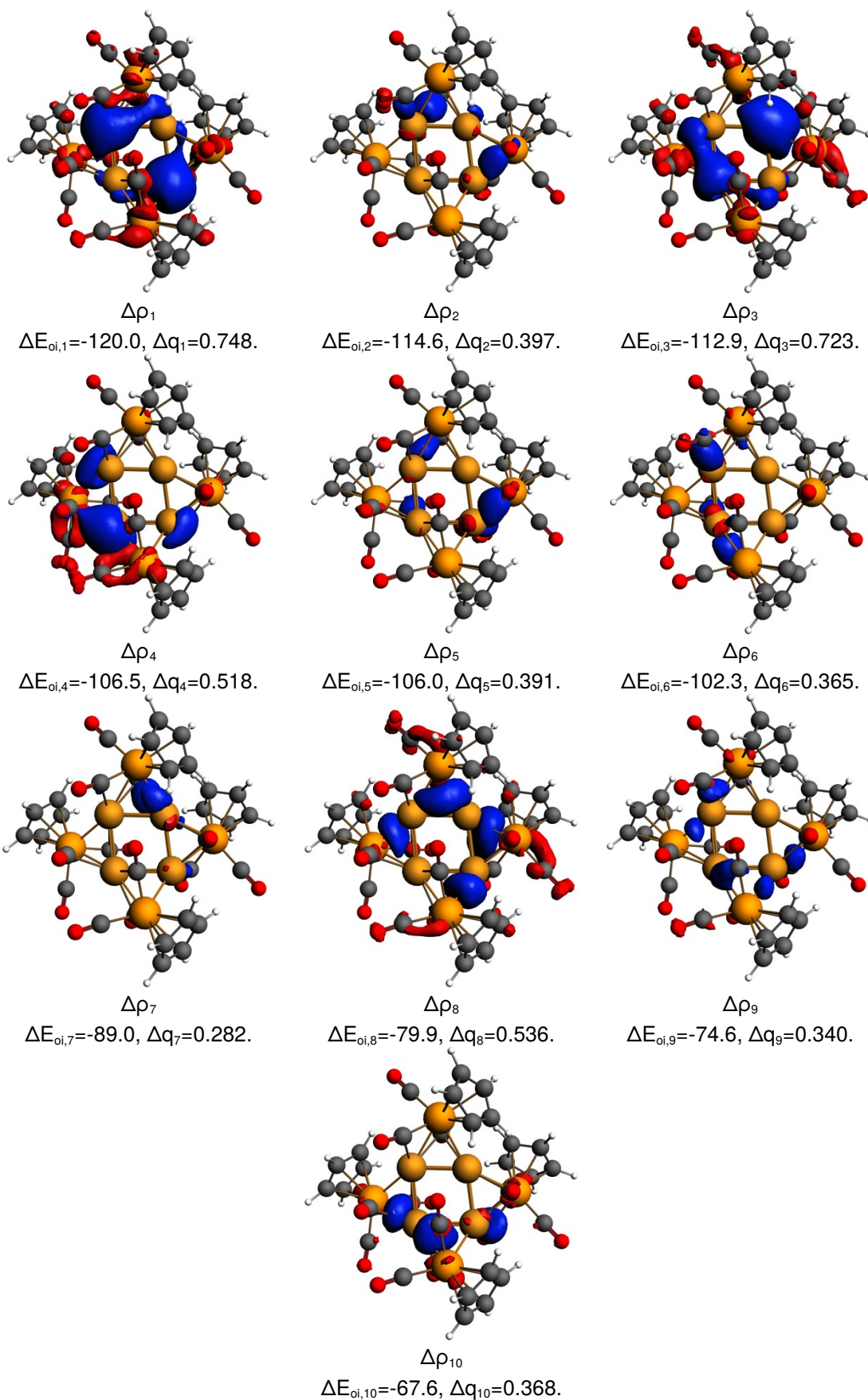


Figure S3: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **1c** in FSI scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge

transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

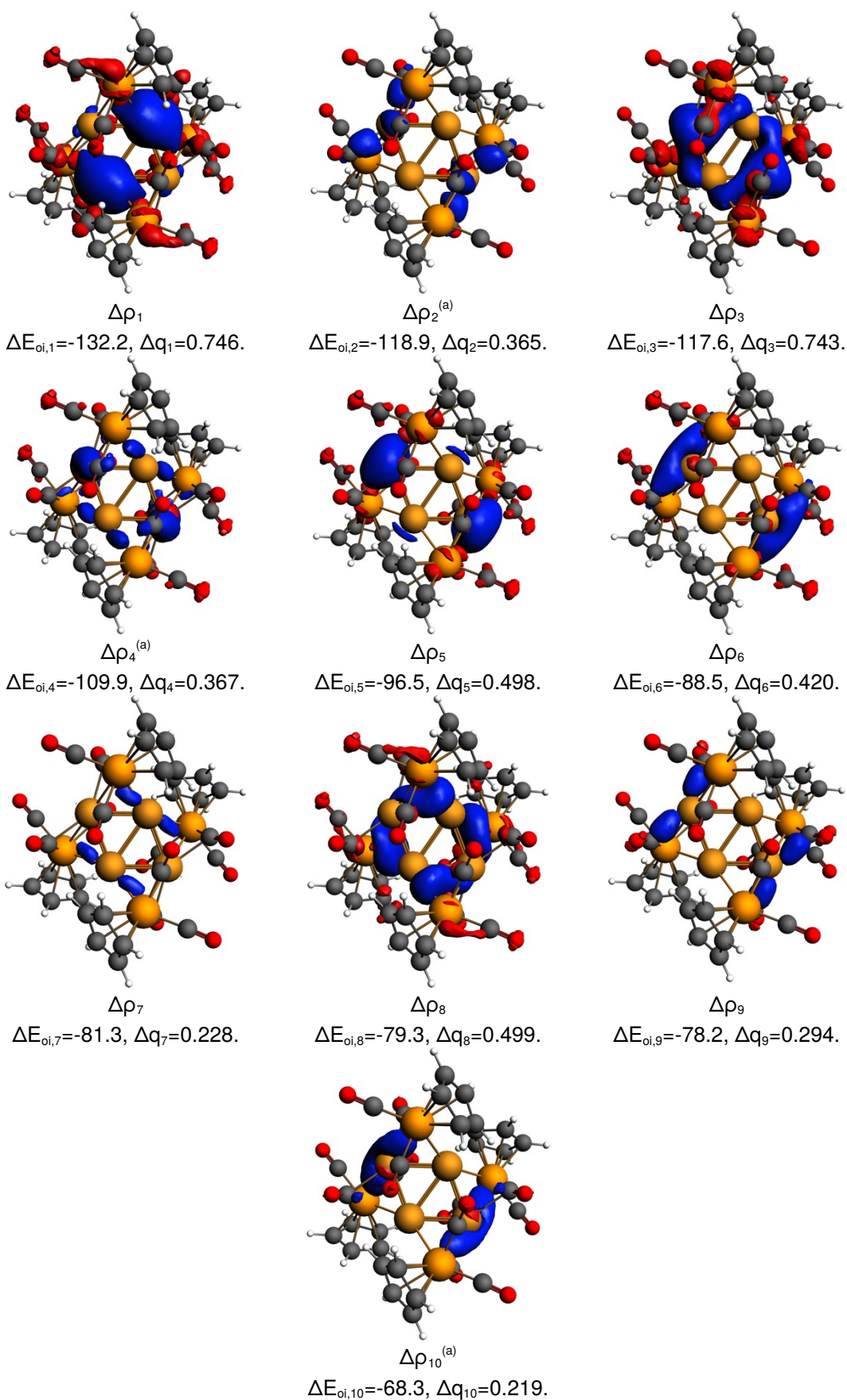


Figure S4: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **1d** in FSI scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge

transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

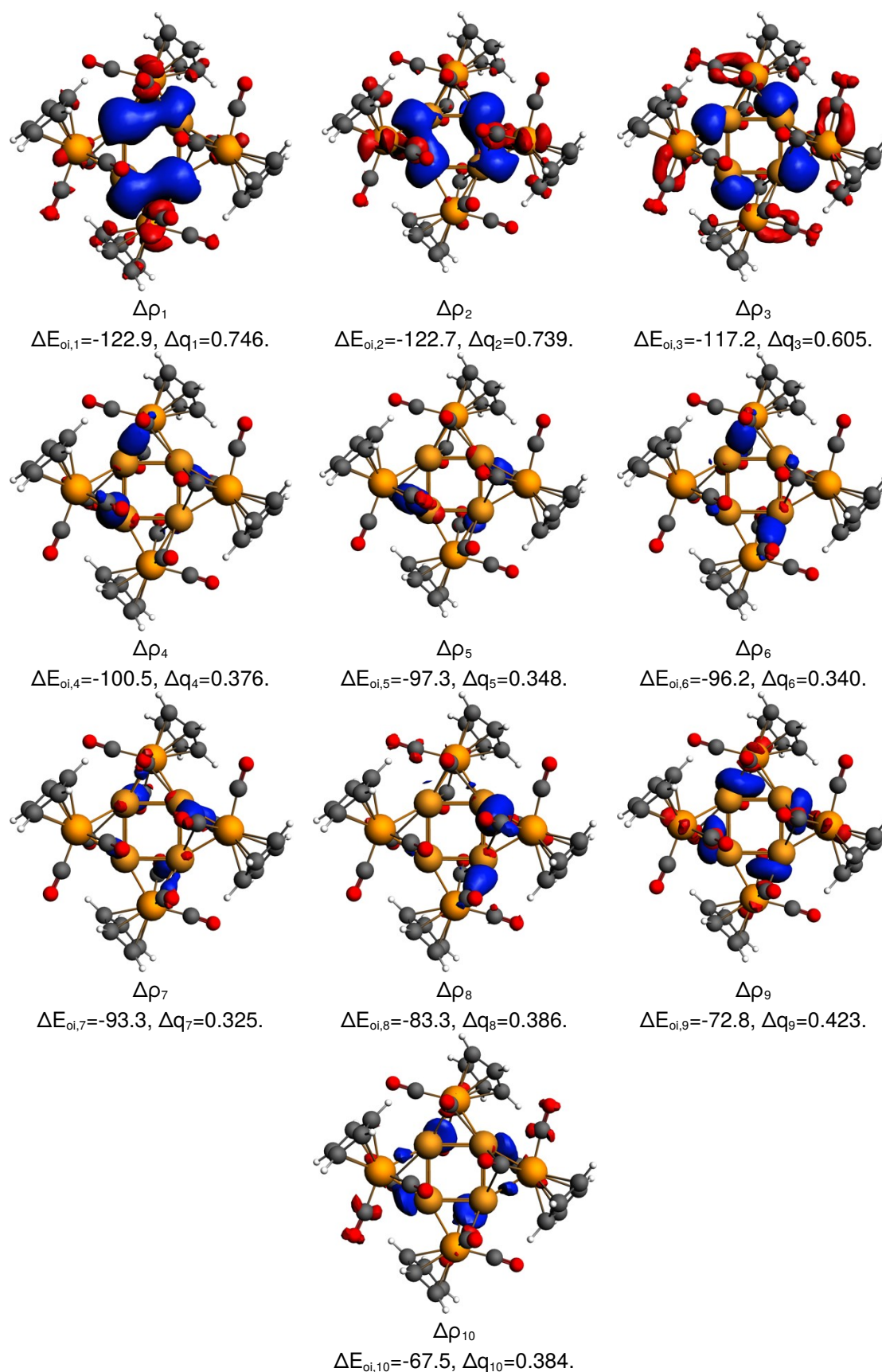


Figure S5: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **1e** in FSI scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

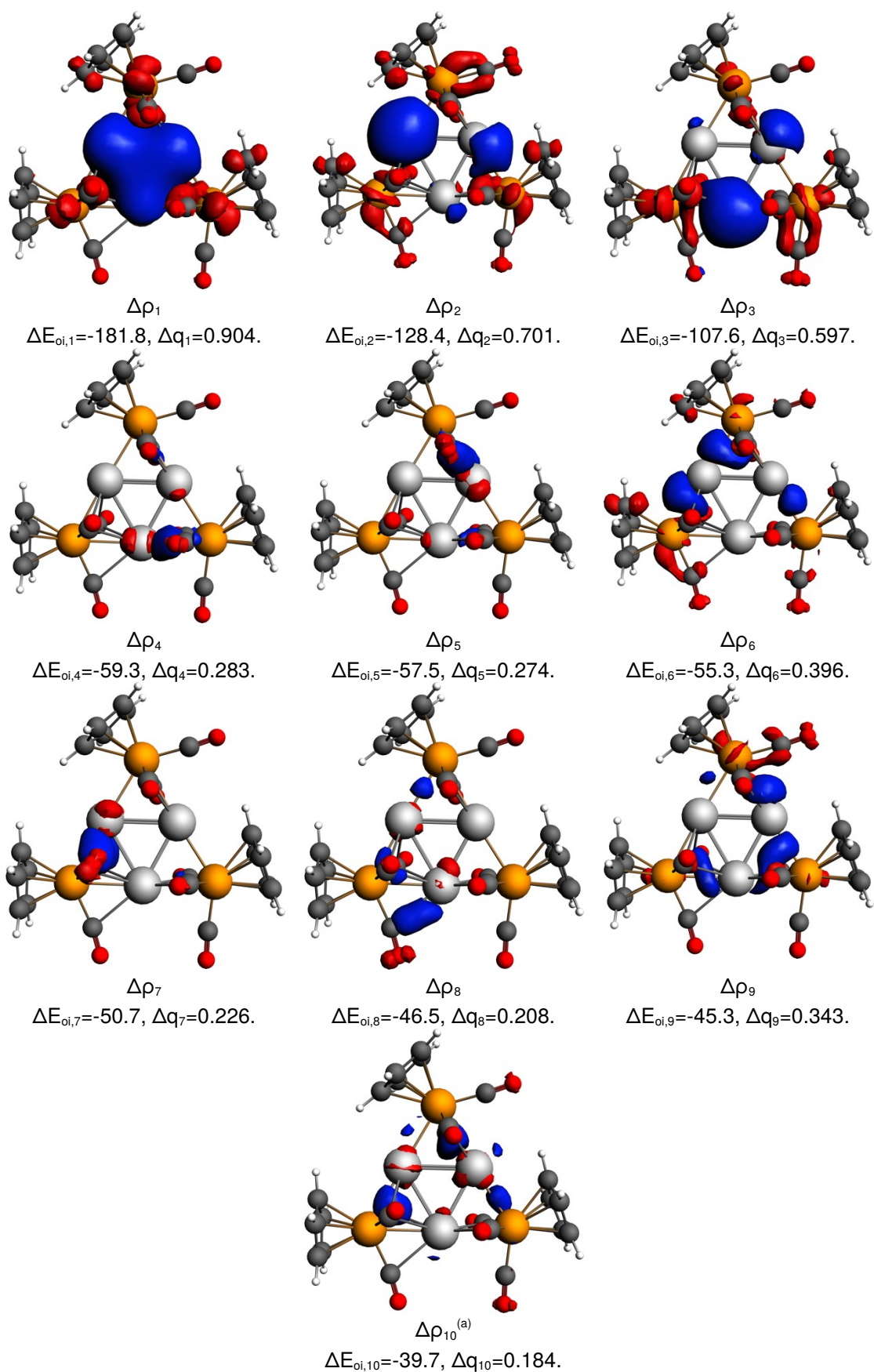


Figure S6: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **2a** in FSI scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge

transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

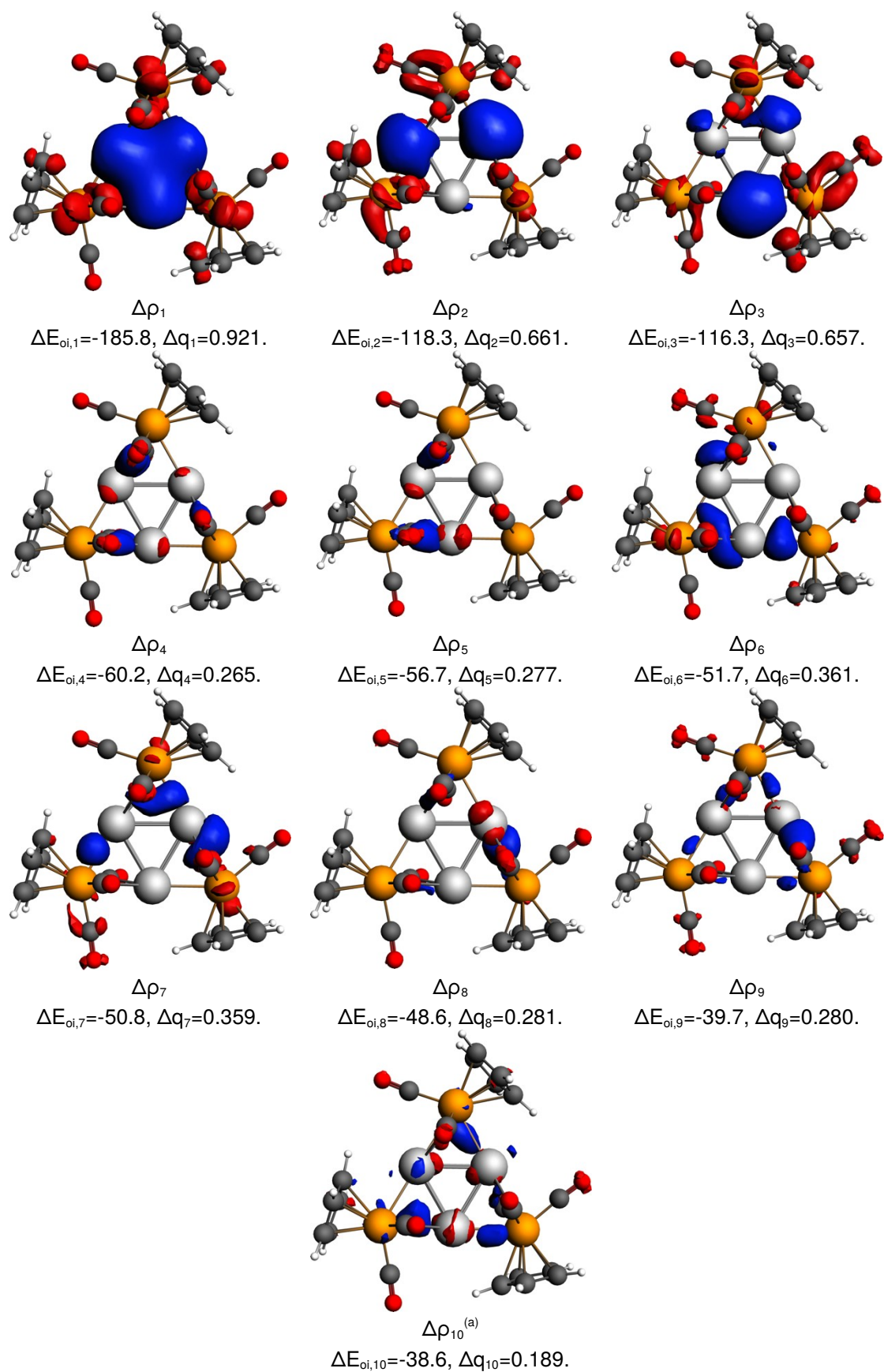


Figure S7: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **2b** in FSI scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge

transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

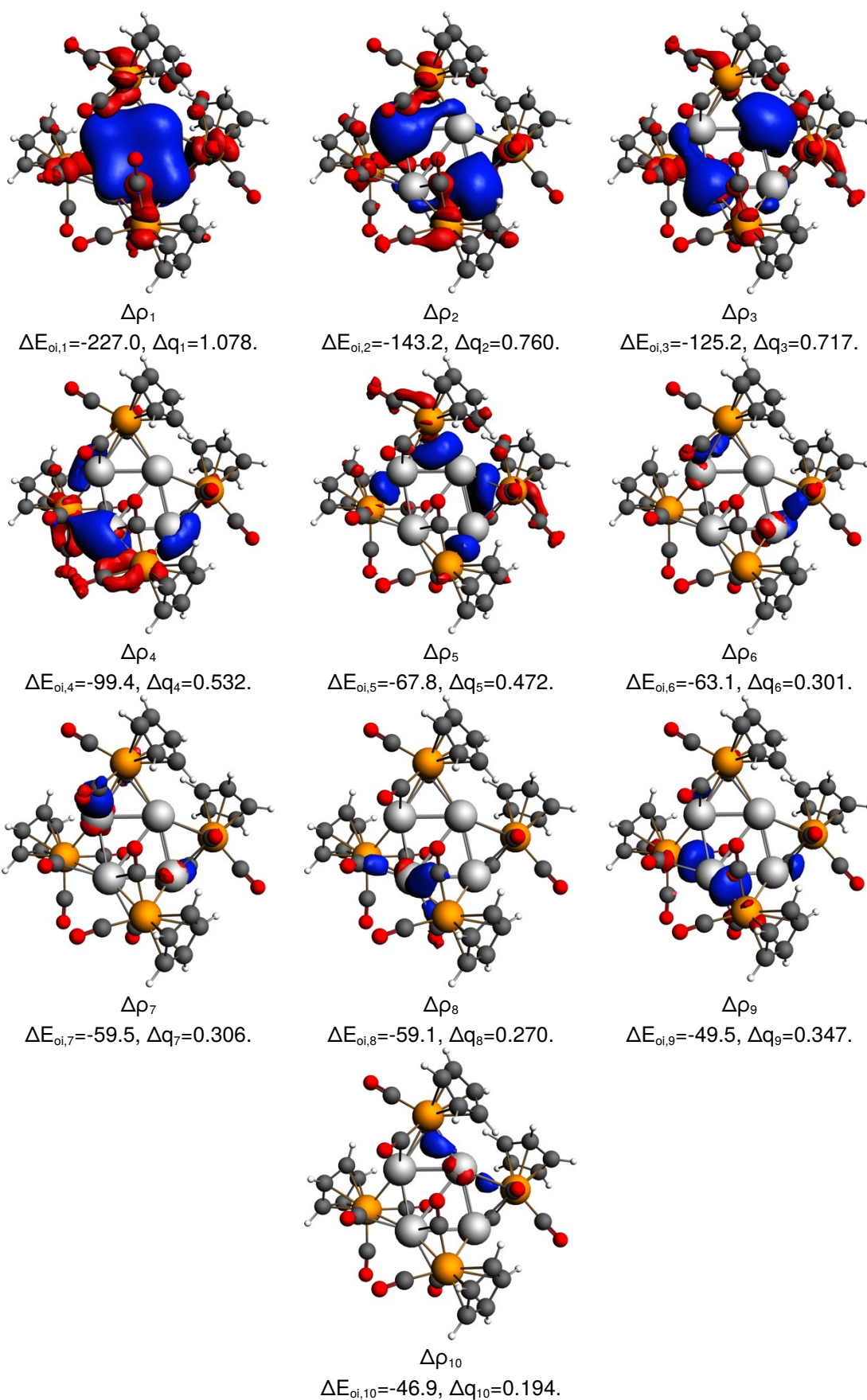


Figure S8: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **2c** in FSI scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge

transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

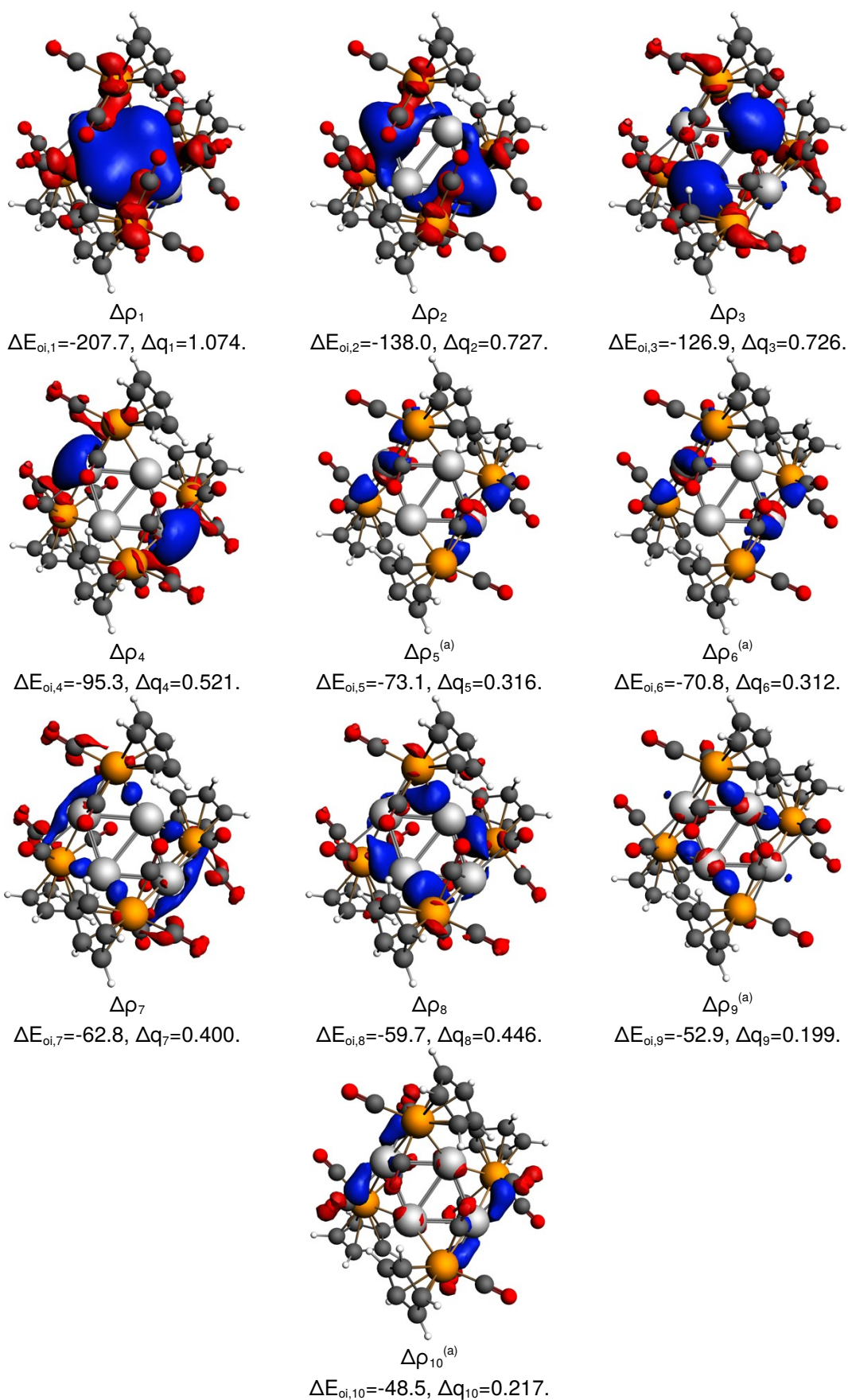


Figure S9: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **2d** in FSI scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge

transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

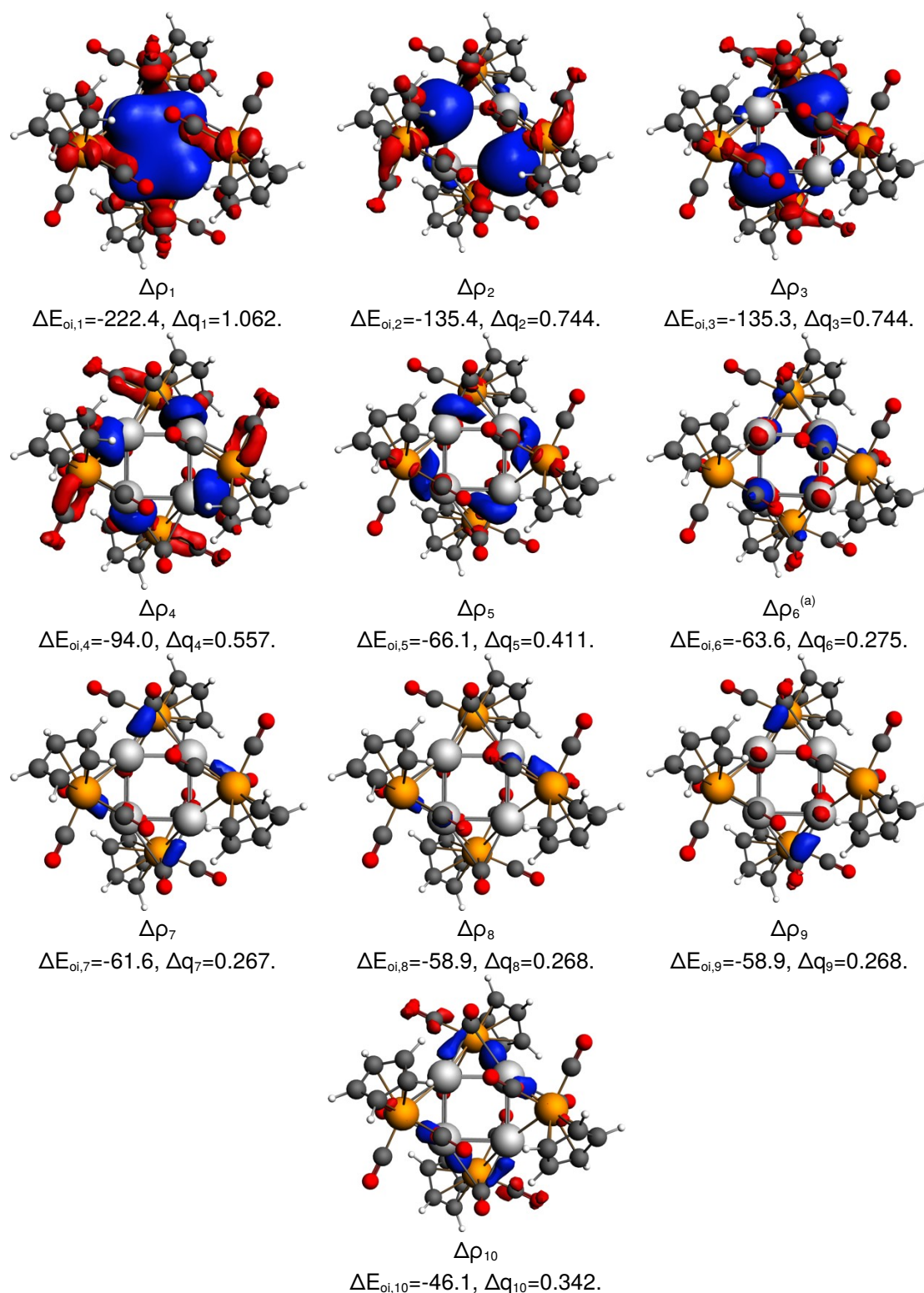


Figure S10: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **2e** in FSI scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

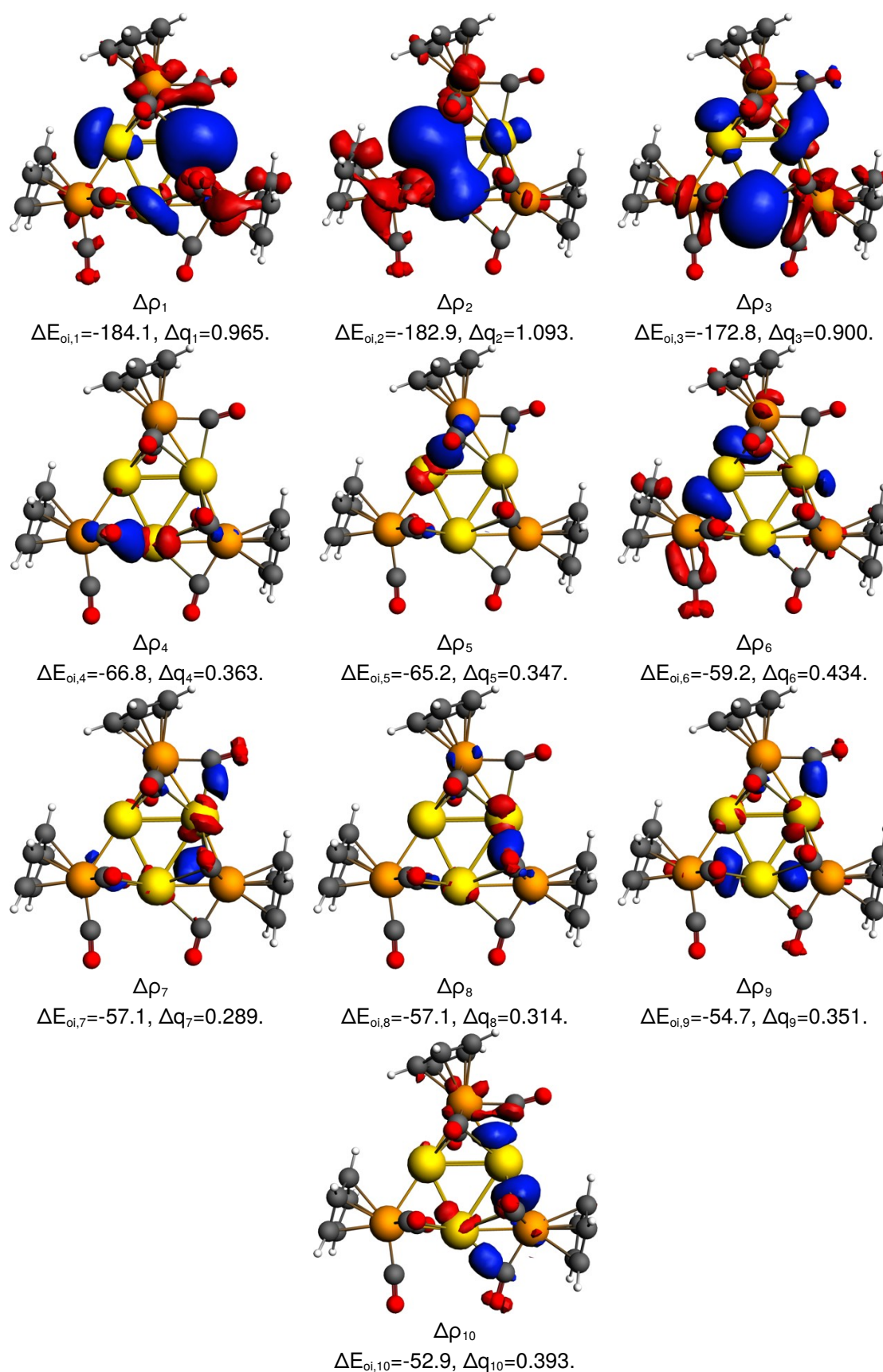


Figure S11: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **3a** in FSI scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

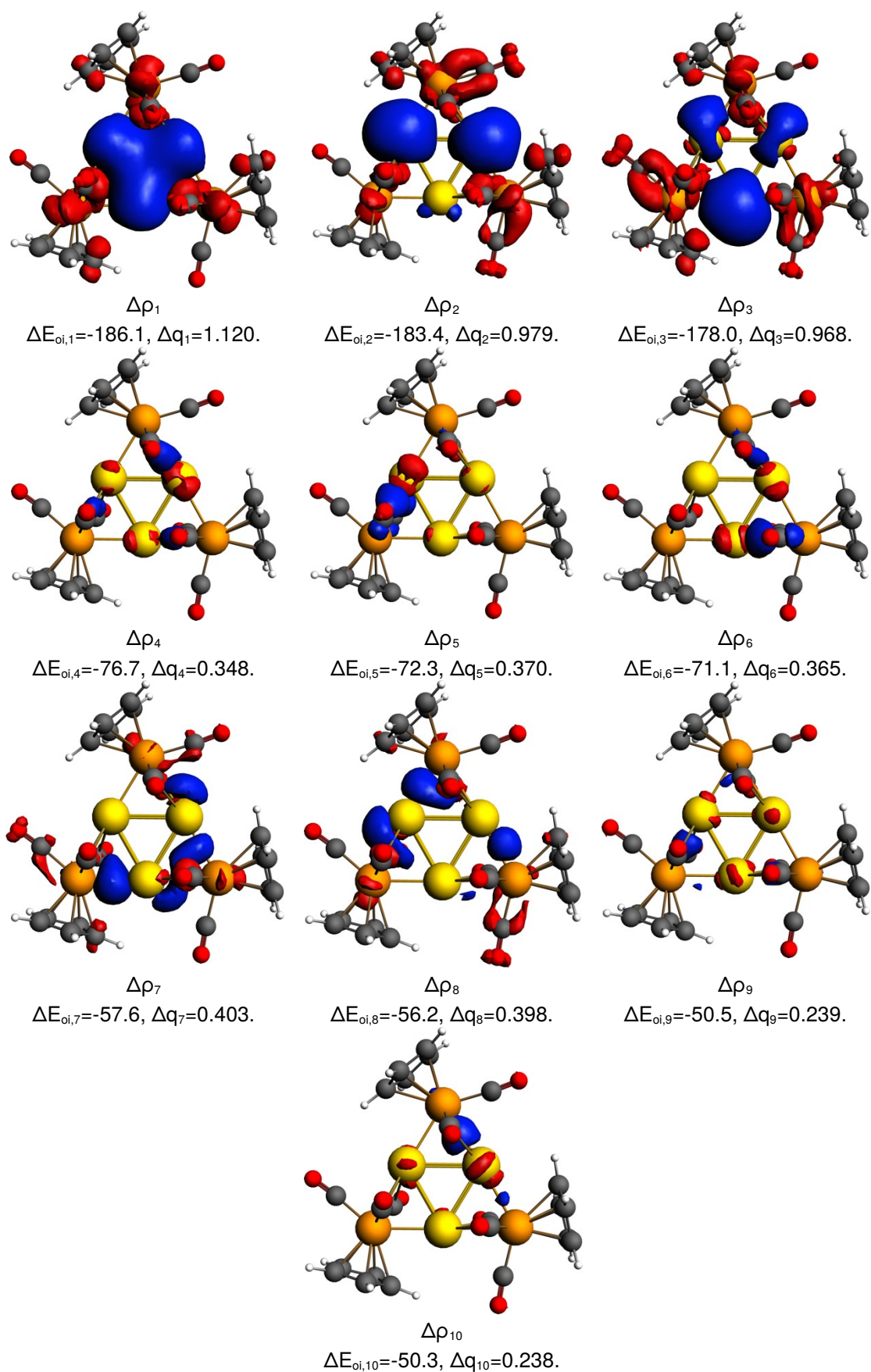


Figure S12: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **3b** in FSI scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge

transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

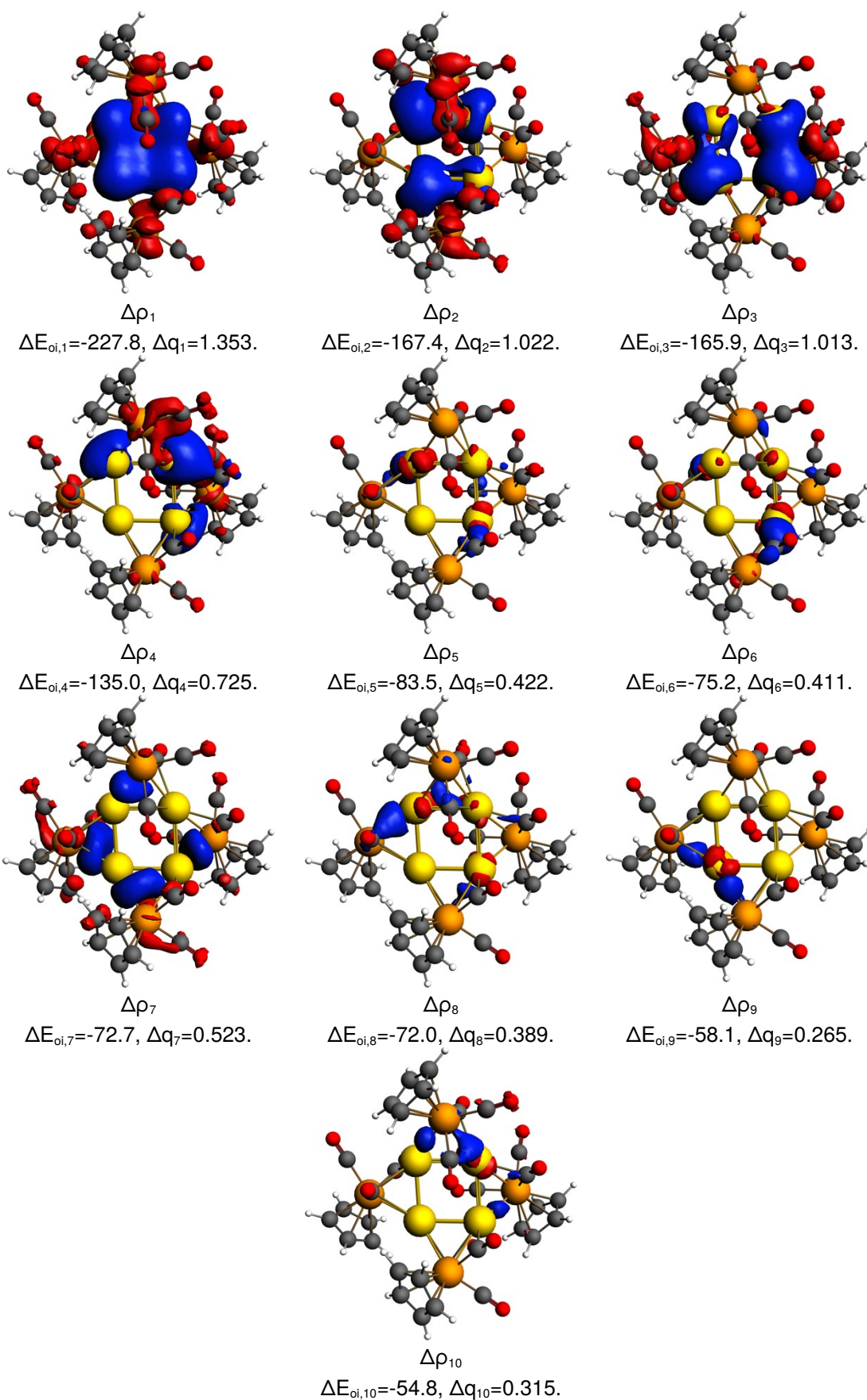


Figure S13: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **3c** in FSI scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge

transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

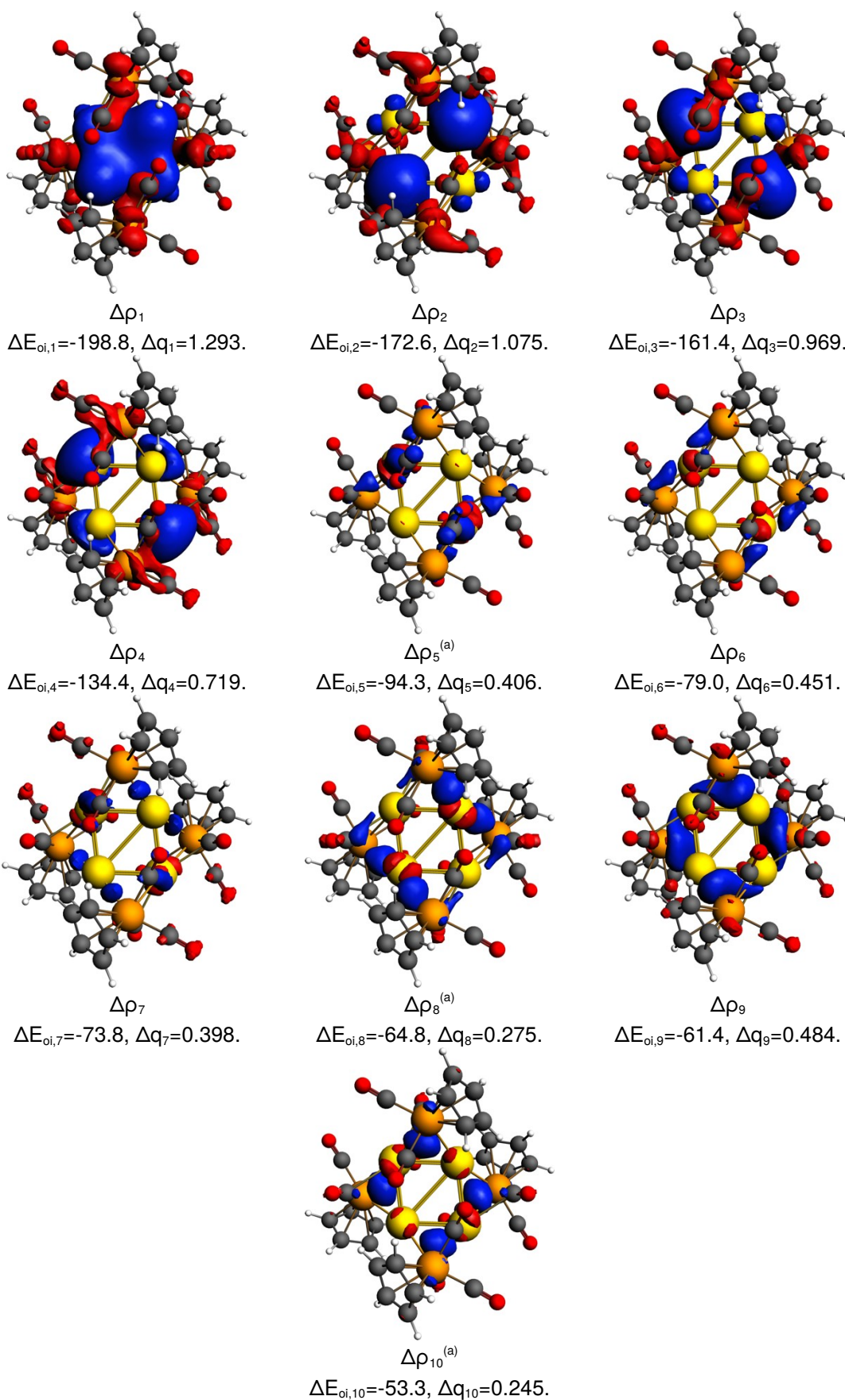


Figure S14: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **3d** in FSI scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge

transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

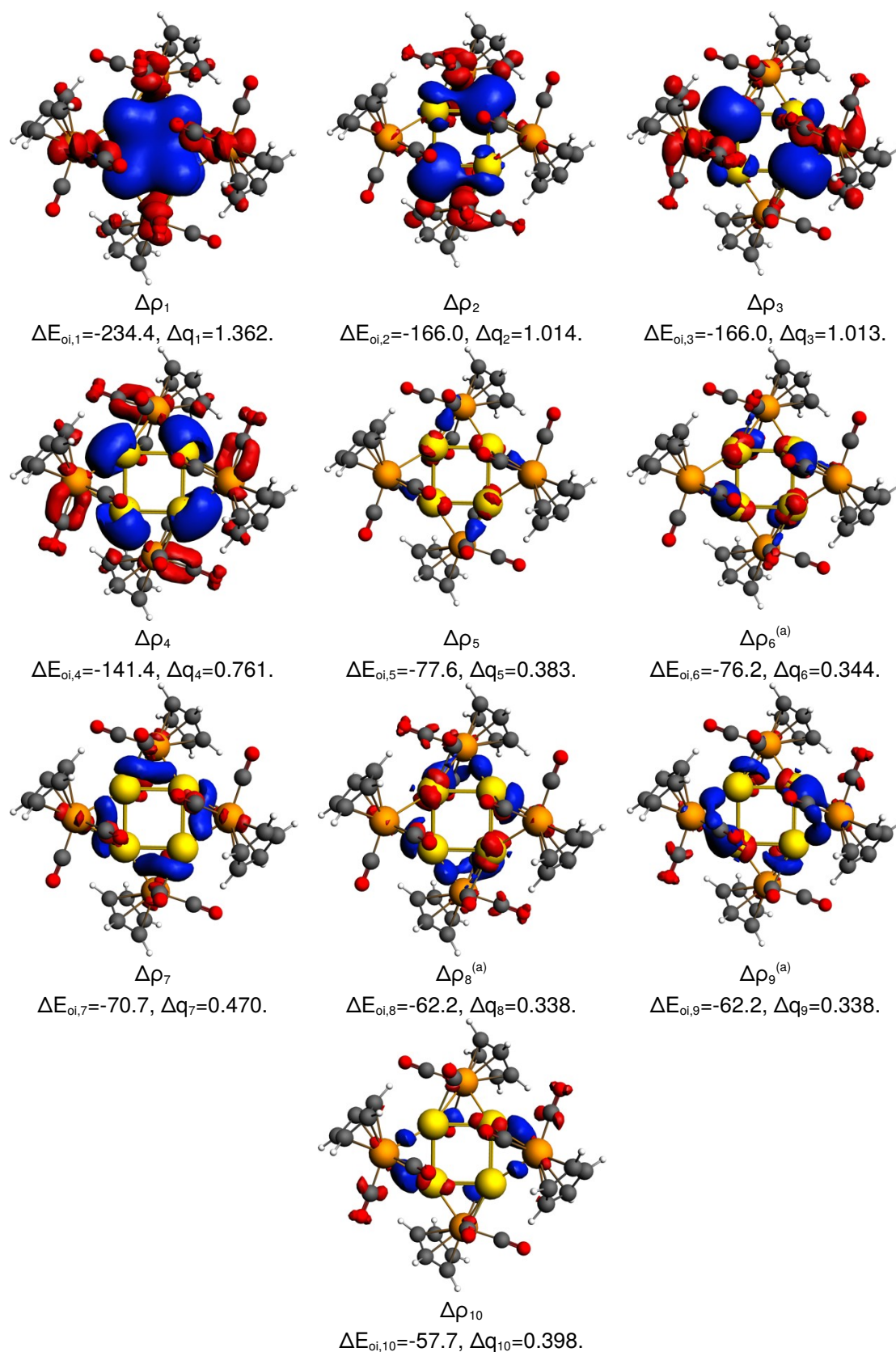


Figure S15: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **3e** in FSI scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

Figures S16-S30 below are respective to the FSII fragmentation scheme.

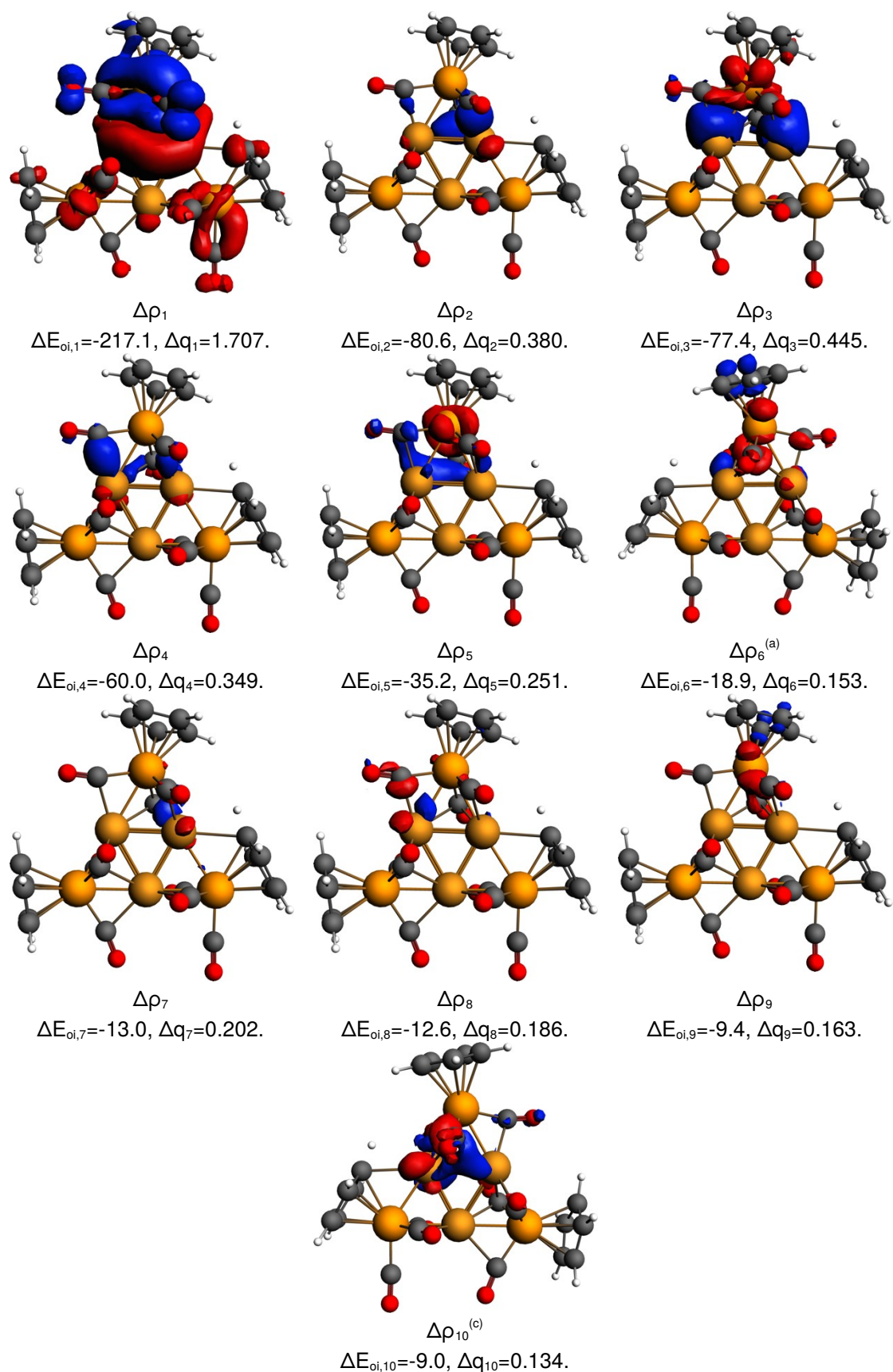


Figure S16: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **1a** in FSII scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

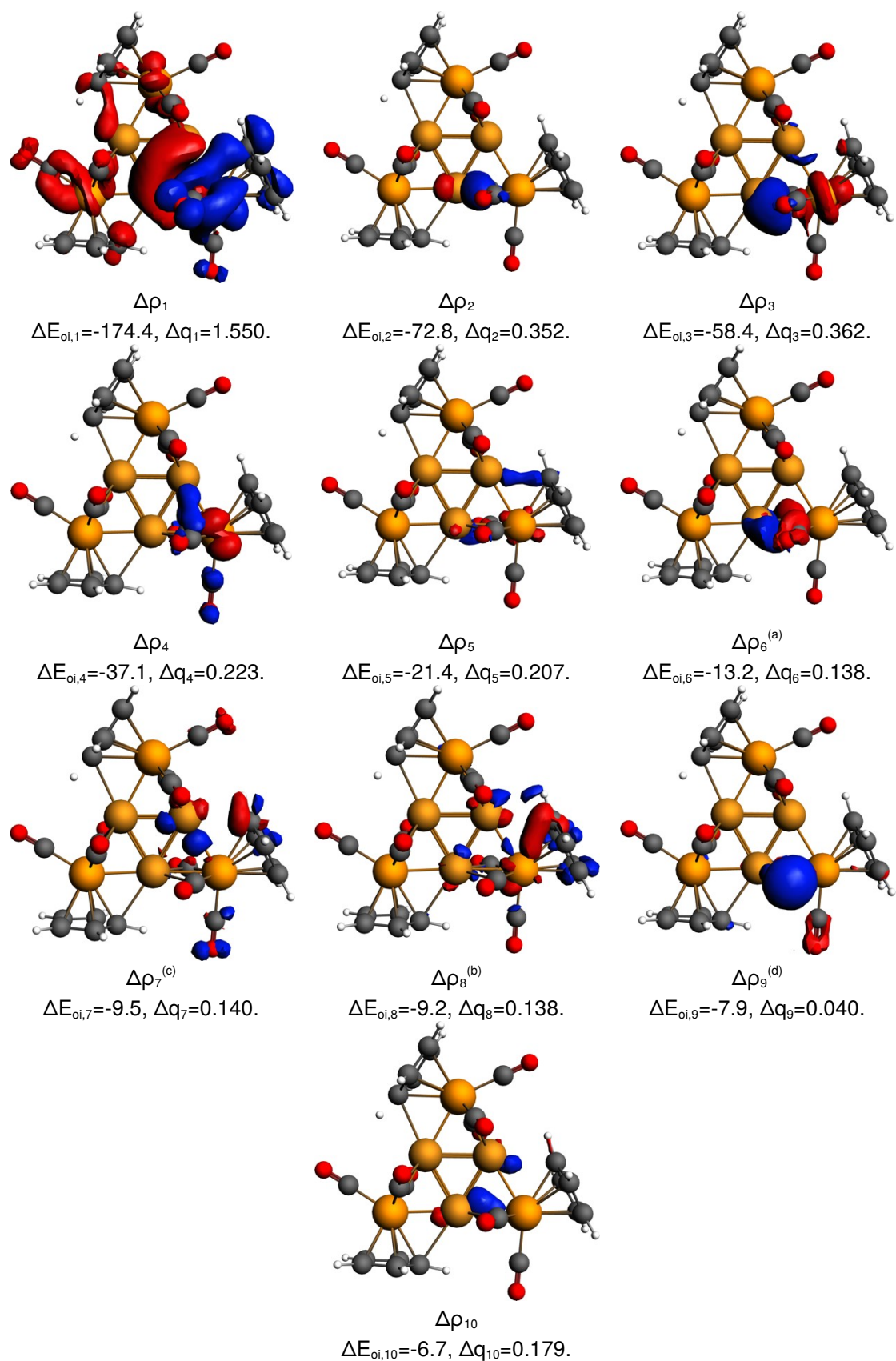


Figure S17: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **1b** in FSII scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

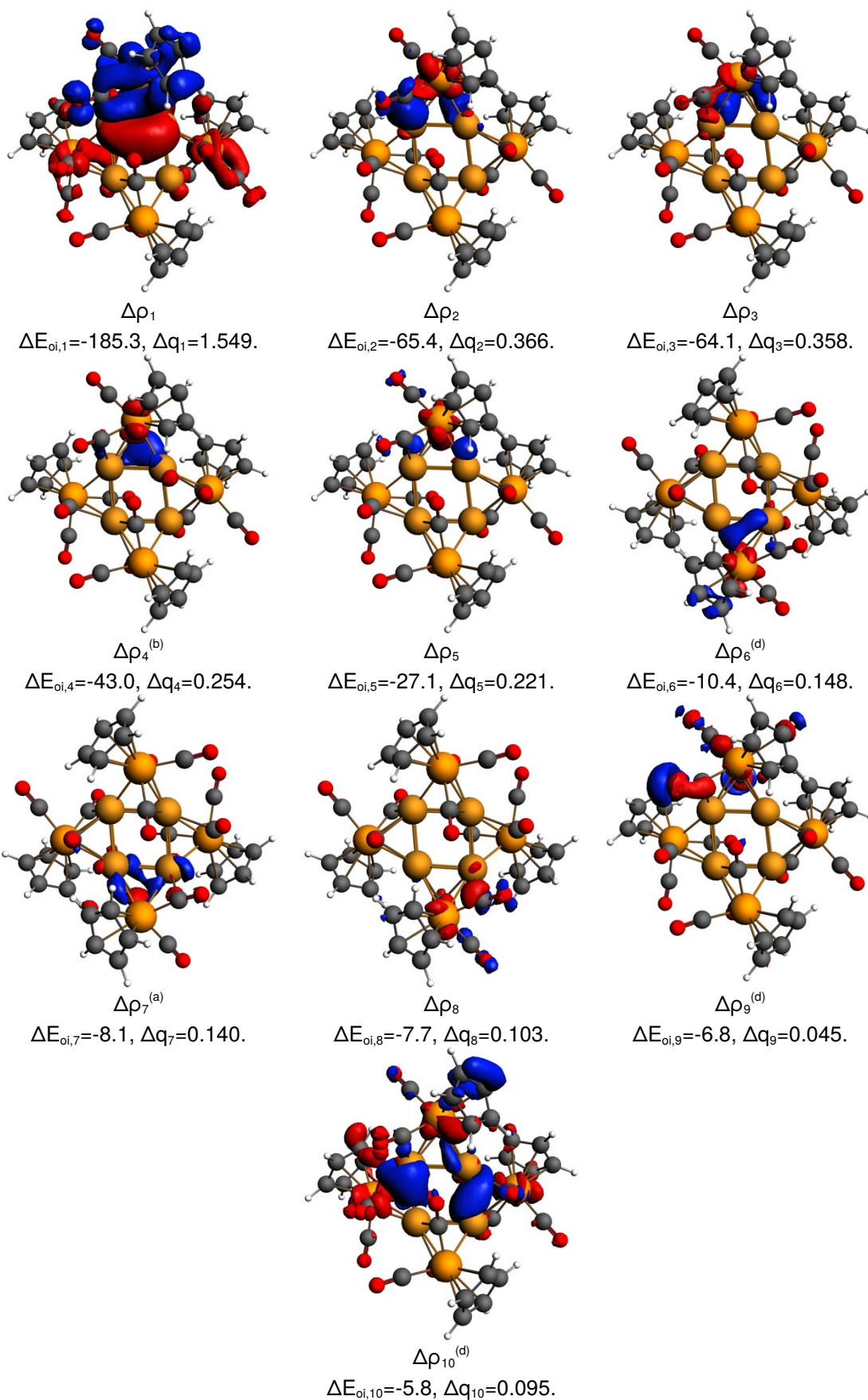


Figure S18: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **1c** in FSII scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and

charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

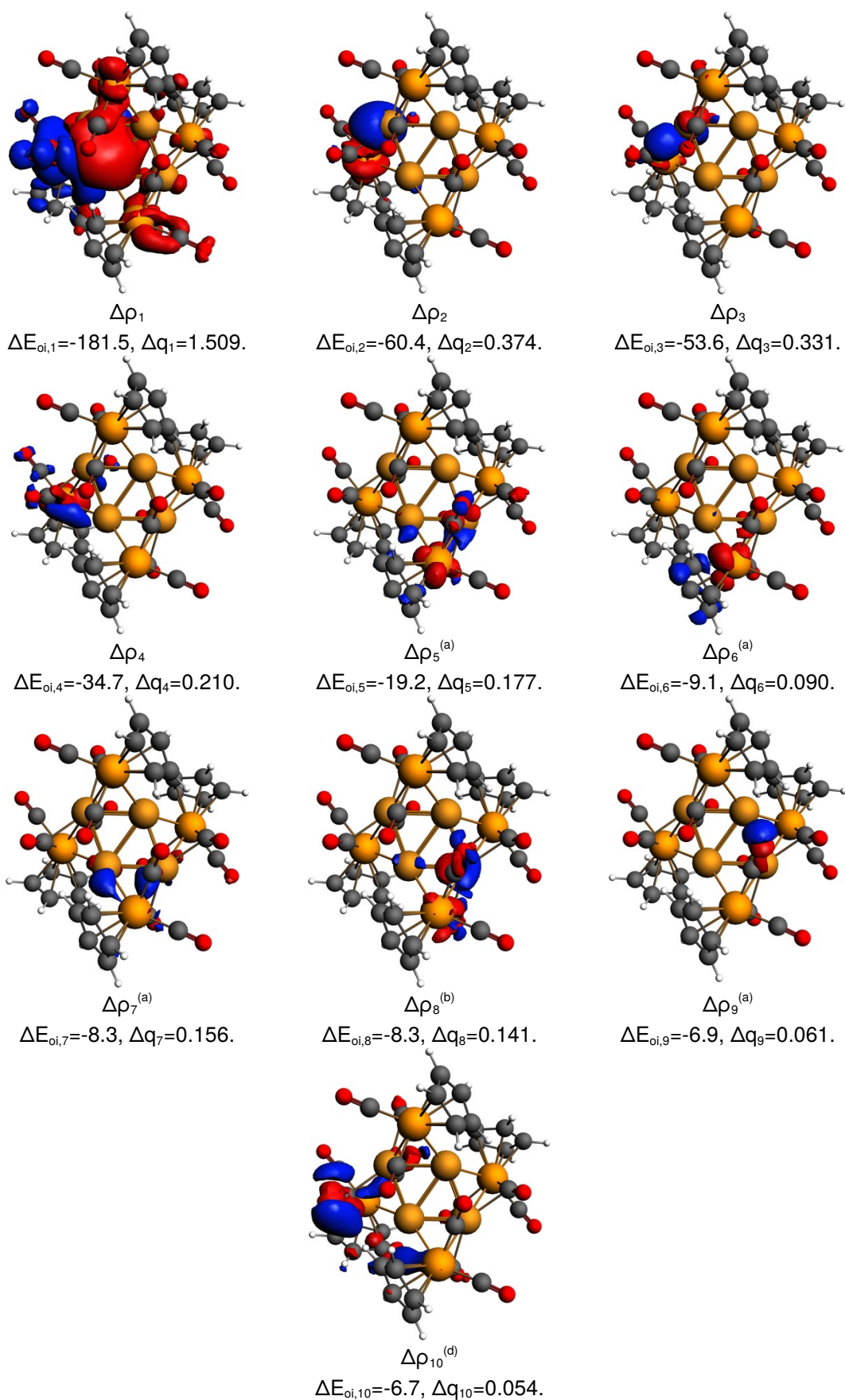


Figure S19: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **1d** in FSII scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and

charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

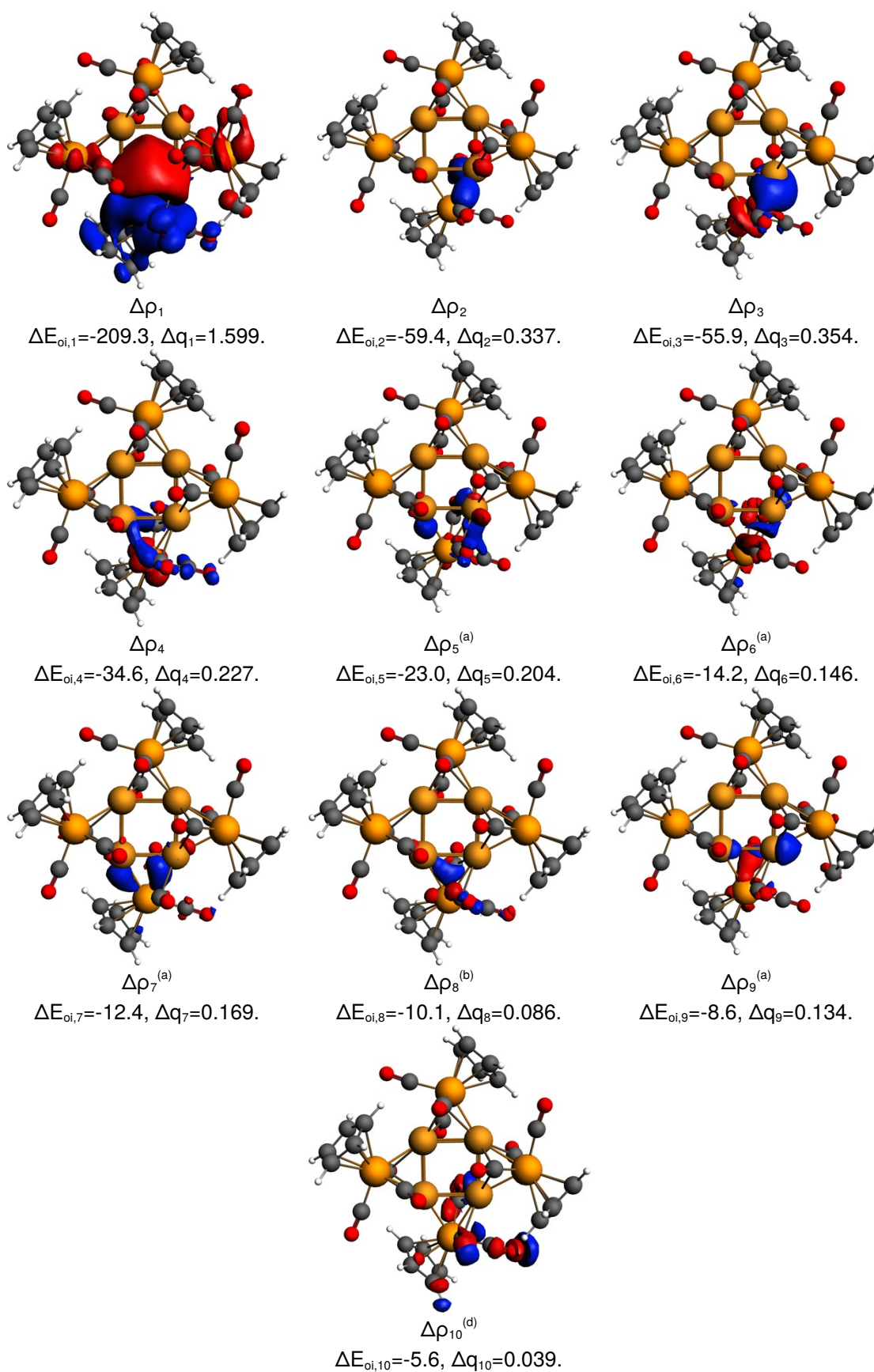


Figure S20: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **1e** in FSII scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and

charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

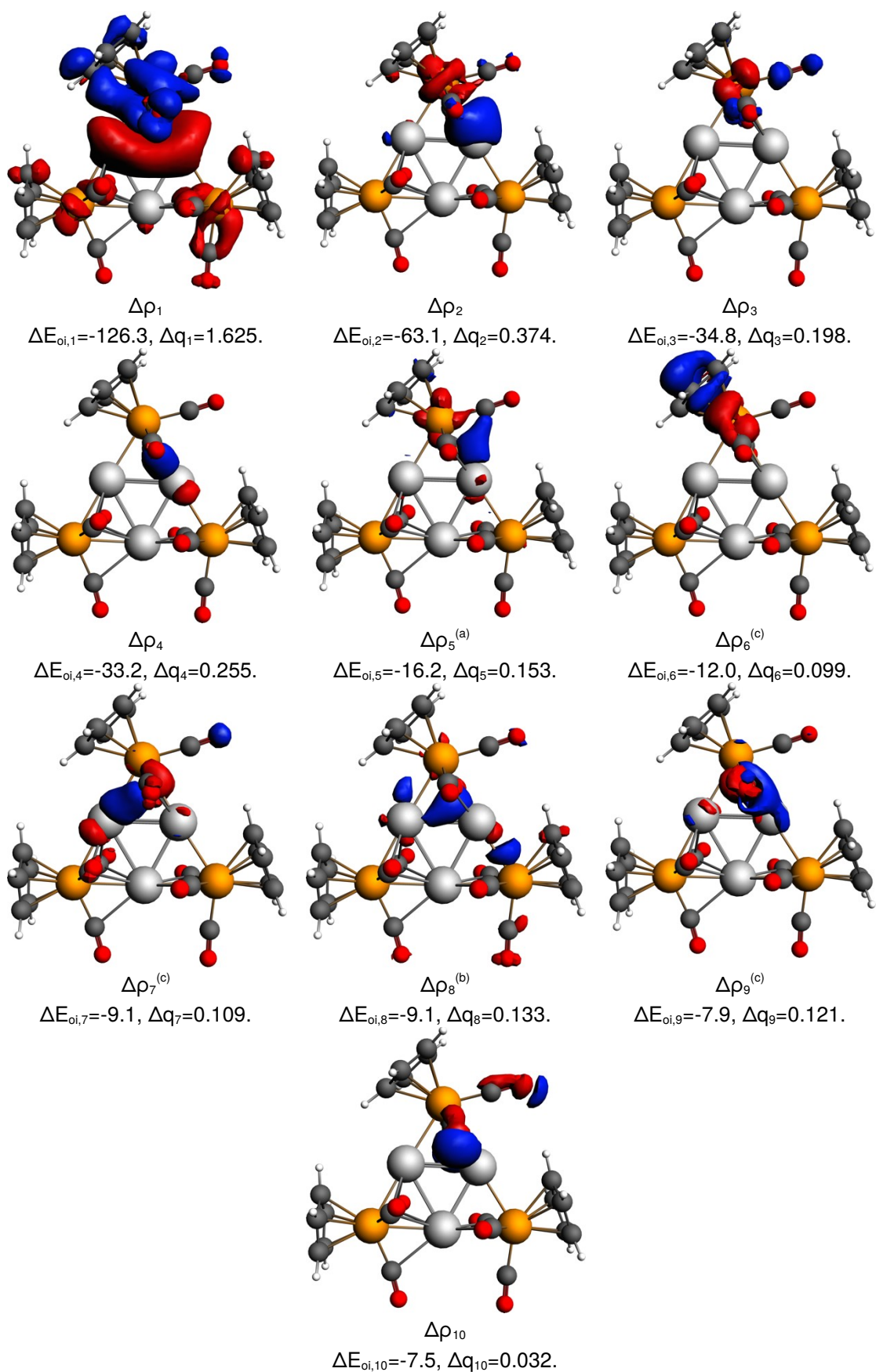


Figure S21: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **2a** in FSII scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and

charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

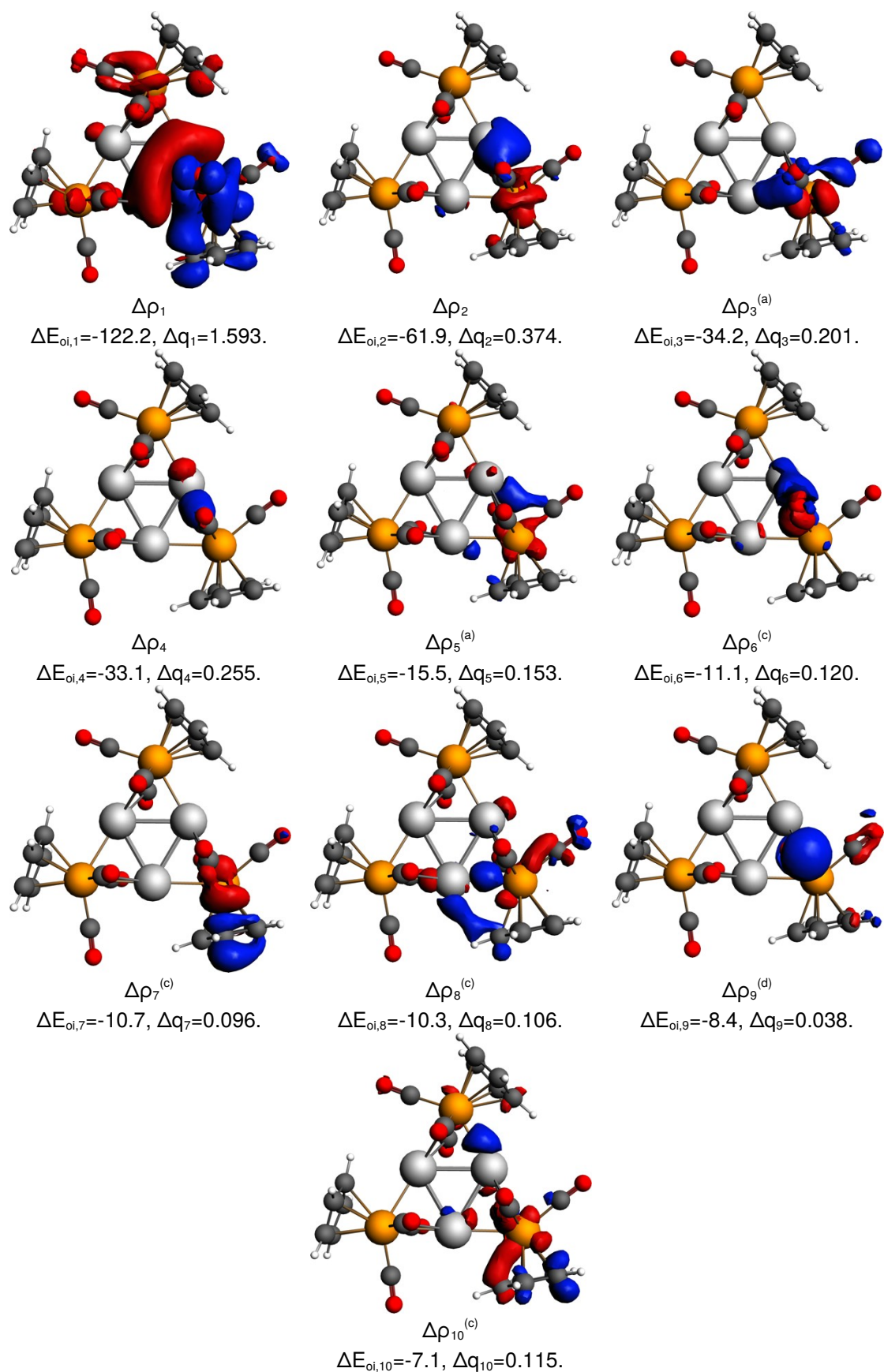


Figure S22: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **2b** in FSII scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and

charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

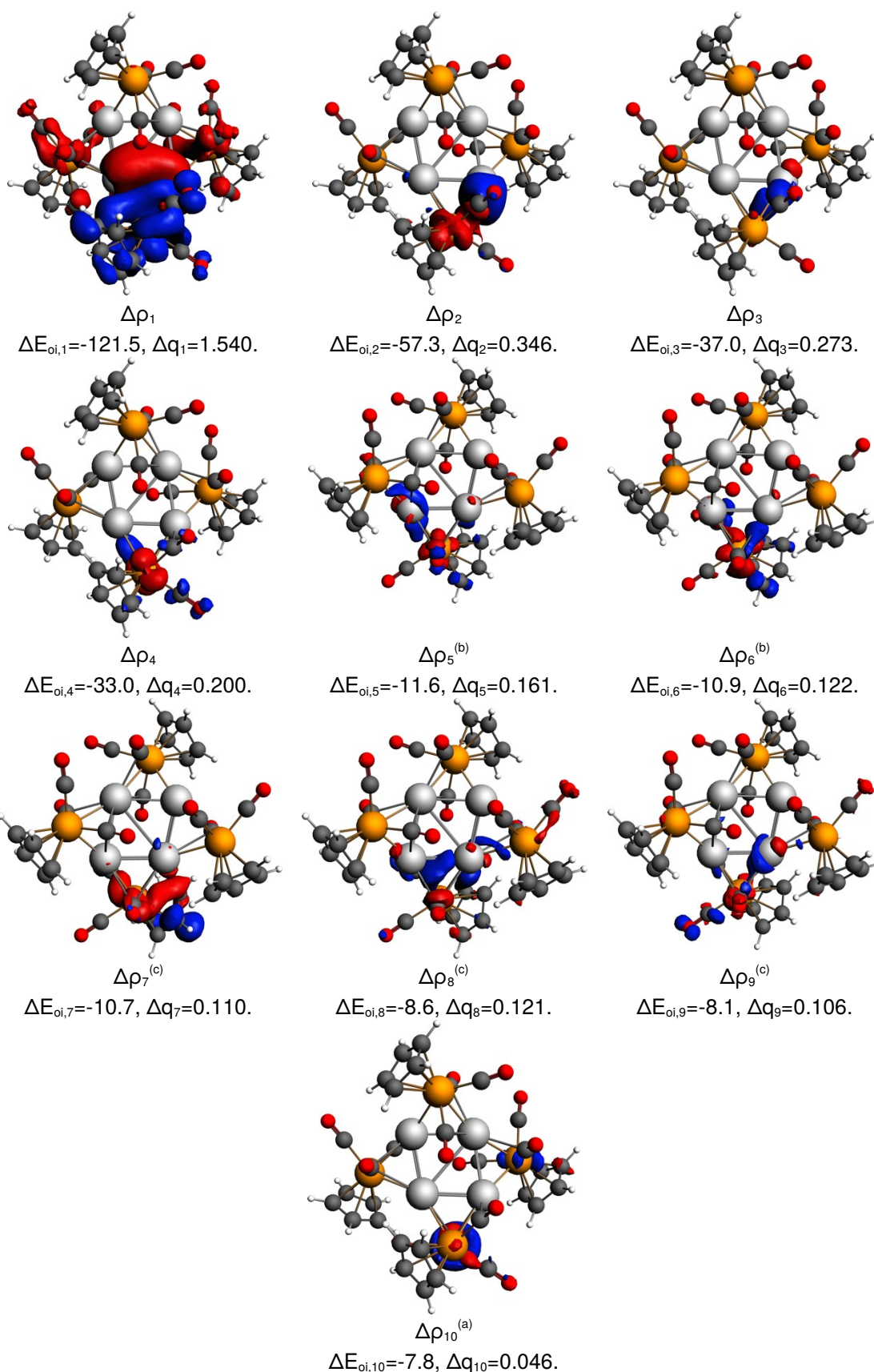


Figure S23: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **2c** in FSII scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

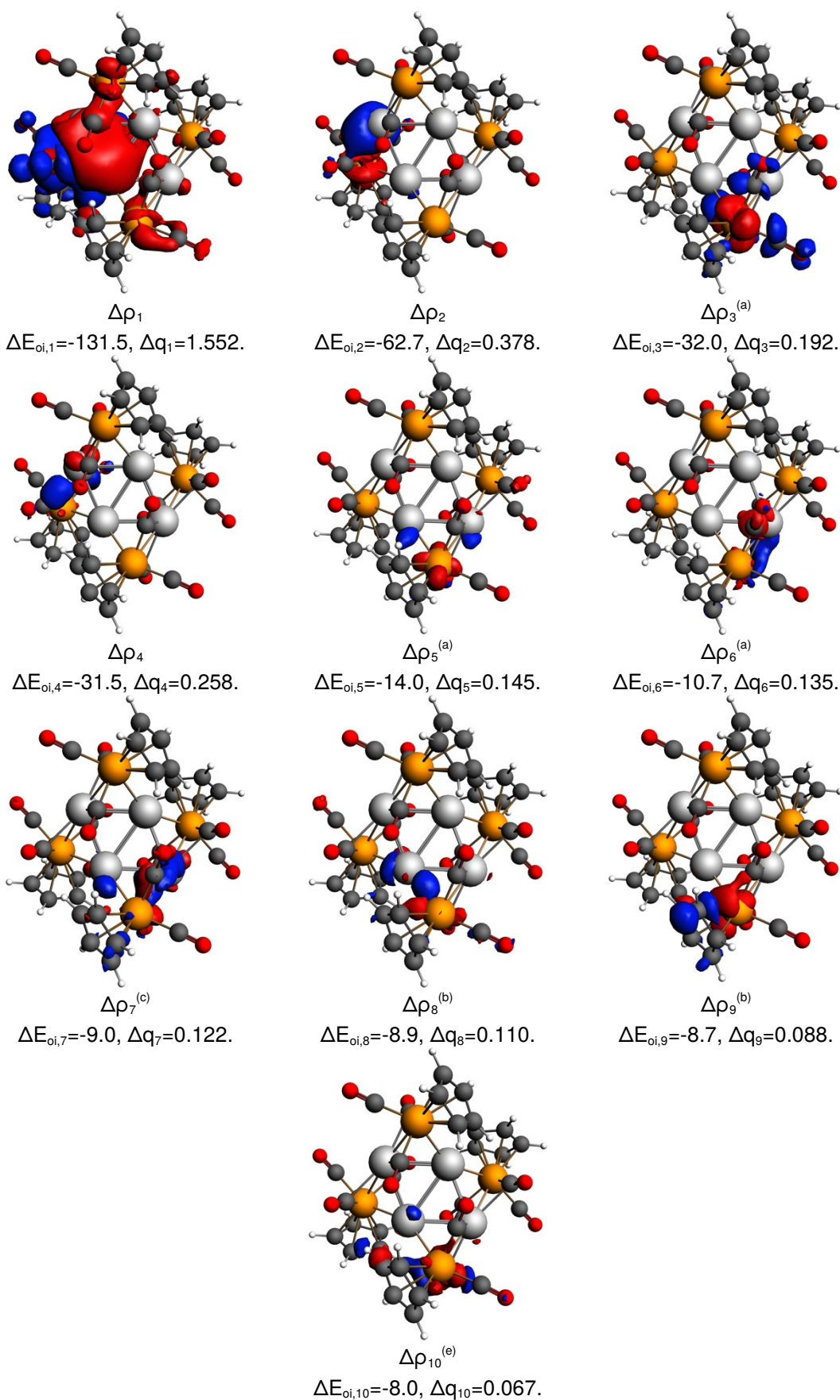


Figure S24: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **2d** in FSII scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and

charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

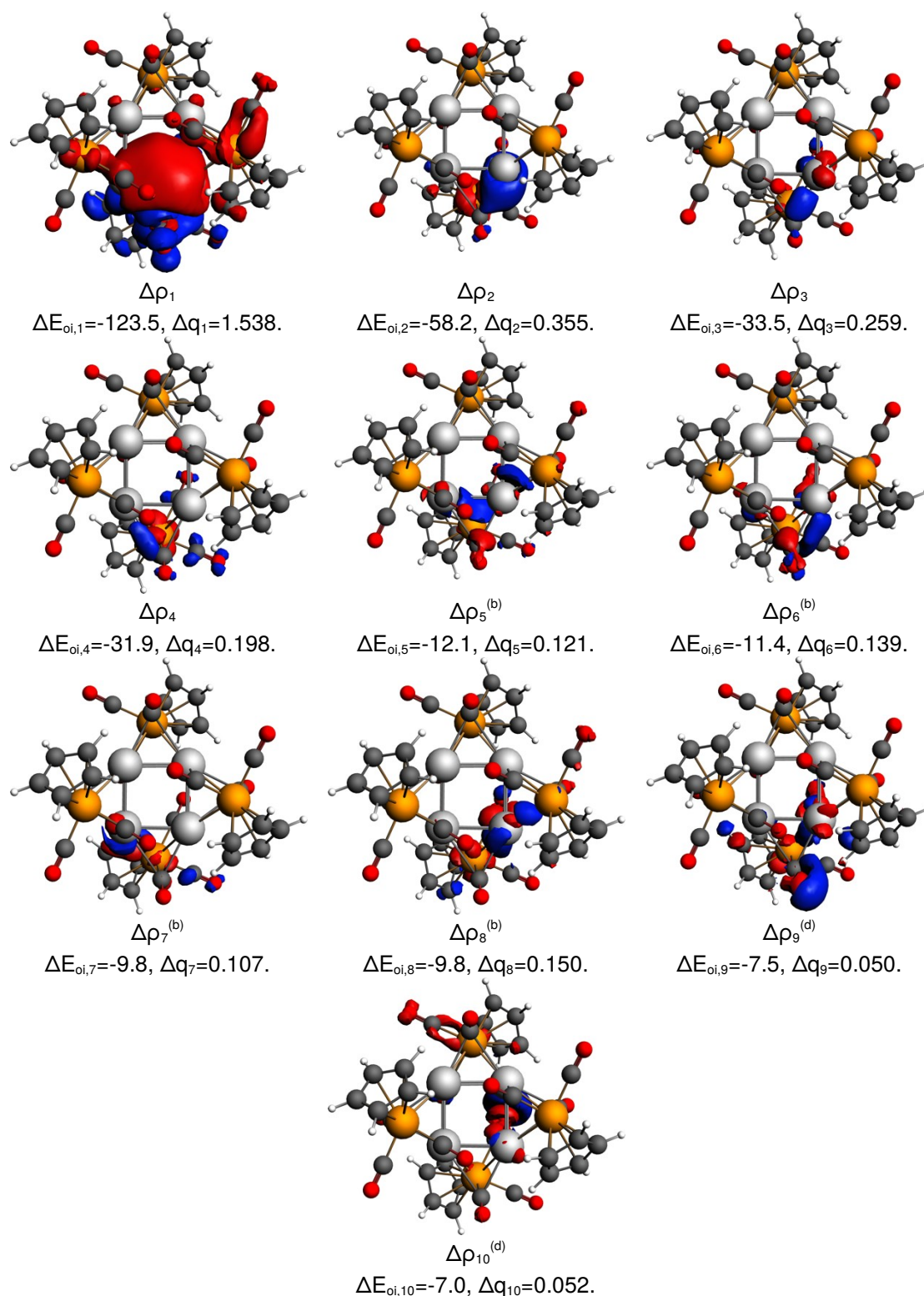


Figure S25: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **2e** in FSII scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

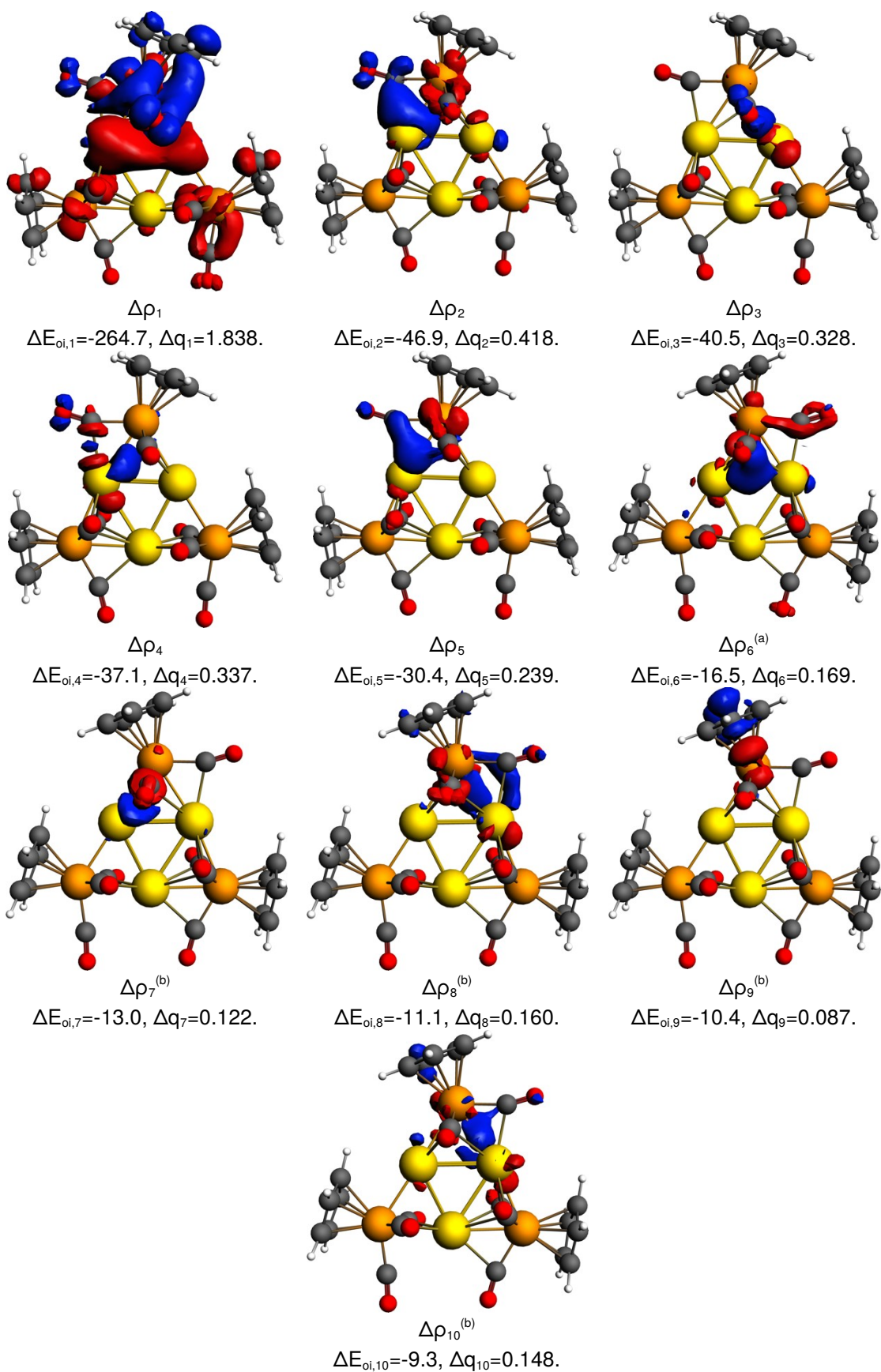


Figure S26: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **3a** in FSII scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and

charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

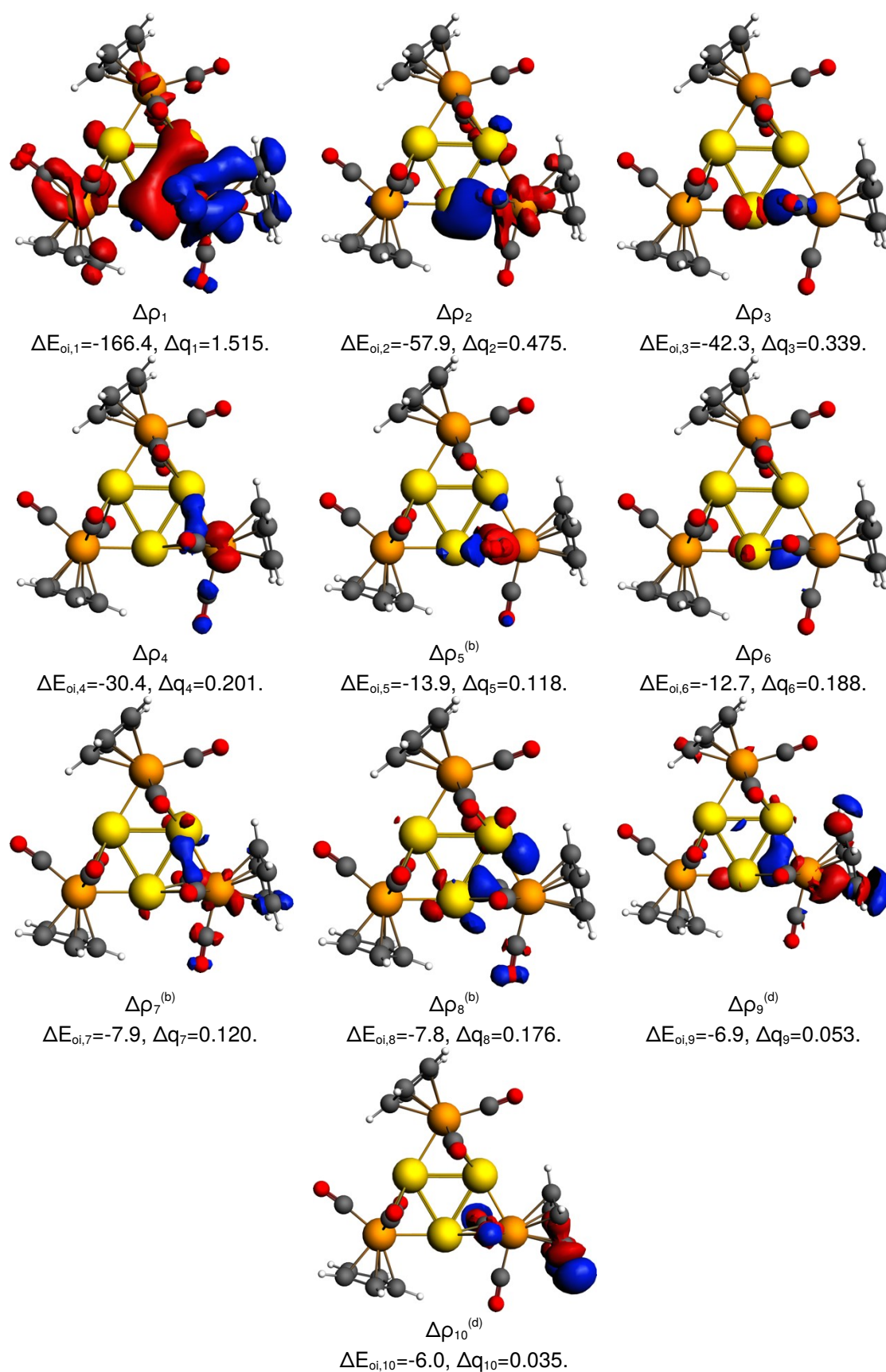


Figure S27: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **3b** in FSII scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

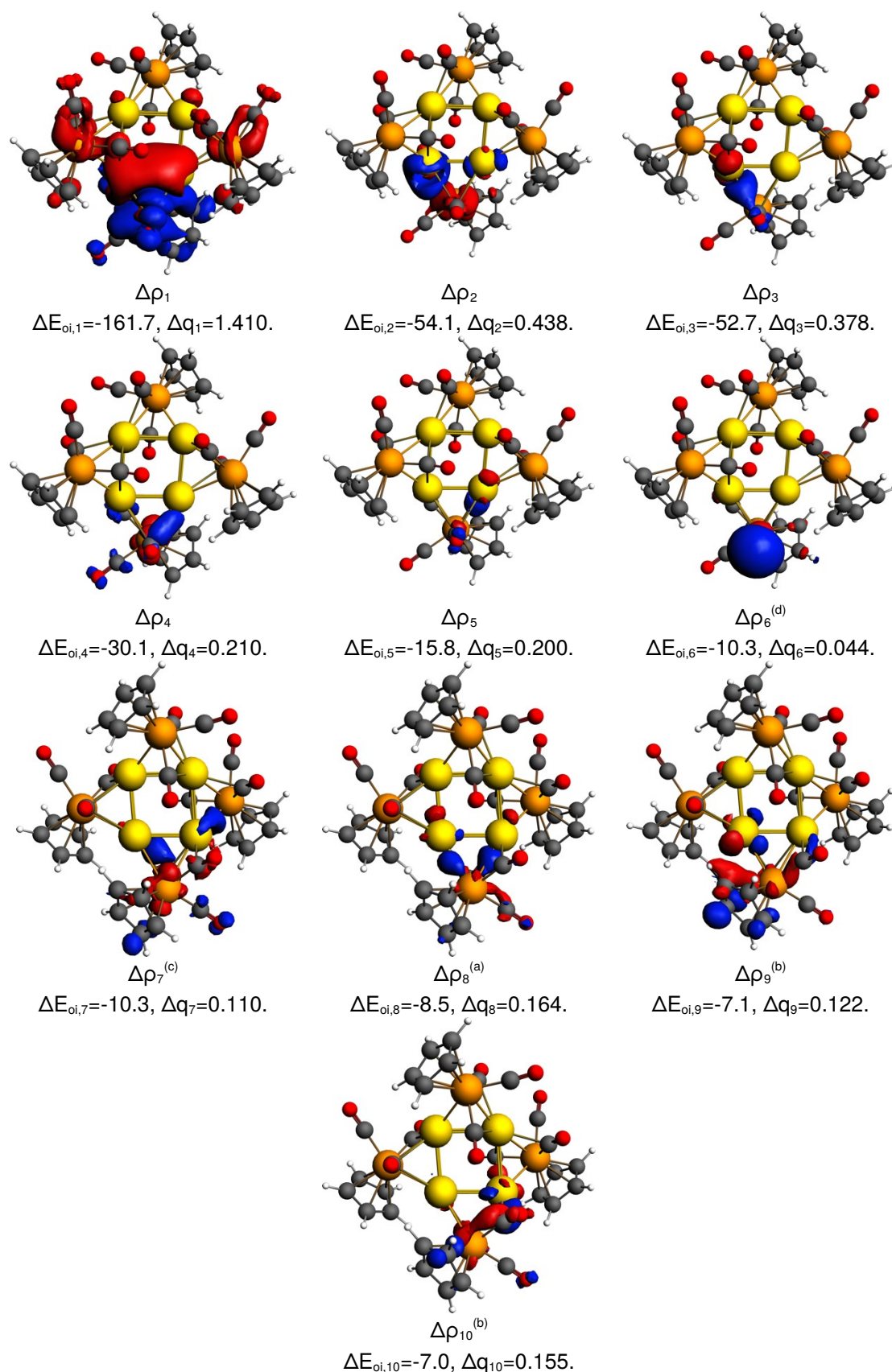


Figure S28: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **3c** in FSII scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

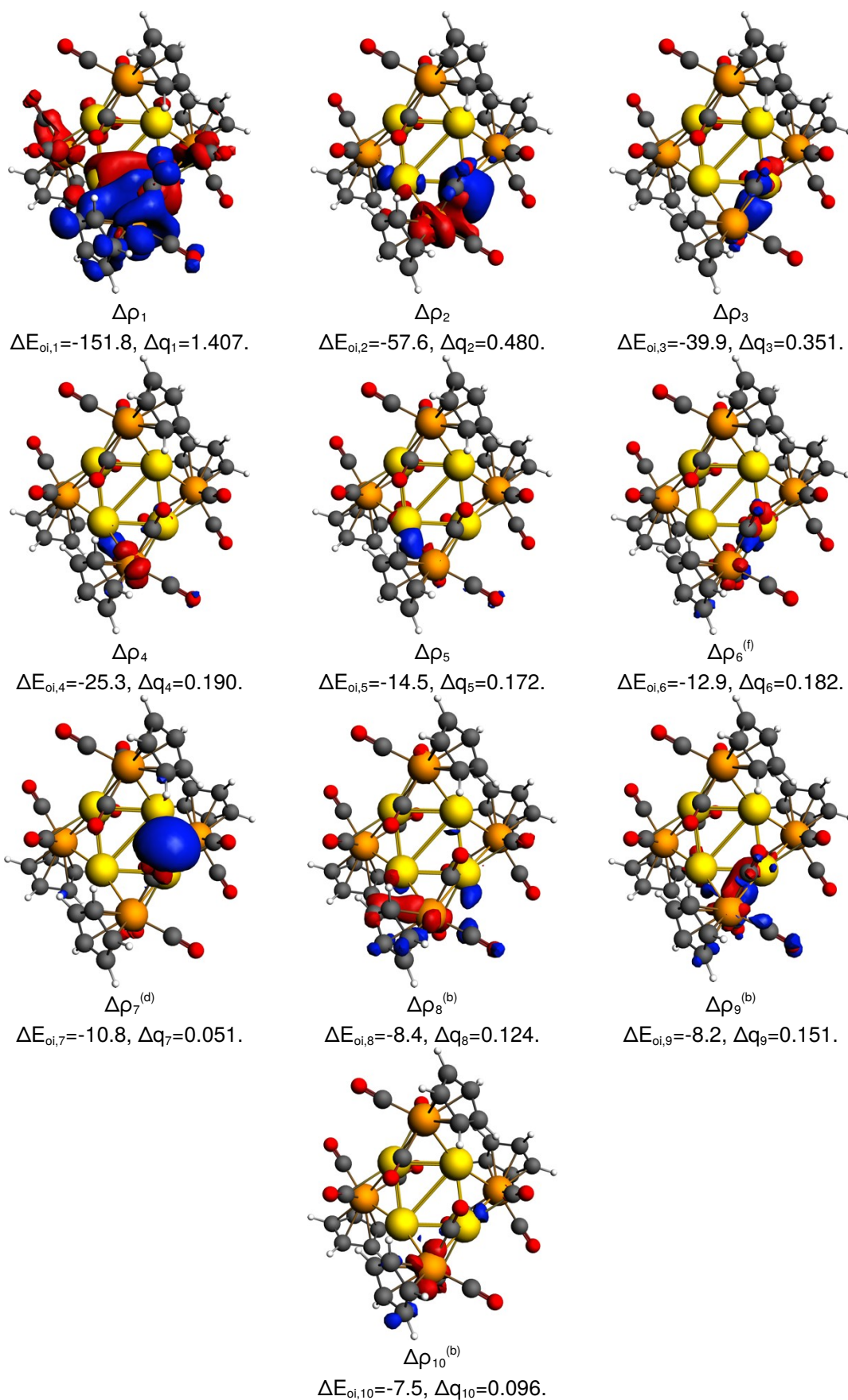


Figure S29: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **3d** in FSII scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and

charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

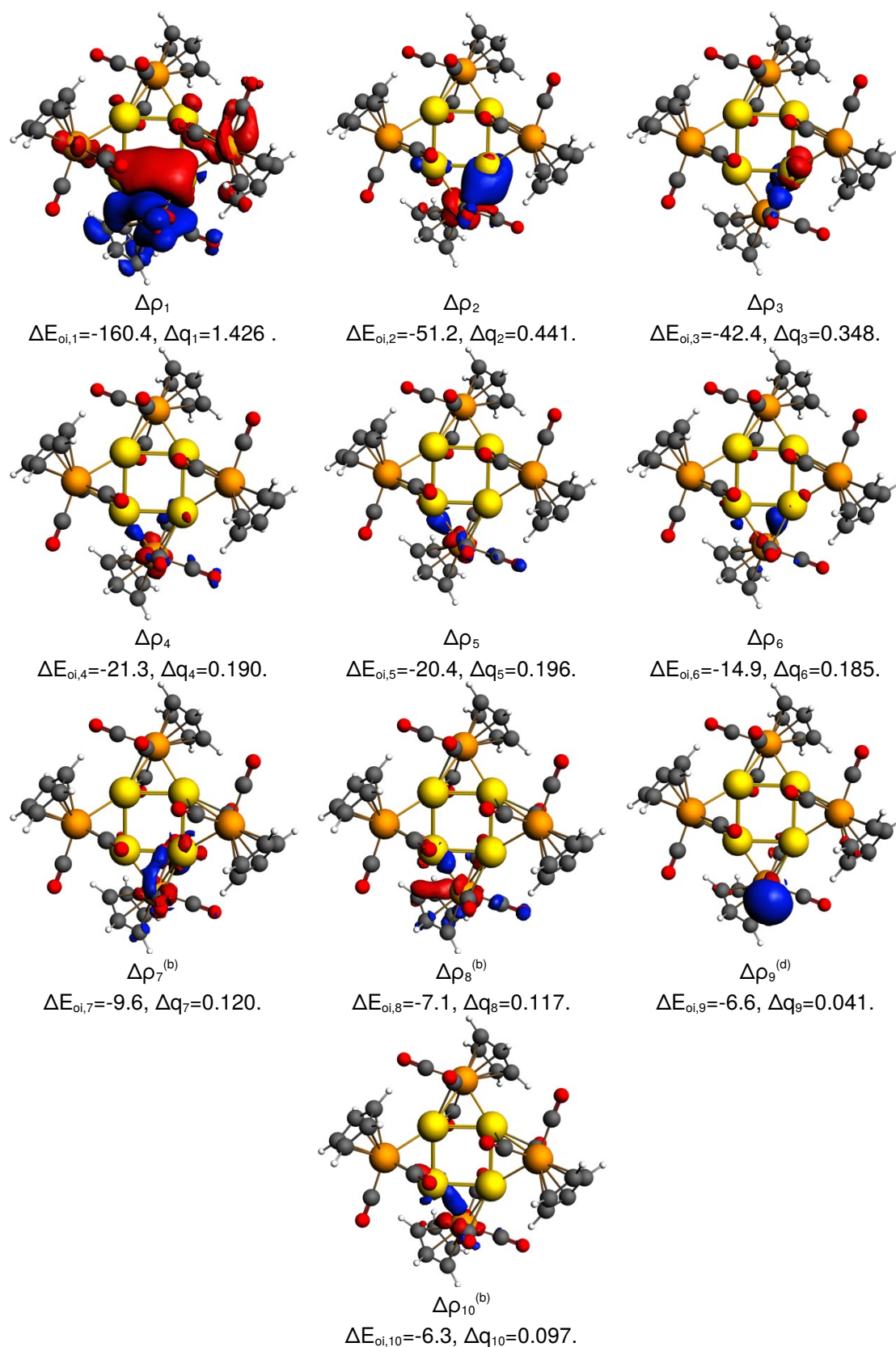


Figure S30: Selected density flow channels ($\Delta\rho_i$), describing the orbital interactions in **3e** in FSII scheme, with their energy, $\Delta E_{oi,i}$ (kcal mol⁻¹) and charge transfer estimation, Δq_i (a.u.). Red and blue surfaces indicate the electron density inflow and outflow, respectively. Contour value of 1×10^{-3} a.u.

List of coordinates for compounds 1a-3e

1a

Cu	1.04025743105119	1.05766016216572	0.31259535838681
Cu	-1.40191347187793	0.35115865520158	-0.10134262867687
Cu	0.33709691257309	-1.49580894229685	-0.05968048493977
Mo	-0.78288396135437	2.93679889832101	-0.02399238647363
C	-0.86361209072954	1.74847698395264	1.56899475651207
O	-1.06181717998036	1.30366944209280	2.62545274228951
C	-1.22288851924313	1.89528359832758	-1.64871516293141
O	-1.56069504479258	1.50322928462199	-2.68772313389017
C	1.12676019929411	3.07796728371166	-0.50090562341689
O	2.17913372633331	3.43234896974109	-0.84475946019098
C	-1.66818942122162	4.55834536031265	1.41693589295485
C	-2.72711064952475	4.10483914235274	0.57899534131048
C	-0.69460473101085	5.18001999070313	0.60504433133376
C	-2.39777550364597	4.45109659701853	-0.75478605856557
C	-1.14380815548804	5.11391793525450	-0.74706681968422
H	-3.62508284357721	3.60566843985709	0.90605284991818
H	0.22225692627246	5.63245250563023	0.94710555802293
H	-2.99858812408211	4.24874808068280	-1.62742306274555
H	-0.62852242057708	5.50941106186051	-1.60748088818821
H	-1.61757390158386	4.44102428348200	2.48798134494835
Mo	-2.23193619895268	-2.13853059931593	-0.09022866880046
C	-1.19721009933020	-1.94330766439839	1.59297040419895
O	-0.76579319500229	-1.88797962274509	2.66319743405214
C	-1.69667294955069	-4.03724339957541	0.04845960663314
O	-1.43493197694683	-5.15122514393743	0.12911681668670
C	-1.08189320424341	-2.12705893085797	-1.70454240439220
O	-0.60896788180007	-2.18665066473795	-2.75820843331464
C	-4.43862727145626	-2.56042457155552	0.48862438936256
C	-4.14876698741760	-1.24929480280568	0.92390574111759
C	-4.34426429483758	-2.58174177483198	-0.93706280769908
C	-3.99464736933311	-1.28213007145119	-1.36769875144274
C	-3.86956611375527	-0.44492200074210	-0.22056101668077
H	-4.70081780306372	-3.39405816453023	1.11997042883820
H	-4.52284391195432	-3.43373190538184	-1.57295160488144
H	-3.76076723689289	0.63170957958238	-0.22923750064458
H	-3.84014970497076	-0.96853138393062	-2.38819318862019
H	-4.13241562425644	-0.90984902411316	1.94769454071537
Mo	2.86239604475759	-0.83659151974322	0.14351350220905
C	2.07897882407276	-0.21371562968811	1.85545366015308
O	1.85589169611369	0.09682626967653	2.94819896897333
C	2.19490844159760	-2.68280632090647	0.37636089589595
O	2.04434135501712	-3.81915204659005	0.54338640473360
C	1.81950098355715	-0.25158135090565	-1.44382734141905
O	1.46608643659094	0.10589672525837	-2.48905694970893
C	4.99336605889292	-1.53572964019175	0.73900489055389
C	4.89633481225595	-0.15869498040270	1.05807120478770

C	4.87433663671226	-1.66488932949748	-0.67699576716013
C	4.71791042848604	0.57036365987302	-0.14664573679326
C	4.70479602390089	-0.36730232704630	-1.21455641986905
H	4.92022040670638	-2.58433102050383	-1.23790466585118
H	4.60860325984074	1.63911684222456	-0.23839016465120
H	4.57811115041962	-0.12809147925195	-2.25871844055395
H	5.14329849386505	-2.34107701252074	1.43991375452745
H	4.94652559414266	0.26426957255047	2.04907075307052

1b

Cu	-0.39013105921683	-1.40408269238829	0.12749806984880
Cu	1.44592831498304	0.30987517229138	0.26337380190149
Cu	-0.97043323966155	1.04557046065441	0.12972970417173
Mo	2.11420969800406	-2.22941197060326	0.20568281199763
C	4.06812747073068	-1.45142708207114	-0.82605974638774
C	4.27286396381282	-2.79241645138798	-0.43347055226464
C	4.20784864964973	-2.84680854093912	0.99280725771871
C	3.96255514243830	-1.53873842139088	1.46580776348207
C	3.87363372752384	-0.66080238251967	0.34523331343290
H	4.46225259650602	-3.62407456756180	-1.09277540980179
H	4.33872594960653	-3.72686745621688	1.60152298289502
H	3.85734262238447	-1.24487579365521	2.49836959592643
H	3.85762458108085	0.41992285575248	0.38555479894515
H	4.05779149942839	-1.07944619519887	-1.83859145400242
C	1.08664996663687	-1.92292104840756	-1.46311325980182
O	0.65009429266475	-1.81549779549919	-2.53094698841893
C	0.94843078047106	-2.05782034578862	1.79982564293025
O	0.42171114896695	-2.03038486268959	2.83166211115061
C	1.39116550706758	-4.05817551041761	0.09184243573785
O	0.97428117619090	-5.12930426590987	0.02422601434209
Mo	0.90212763369635	2.89019004092964	0.29812768633892
C	-0.61604259109342	4.23526139635347	-0.87548613708392
C	0.38690941268400	5.06484383590283	-0.32937419287653
C	0.29735193578698	4.98443902756844	1.09452545863199
C	-0.76046005894164	4.10376823219696	1.41247703448016
C	-1.33710057808088	3.63017492388053	0.19690937099326
H	1.08538607654218	5.66641264391089	-0.88839720497165
H	0.91549491811554	5.51454055285149	1.80097540478230
H	-1.08401922673841	3.82989009006911	2.40440883863867
H	-2.26374562349065	3.07930105762381	0.10656939994864
H	-0.81016302649799	4.07868737006293	-1.92499042886984
C	1.31292864478107	1.86518740798058	-1.35059711428578
O	1.54043938050575	1.44141916581562	-2.40455244958507
C	1.18808110669232	1.77729874840855	1.91394091625393
O	1.33085482457704	1.29831646843167	2.95955380164907
C	2.84671606485741	3.19832834940864	0.37777190135516
O	3.98005471759606	3.39484123259983	0.42392357151686
Mo	-2.92739030221655	-0.73385580401799	0.04064898605334
C	-3.22137777513870	-2.78171146260477	1.13928906830143

C	-2.40250224383032	-3.03674237300450	-0.00079588627526
C	-3.18165761773177	-2.73269427233415	-1.15661351564640
C	-4.45670898469831	-2.29726663625036	-0.73534620590221
C	-4.48202389767913	-2.32798885082614	0.69338332621809
H	-1.45207562667494	-3.55302341144554	0.00389248537337
H	-2.84544833248950	-2.82189991395525	-2.17764413373344
H	-5.27262493583674	-2.00971771499925	-1.37871389634515
H	-5.32007530647643	-2.06787820869370	1.31968459312397
H	-2.91989628578759	-2.91527874075600	2.16638641842361
C	-2.12951232037418	0.14833036737134	-1.54719376968335
O	-1.79858638971496	0.55902759910632	-2.57926144967399
C	-2.25312417805934	0.09591609878617	1.71067368537962
O	-1.99817114130949	0.47664007007824	2.77491203074386
C	-4.21391479508658	0.75731644164710	0.01446376597675
O	-4.98837026715569	1.60852016185076	-0.00251525305380

1c

Cu	-1.74733231062189	-1.02227897778622	-0.48506105467676
Cu	0.68737509709230	-1.51893870554623	-0.17852636534339
Cu	1.52014708241796	0.83692112484706	0.04808652480047
Cu	-0.96036188776384	1.41083334998462	-0.29218197716935
Mo	-0.85144692735462	-3.31189489983250	-1.43620157697650
C	-2.48268168527362	-4.30538557457158	-0.99462861761651
O	-3.42776122820057	-4.91040850779416	-0.73954685326183
C	-2.08647507446389	-2.06643895360942	-2.33965502359970
O	-2.79386720245719	-1.52527705242345	-3.08148438367791
C	-0.95173575094663	-3.00758410915435	0.52549382299628
O	-1.06380082789485	-3.03430874135614	1.68630187556058
C	0.82617711723807	-4.94625494087467	-1.70444691596716
C	1.42142460449536	-3.67857220976062	-1.94546439829611
C	0.80489494642678	-3.10552067555620	-3.08947637698389
C	-0.16518701709750	-4.02941659190485	-3.56329720933969
C	-0.15561401606575	-5.15482294582468	-2.70444599885707
H	1.08872820361458	-5.63854377864363	-0.92044623501961
H	2.25132418190919	-3.25659802688578	-1.40449793646334
H	1.04585109165639	-2.14761641856045	-3.52086065167208
H	-0.80490807832905	-3.89195587319668	-4.42050273189583
H	-0.78436906196708	-6.02610690551997	-2.79984869651532
Mo	2.98181964736791	-1.08639849401791	1.11507897378576
C	4.54742946682383	0.07704920728829	0.91728182294102
O	5.49052506824348	0.72866203786095	0.80854418969238
C	2.88557417770396	-0.81008450277750	-0.84689803819298
O	3.02120018742457	-0.73142328839183	-2.00275576769617
C	2.18538080149146	0.44458006845359	2.08483105810890
O	1.85478959318499	1.23206636003151	2.86404347862823
C	2.14178345809219	-2.58177451063343	2.70854772959572
C	3.44228039105837	-2.18297639574300	3.12231932213580
C	4.36968972579284	-2.65332382032291	2.15574189158590
C	3.65403675334280	-3.34770064104832	1.15394510459291

C	2.27419989835867	-3.30739797052722	1.49685549503046
H	1.21390062918522	-2.38498855977632	3.22094696820162
H	3.68210633611441	-1.62530538637979	4.01331791640305
H	5.43850851571320	-2.51114299333274	2.18367220852841
H	4.08425424713412	-3.83440222747310	0.29292065705286
H	1.47621496962759	-3.80493082453372	0.97196818127672
Mo	0.90838674216896	2.96027492165063	-1.31707655808388
C	-0.78394566671540	3.83414895954165	-1.85367100120165
O	-1.71672445918748	4.41148770353923	-2.19031758765360
C	0.28683477397730	3.15748605898166	0.56209546416713
O	0.04108029242601	3.46212383531180	1.64911229075427
C	0.30415853618055	1.31397576297264	-2.23493186073950
O	0.09096046356864	0.42231684546926	-2.94496017229278
C	2.86054650202092	2.82364823153701	-2.58941546774306
C	3.26757526858460	2.93191394111394	-1.23275495684882
C	2.81953088039319	4.19158774524474	-0.75140106252102
C	2.14766095861511	4.85970851930297	-1.80215714653722
C	2.17364428561895	4.00978686724288	-2.94804455148772
H	3.04579077820755	1.97550706512462	-3.22943618301433
H	3.87277588247636	2.22373917653313	-0.69134648821235
H	2.96618637635704	4.56967537303403	0.24820873465373
H	1.70781336198822	5.84263473704196	-1.74944652645464
H	1.75912952818319	4.23595703737818	-3.91709283900370
Mo	-3.35668611290456	0.72657002778736	0.55399125827628
C	-3.21703936233514	2.64828064094413	1.00474430211532
O	-3.21541838692926	3.75981090845403	1.29129958033954
C	-1.73045736290070	0.39044701658785	1.63465044001122
O	-0.93992890715271	0.12226757968990	2.43975721742471
C	-3.03624215641903	1.23120487787047	-1.33986518840972
O	-3.07034306934352	1.50849311509301	-2.45982535898253
C	-5.19356276184096	0.43144565178523	1.93820013177325
C	-4.47163567837886	-0.78455752691796	1.95124004543087
C	-4.49606564333384	-1.33646265847577	0.64061073905937
C	-5.23359996237340	-0.44656010683893	-0.18385442597253
C	-5.66991811675905	0.64444200881133	0.61037582519127
H	-5.36323102475121	1.07690062161346	2.78489118249043
H	-3.97904635198678	-1.22216842904014	2.80521676988073
H	-4.09135935051002	-2.29110721920122	0.34570985381083
H	-5.42430199900101	-0.58150190981929	-1.23702106037984
H	-6.26802338101779	1.47577397592942	0.27381418846401

1d

Cu	-1.40371633790987	0.00002266438469	-0.00001316085886
Cu	0.00002458867794	-2.04905321651682	-0.00016271084217
Cu	1.40365127851910	0.00011888185546	0.00008071566087
Cu	0.00001299272506	2.04925901210271	0.00004068642984
Mo	-2.10076114539759	-2.08020245877248	1.60688810155482
C	-0.30002713411344	-1.65819612685652	2.29975004201249
O	0.65017645497308	-1.41329366548539	2.91136340234242

C	-1.62183462590840	-3.93103994620826	2.08327785590886
O	-1.38814499505471	-5.00927307705687	2.40031409756667
C	-2.12573836098392	-2.79026055009290	-0.23927816289530
O	-2.37692527800271	-3.26594003665400	-1.26707895815415
C	-3.02430247362924	-0.64252259578084	3.21660916174258
C	-3.53676121584427	-1.94178874284374	3.42547001198650
C	-3.46783996264299	-0.18234489086617	1.94786808104430
C	-4.30890427203302	-2.30111965310044	2.28133019352490
C	-4.26164871438341	-1.21589680197739	1.37398318406463
H	-2.39277176146407	-0.08750895969863	3.88989500448245
H	-3.38143136165239	-2.55032694867916	4.30194887108787
H	-3.30504760359168	0.80735438293632	1.55287958165846
H	-4.84489057312014	-3.22558388909818	2.13915289104900
H	-4.75786802781662	-1.17905182788274	0.41745459611399
Mo	2.10071199820832	-2.08021570386580	-1.60704373474076
C	0.30002361819973	-1.65819014600015	-2.30009909306779
O	-0.65013712268477	-1.41323449333542	-2.91174837034300
C	1.62196227066849	-3.93092030249320	-2.08410085800896
O	1.38835901737797	-5.00905344479353	-2.40154995606768
C	2.12531225438347	-2.79087391476702	0.23892278323694
O	2.37632253845120	-3.26692936685014	1.26659138765831
C	3.02446706881437	-0.64225385111634	-3.21640469386745
C	3.53698815807725	-1.94149282250176	-3.42531830351616
C	3.46777059866346	-0.18222874055392	-1.94749302263127
C	4.30899415468065	-2.30090220714304	-2.28113294857396
C	4.26151547552976	-1.21586516293532	-1.37362437543006
H	2.39300932108773	-0.08721286521178	-3.88973801994708
H	3.38183325433427	-2.54993757752891	-4.30189364191355
H	3.30488763615792	0.80740875273754	-1.55238229971910
H	4.84503633516298	-3.22534632333845	-2.13902797796047
H	4.75755907725602	-1.17919545857800	-0.41699839719667
Mo	2.10082895220426	2.08025190741187	1.60703578285846
C	0.30013970271580	1.65832718558562	2.30008952485941
O	-0.65002440045958	1.41344484004880	2.91176150558307
C	1.62228242113002	3.93111446844642	2.08367155543630
O	1.38884194939923	5.00935050146534	2.40089329502600
C	2.12544737372159	2.79047644765955	-0.23907088597734
O	2.37647731822117	3.26627308641324	-1.26686466400744
C	3.02437709634585	0.64243536252997	3.21667703638806
C	3.53702313148994	1.94163651142247	3.42544071693696
C	3.46765625868426	0.18219515309436	1.94787044311670
C	4.30911432662139	2.30084423032559	2.28122077669478
C	4.26156145003781	1.21563801258523	1.37388652979670
H	2.39283532937167	0.08753791941310	3.89005025179453
H	3.38186013215686	2.55021082433263	4.30192517979933
H	3.30467580813919	-0.80748219780116	1.55289185069869
H	4.84520624571829	3.22523577621599	2.13897200228063
H	4.75769118088881	1.17873581668112	0.41731495303752
Mo	-2.10083510106416	2.08029069986484	-1.60691691729405
C	-0.30014588828231	1.65828283739484	-2.29991006511822

O	0.64999263317866	1.41328239512158	-2.91157965186945
C	-1.62205803628877	3.93112245930720	-2.08350564750159
O	-1.38846530818492	5.00932267614780	-2.40073059052952
C	-2.12570840358331	2.79038758387388	0.23925096046378
O	-2.37683845594409	3.26604420949331	1.26707677310455
C	-3.02430014022198	0.64242911170684	-3.21651058348266
C	-3.53682111362752	1.94165255834934	-3.42548913332068
C	-3.46781378234580	0.18233672788490	-1.94772945218380
C	-4.30900019849088	2.30103310095460	-2.28138777981475
C	-4.26167922436090	1.21590111013546	-1.37394099321157
H	-2.39272195650009	0.08739891292350	-3.88973888158080
H	-3.38151865507996	2.55012142620391	-4.30202091261534
H	-3.30499381639369	-0.80732589297498	-1.55265739613789
H	-4.84504997400216	3.22547319176441	-2.13929459277270
H	-4.75790398091023	1.17911312058507	-0.41741295384918

1e

Cu	-1.56124310132728	-0.89530849377677	-0.01538571191865
Cu	0.88977735031284	-1.56578507318895	-0.04207262498435
Cu	1.56855986658557	0.90674764385500	-0.01452572874509
Cu	-0.90328661685571	1.56563723170174	-0.07103030374130
Mo	-0.90934390835981	-3.34979388225164	-0.73556066332663
C	0.77725798553965	-4.31515069308212	-1.00704962907991
O	1.72094249952909	-4.94628350157085	-1.20985258885285
C	-0.17100241859633	-2.01209562507252	-2.00400425543349
O	0.16803921362279	-1.39036830614324	-2.91677095504151
C	-0.35741838635331	-3.09409174836518	1.15210095224414
O	-0.12243415007659	-3.13941614897855	2.28464095251033
C	-2.00460944394550	-5.12696335114708	-1.77043515893389
C	-2.52708516343707	-3.94044664333579	-2.33288880448820
C	-3.18896969371599	-3.21700681375653	-1.30392176333498
C	-3.06991494762462	-3.96387497013896	-0.10302471983749
C	-2.33992984983829	-5.14925983114545	-0.38893461682580
H	-1.44981394157071	-5.88601274591080	-2.29898494728877
H	-2.43445976865654	-3.63024162929928	-3.36167932806059
H	-3.72853803468718	-2.29440429776844	-1.43226340579367
H	-3.48535097419304	-3.68614508079080	0.85181646294627
H	-2.09719432666407	-5.93235768808571	0.31109448507142
Mo	3.30887231235684	-0.90548495874558	0.73747513635230
C	4.19646418861813	0.81600460385865	1.04998818207655
O	4.79738234661590	1.77093678921855	1.29205640590976
C	3.04731054678072	-0.41205750680007	-1.16722393392616
O	3.08293351146373	-0.22229810581551	-2.30971651523783
C	1.86909672731015	-0.25542247272218	1.93997092259445
O	1.17125004608639	0.03197138411680	2.81546426535206
C	3.83493105441295	-2.54103014345281	2.33622344129670
C	5.03614074613248	-1.92647243533802	1.91530141698255
C	5.21894572838478	-2.21125995947697	0.53250855306263
C	4.11859998558088	-3.00253550736291	0.10708302869102

C	3.26464785690927	-3.21106414092735	1.22038648770109
H	3.41396135934393	-2.50169241257433	3.32853370141378
H	5.70108190371568	-1.34664714185871	2.53562999078773
H	6.05152393020908	-1.89755613420477	-0.07622198044097
H	3.95958241601447	-3.39520897800401	-0.88409162090784
H	2.37046518546001	-3.80972189899215	1.23513581904918
Mo	0.91954441392637	3.33913089593512	-0.76903442284101
C	-0.77560713478198	4.30487528601182	-0.97172294906285
O	-1.71765709496976	4.94859879257178	-1.14245141242773
C	0.45329591561578	2.98410017033105	1.12655048693126
O	0.27744249185651	2.97313661909083	2.27260934355398
C	0.19072183091365	2.02352776176619	-2.06688325111818
O	-0.12974268675364	1.41628552927034	-2.99345575824358
C	2.58123415626565	3.83065237173240	-2.35235589189318
C	3.23225378205141	3.25869211012911	-1.22720597466856
C	3.02069754627880	4.12304134944623	-0.12089994935676
C	2.24766097149944	5.22863311256211	-0.56054235924246
C	1.97556276607923	5.04186018483502	-1.94676526534012
H	2.54819279207310	3.40420546574875	-3.34259739881759
H	3.82299061408226	2.35879872480007	-1.23061903017904
H	3.39943005197864	3.96447206439556	0.87560124542705
H	1.93826910819728	6.06853503210455	0.04030737175708
H	1.41319305666902	5.71104227552908	-2.57833360961409
Mo	-3.34102324609264	0.90519393670909	0.71386087008458
C	-4.47095419569992	-0.69565896941416	0.71946225219630
O	-5.20934441203199	-1.58016588091586	0.76086717355315
C	-2.17134917541737	-0.07391373877209	1.98493416318786
O	-1.65447709709597	-0.54445265507670	2.90354746330582
C	-2.98819312072143	0.49237870240855	-1.19674243528168
O	-2.97852537618362	0.32607519046964	-2.34384757195411
C	-3.65742238048353	2.50576733948136	2.40188745526466
C	-4.91734029885375	1.98150553267353	2.03099239139157
C	-5.15912099896163	2.33957840916549	0.67116342179552
C	-4.04166550245408	3.08107912798153	0.21538500062210
C	-3.11171693984178	3.18887928563212	1.28457669275038
H	-3.18236509550804	2.39972606314561	3.36450533609589
H	-5.58328284325710	1.42172022741186	2.66809675507521
H	-6.04293911518215	2.10444534378289	0.10032875595150
H	-3.91474439761606	3.50622794123970	-0.76686085998458
H	-2.19019042066394	3.74418706515070	1.27587101323964

2a

Ag	1.34602753761226	0.90789669130160	0.00331480243605
Ag	-1.52054842622993	0.76128531271654	0.01909115853821
Ag	0.17503651890347	-1.70053013854914	0.00657350713753
Mo	-0.26166927968145	3.28048235795071	-0.02029979363642
C	0.18000797178772	2.36039631369323	1.69340253552556
O	0.35100815567327	2.02766730622080	2.78677712608621
C	0.15355423774573	2.31047790923834	-1.71352987231349

O	0.30907405662569	1.94654811687550	-2.79901773015528
C	1.58994286168054	3.94068973700882	-0.04534970160726
O	2.64965766662622	4.39510964688674	-0.06042455939542
C	-2.00883636481902	4.32660274753982	1.12434382680403
C	-2.59326186215522	3.69669866372486	-0.00908931589155
C	-1.10542164786165	5.31799713892974	0.67151826256375
C	-2.02524195853117	4.29554524727444	-1.16740057982957
C	-1.11567406895570	5.29861965127629	-0.75459341585391
H	-3.38123605837479	2.96136846030057	0.00634634173376
H	-0.52648651490792	5.98021070206939	1.29473330334170
H	-2.25569540777214	4.03291719371109	-2.18790509181350
H	-0.54532945928463	5.94323249732327	-1.40366692061702
H	-2.22531583508517	4.09278098430872	2.15486751348251
Mo	-2.66647992541897	-1.82673024588760	0.03446729033576
C	-1.83041677840142	-1.17952485116671	1.72752063248826
O	-1.56195799097629	-0.88400321249919	2.81155765067940
C	-1.68752251672374	-3.54349307371028	0.01643818131882
O	-1.29995985169226	-4.63059337790340	0.00650484860566
C	-1.88176960771144	-1.19007231267081	-1.68676014996174
O	-1.64399770376249	-0.90188182199760	-2.77946668665133
C	-4.54156698791211	-2.98548454804062	0.73581528746222
C	-4.66311253167950	-1.66479870723829	1.23007033227409
C	-4.56880565872735	-2.92329996576408	-0.68929164250449
C	-4.70508500923892	-1.56211230656573	-1.05902242459877
C	-4.77363648063902	-0.77902593181922	0.12407931442279
H	-4.45835784141218	-3.87982254703176	1.33192179561834
H	-4.51253344379759	-3.76196363333496	-1.36409751639526
H	-4.91558878314422	0.28767839190325	0.17489322576025
H	-4.75755023845161	-1.18526255830709	-2.06826027565712
H	-4.67518969794364	-1.37975293364576	2.27022823460402
Mo	3.01539966412277	-1.32020364817629	-0.02158254408962
C	2.01833584339535	-1.37652595688901	1.70643274476252
O	1.65985432881817	-1.40778996497624	2.80291980553932
C	2.90837830189301	-3.29079178653297	-0.03154073395107
O	2.93559878292640	-4.43954084946754	-0.03843263509947
C	1.98227913927142	-1.35821003158873	-1.72890220838990
O	1.59973543912418	-1.37798727676003	-2.81740024528684
C	5.21666804822458	-1.36454876177782	0.66034503429592
C	4.67780557318760	-0.13759356263006	1.11719578821828
C	5.19679130045721	-1.34516314546515	-0.76585668864961
C	4.33369925909093	0.65527959031423	-0.01294125071425
C	4.64538818522711	-0.10622672549567	-1.17354330395608
H	5.55455873210166	-2.12542402541713	-1.41793335495266
H	4.00885486971048	1.68398175921078	0.00575883920536
H	4.49712928946370	0.21559541759247	-2.19233554786183
H	5.59176991270570	-2.16238632938981	1.28067985369818
H	4.55746625491634	0.15553039332751	2.14826295289498

Ag	0.47669628155101	1.54598452364960	0.03657096300820
Ag	1.15949923791964	-1.23867245692118	0.09791211719454
Ag	-1.60498393489445	-0.42854913206183	0.06157745155773
Mo	3.17234924695637	0.79556566856836	0.07099314622495
C	3.75273261574893	2.72630043589265	-1.10813548696883
C	4.93627858613793	2.08942043415392	-0.66388517788977
C	4.93588227264438	2.11451616088229	0.76209627723758
C	3.75204931370926	2.76670627546856	1.18316886183231
C	3.01792079962912	3.16274753070304	0.03004556749704
H	5.70777991189127	1.67550961954540	-1.29284192356936
H	5.70713790974746	1.72304281085055	1.40552577469056
H	3.45805974194832	2.94611773625156	2.20534806484086
H	2.13167311680189	3.77799506606039	0.01919166513840
H	3.45907846001151	2.86916382989422	-2.13617538669241
C	2.37402952722698	0.11369877455549	-1.62474961495979
O	2.08125847893847	-0.15724674960146	-2.70887650002723
C	2.36078884672294	0.17809847770846	1.78598617195329
O	2.05890950401633	-0.04981933400344	2.87737350261367
C	4.25540987036684	-0.84960607875156	0.10072798533849
O	4.94738206895135	-1.77045832196420	0.11522531839314
Mo	-0.84227088491868	-3.18591651438084	0.08333500791552
C	0.50626321052536	-4.71764665640224	-1.05126229060387
C	-0.67023979157585	-5.37753459100764	-0.62117234402419
C	-0.67601308444262	-5.37275008767703	0.80494835037862
C	0.49721029385712	-4.70983415709263	1.23999439681310
C	1.24381968977979	-4.31260176500325	0.09591841726295
H	-1.41840023403625	-5.81977650525029	-1.25895145102699
H	-1.42939495918029	-5.81072199463173	1.43949470186070
H	0.78601534869926	-4.54263869183684	2.26573717201770
H	2.22954120227094	-3.87494966755222	0.09822827215202
H	0.80274604162144	-4.55649281494339	-2.07580742478465
C	-0.95201885681734	-2.14989838888740	1.78519438091125
O	-0.99776989411951	-1.75700378629394	2.87049582698432
C	-2.81180264257316	-3.22365538996273	0.07272346823187
O	-3.96047656046592	-3.31781301944640	0.06651215216516
C	-0.93359490153713	-2.16555711795481	-1.62890640796263
O	-0.96587279746220	-1.78440993496588	-2.71869675130057
Mo	-2.30129227364213	2.27492991789950	0.00764450801224
C	-4.30558466605403	1.84855087848346	1.13067140028552
C	-4.29419700267395	0.98787503327412	-0.00260243064157
C	-4.27192922623877	1.81461230005024	-1.16050209879882
C	-4.29139187586511	3.16855987421483	-0.74806524701559
C	-4.31238651729756	3.18945239640382	0.67802371936943
H	-4.39437813610121	-0.08616469813917	0.01173056283216
H	-4.25503145895686	1.46467018497877	-2.18065043660548
H	-4.30669069695743	4.02896812195276	-1.39732188908792
H	-4.34593210684573	4.06857865449382	1.30103311149840
H	-4.31909341124561	1.52906824033635	2.16082400725336
C	-1.32626919909030	1.86531933432862	-1.68371821599162
O	-0.95778282278529	1.71216959228005	-2.76793641792569

C	-1.39528940832279	4.02383380746001	0.00295916035696
O	-0.92867640397735	5.07730666356935	-0.00149059222138
C	-1.36203632099471	1.89687006630257	1.72685979974908
O	-1.01009453060173	1.76492615151933	2.81929078452726

2c

Ag	-2.03776990019331	-1.09952718487550	-0.57350311808403
Ag	0.68188801780130	-1.53068728854588	-0.17178309737478
Ag	1.62805646784946	1.05916097539052	0.23350270899599
Ag	-1.11056845135100	1.59825463531918	-0.31551068929310
Mo	-0.85911563614048	-3.45007443264744	-1.66669352327256
C	-2.66248111578098	-4.20805190556400	-1.73221748341343
O	-3.70560274848529	-4.69345522573091	-1.78886244642017
C	-1.65752444617168	-1.96809618469006	-2.72879158916976
O	-2.06273544769894	-1.28469224147653	-3.56791082016381
C	-1.22635210611750	-3.41689107517521	0.29142778780273
O	-1.42373243792055	-3.60142776440407	1.41951698350831
C	1.03506324333596	-4.83161895179990	-1.47079669078842
C	1.47158816393891	-3.65431749636281	-2.14266935234772
C	0.75699808761650	-3.56962937438281	-3.36330015580490
C	-0.10178952590703	-4.69409507492630	-3.45946514661114
C	0.07301862051486	-5.47696013759065	-2.28073958087115
H	1.39384318355989	-5.18789855019194	-0.51849296505122
H	2.25903423960653	-2.98773538482043	-1.83248013091639
H	0.85971554819604	-2.78177877025019	-4.09262917906287
H	-0.75486089152386	-4.92450917585202	-4.28559177261159
H	-0.42495500483532	-6.40610708876900	-2.05501224190430
Mo	3.11967220719286	-1.11992833538347	1.29239228533093
C	4.57159108415314	0.18568860498606	1.44370175331089
O	5.45866995801568	0.91355616841706	1.54694533987325
C	3.27693294759647	-0.72193485350442	-0.65227857167344
O	3.53906619497474	-0.60762161915135	-1.77665959806458
C	2.07349358117376	0.17103845291818	2.39197279462068
O	1.59372531636195	0.77526187711146	3.25160837649132
C	2.54771169851813	-2.70321316999403	2.92680698588091
C	3.93492118415207	-2.42612770327877	3.01465999158641
C	4.54460786687853	-2.86597591057251	1.80326446439640
C	3.52969686755705	-3.40822281002250	0.98048520375542
C	2.29113953386612	-3.32141913802892	1.67723933376136
H	1.80708543710779	-2.48867618567750	3.68090299202053
H	4.44060702523969	-1.97871800236640	3.85507615300036
H	5.59465655903999	-2.81378415496710	1.56502914798855
H	3.67717067172531	-3.83517398322766	0.00119146625884
H	1.34066452453360	-3.71521488414979	1.35771980812558
Mo	0.98522163547860	3.16348603815141	-1.45478786729847
C	-0.65588574304224	3.95857845335149	-2.21020948329259
O	-1.54695438185230	4.48965933479139	-2.70367890127082
C	0.29073490080897	3.56739222372754	0.37732949088869
O	0.03217095339472	3.99379673080217	1.41929514497551

C	0.49597694647016	1.44474645849541	-2.33103041366758
O	0.38198494069008	0.51256077632472	-3.00396959465910
C	3.03977422676535	2.91931244671972	-2.52388583865095
C	3.33586936800716	3.25143107138951	-1.17543644100433
C	2.79996821962660	4.54503378933100	-0.92746637338632
C	2.19521600600425	5.01591040342388	-2.11689376682162
C	2.34526895567219	4.00756086503461	-3.11347365344712
H	3.31052144856005	1.99661376373704	-3.01252385299804
H	3.92371448019396	2.66376629091268	-0.48848430527088
H	2.85281385619118	5.07878187178992	0.00842828892548
H	1.72010396704329	5.97459900675704	-2.24929451662005
H	2.00819395950231	4.06748790649125	-4.13561792108163
Mo	-3.63342013238128	0.76379703559259	0.71048696067310
C	-3.43883709137971	2.64831280810932	1.26861348985123
O	-3.42184845032762	3.73487216433786	1.64133009579755
C	-2.00768017939921	0.32220766467232	1.77487826304117
O	-1.22464291543581	-0.01341730587441	2.55524043194850
C	-3.43880290521102	1.33640072069013	-1.19535582231237
O	-3.56993765879906	1.64745424361288	-2.29937589798624
C	-5.30171043835747	0.36676104415765	2.25169113725930
C	-4.69389068711446	-0.88339456861891	1.97453463660263
C	-4.93625625189997	-1.21270231271385	0.61356967965372
C	-5.68124123333261	-0.14450183660279	0.04509252948546
C	-5.91512771713747	0.82682701050681	1.04928311699690
H	-5.31159444012824	0.87041306975531	3.20465105965450
H	-4.14620771040904	-1.49163812319983	2.67711175466969
H	-4.66773167998288	-2.13444010397453	0.12248278156372
H	-6.01739284358558	-0.08891896615794	-0.97839480340561
H	-6.47288192301353	1.74144336871408	0.92877516737742

2d

Ag	-1.54285390401747	0.00018893650133	0.00001735968452
Ag	-0.00009441199051	-2.33191077682145	-0.00022078246417
Ag	1.54275902132964	0.00012570866483	-0.00035121245927
Ag	0.00009773651434	2.33235552203083	-0.00029208898500
Mo	-2.23908682257320	-2.16448115789553	1.74323879406661
C	-0.41030119276685	-1.75517372635419	2.41060406095325
O	0.54570305289888	-1.49716647376691	3.00676671613774
C	-1.82035409764241	-4.04780958446152	2.12950007262828
O	-1.63961689764015	-5.14920784700264	2.40356307121449
C	-2.44886100063458	-2.75843765477790	-0.14311209749145
O	-2.81256222329857	-3.13784889360109	-1.17656783563516
C	-3.03259662890029	-0.71349724165262	3.40294066795678
C	-3.53242106580587	-2.01452634116554	3.64906868769821
C	-3.57672524983184	-0.24466965390126	2.17829997133422
C	-4.38691795215286	-2.36781540096546	2.56356331022706
C	-4.40201578979017	-1.27977818193979	1.65657101019943
H	-2.35566222640155	-0.15854186104220	4.03186318907022
H	-3.31839781087878	-2.62346929387962	4.51262996037333

H	-3.45417086558997	0.75015400340868	1.78210641717901
H	-4.93535505274535	-3.29002035844730	2.45917113822915
H	-4.96242179820473	-1.23801869926150	0.73584548849149
Mo	2.23930415456710	-2.16480239946180	-1.74311204379923
C	0.41057415578708	-1.75557803019860	-2.41071434996228
O	-0.54531456274432	-1.49756938728513	-3.00707264941923
C	1.82081826080710	-4.04808931822444	-2.12978289810823
O	1.64021120888630	-5.14944404959674	-2.40410813021152
C	2.44870836720126	-2.75906517509241	0.14318370893434
O	2.81213999807805	-3.13849964621812	1.17671454304117
C	3.03292721493815	-0.71324786135136	-3.40230957651280
C	3.53266507692980	-2.01423733405188	-3.64887786588188
C	3.57709259856739	-0.24489298615766	-2.17749797329839
C	4.38709444847559	-2.36796113619441	-2.56347690291095
C	4.40229513933245	-1.28025430531314	-1.65610132735526
H	2.35603434932521	-0.15802604927092	-4.03103919667610
H	3.31860786185621	-2.62287788689549	-4.51264376695281
H	3.45471116953451	0.74983975486449	-1.78101791329894
H	4.93546432692976	-3.29024397951685	-2.45940348070758
H	4.96269973913548	-1.23885722364957	-0.73535938876158
Mo	2.23895923980143	2.16465701520264	1.74315469013216
C	0.41019660317512	1.75554257584894	2.41075827615900
O	-0.54576827713069	1.49759230880028	3.00699485902382
C	1.82060483625269	4.04802661202180	2.12962276210077
O	1.64014273774526	5.14943830483918	2.40381599515719
C	2.44864161305793	2.75865507662507	-0.14320569228717
O	2.81243260682346	3.13804092397896	-1.17664561258902
C	3.03252632955663	0.71341319567303	3.40260578070050
C	3.53252773932332	2.01436363181800	3.64879791213753
C	3.57644787524367	0.24464949101521	2.17785163505674
C	4.38692183786723	2.36767138471338	2.56322005738515
C	4.40178120683372	1.27972687423654	1.65611335599828
H	2.35561668201432	0.15846769613145	4.03156131807452
H	3.31869370466158	2.62323613420040	4.51245592894779
H	3.45374336493628	-0.75012420537798	1.78157681228026
H	4.93544975097850	3.28982448422690	2.45885052905718
H	4.96207036575886	1.23799817114117	0.73531554727028
Mo	-2.23921649577852	2.16467723146951	-1.74328916474061
C	-0.41049706155502	1.75542992643842	-2.41090818295140
O	0.54542519628094	1.49739146945752	-3.00719172828442
C	-1.82076279126541	4.04805374981851	-2.12964922066471
O	-1.64023573011579	5.14946141256257	-2.40381340066343
C	-2.44882200050079	2.75853966688310	0.14310633035138
O	-2.81244284706103	3.13789452276492	1.17661050796250
C	-3.03282412987327	0.71338873377479	-3.40266911033066
C	-3.53261842545354	2.01438929637586	-3.64903484834831
C	-3.57693061589382	0.24482026542707	-2.17792069035446
C	-4.38706618586271	2.36791656298131	-2.56356621498517
C	-4.40217144657012	1.28006181374183	-1.65636387805906
H	-2.35593543609324	0.15828309584644	-4.03150875801593

H	-3.31861954450737	2.62315142395308	-4.51272963492455
H	-3.45443508335954	-0.74994449342760	-1.78156344527359
H	-4.93547189261531	3.29015830923465	-2.45933206952319
H	-4.96254205415958	1.23850332754792	-0.73560733232681

2e

Ag	-1.66723659311534	-1.03344399208449	-0.13472179675001
Ag	1.03584682370776	-1.67212123583602	0.13575572189102
Ag	1.67129361936109	1.03203280427799	-0.13972366579132
Ag	-1.03135968000275	1.66951140398636	0.13840587328942
Mo	-0.60692947081102	-3.06660066039839	-1.77776532218932
C	0.95306992745473	-4.25125912978458	-1.94153775405726
O	1.84103877684003	-4.97111000333454	-2.07370084354758
C	0.65601633219822	-1.63316741863132	-2.32176854894355
O	1.32013646889276	-0.86335646994429	-2.87362237352006
C	-0.59382739501156	-3.63436052703435	0.12891665790992
O	-0.69857961459258	-4.14891420466637	1.16167469138101
C	-1.47466508963770	-3.73713428313294	-3.80754263246105
C	-1.93504322066195	-2.41555433607709	-3.59277563246866
C	-2.79270048280180	-2.41497949890588	-2.46055238670838
C	-2.84252116925965	-3.74899532035944	-1.96452136775818
C	-2.03979626458858	-4.56720265049600	-2.79396557339520
H	-0.82893146667378	-4.06162581872896	-4.60749701596629
H	-1.68815003764664	-1.54824120805500	-4.18360238580919
H	-3.38794450098171	-1.57983957238965	-2.12617955410712
H	-3.41098612838514	-4.07836550404043	-1.10882346022757
H	-1.89641711686972	-5.63049776546603	-2.68933408629224
Mo	3.06663071759471	-0.60647743386353	1.77750763172689
C	4.25170851512401	0.95338795499395	1.93904204676184
O	4.97187293206240	1.84132321960648	2.06971604143618
C	3.63485755296184	-0.59557901321234	-0.12910409010187
O	4.14980039777893	-0.70134412100601	-1.16158378466376
C	1.63319202686062	0.65738004384171	2.31948883057143
O	0.86327692670109	1.32196270671391	2.87058812506859
C	2.41545902222584	-1.93101595220039	3.59517945474406
C	3.73741623573409	-1.47111846846238	3.80847735873092
C	4.56667429346289	-2.03871504301073	2.79560171718135
C	3.74759894524679	-2.84230280180494	1.96791739533276
C	2.41372692040935	-2.79056415044314	2.46439709816552
H	1.54852245377693	-1.68225886040188	4.18578235866661
H	4.06270359232270	-0.82411539051343	4.60708065707261
H	5.62999429330504	-1.89612660416280	2.69012366772364
H	4.07630622299367	-3.41251701260769	1.11313134619861
H	1.57819161576747	-3.38638375808609	2.13198938045265
Mo	0.60656481029626	3.06588055422286	-1.77861822816964
C	-0.95322805072654	4.25115720676059	-1.93969079833046
O	-1.84123479352457	4.97128565660390	-2.07010948756040
C	0.59593506403641	3.63391600314824	0.12796453514526
O	0.70186620021437	4.14843481376355	1.16059701153939

C	-0.65760505378333	1.63260386277060	-2.32044687847059
O	-1.32247340921335	0.86286258479782	-2.87144872178095
C	1.92982989115512	2.41628592913106	-3.59784293267443
C	2.78967052831177	2.41118967753343	-2.46725297632255
C	2.84328655846625	3.74403550448986	-1.96824568206334
C	2.04078077888016	4.56584242077593	-2.79428365873327
C	1.47176414668468	3.73929024750667	-3.80853862250404
H	1.67973409647318	1.55081142712870	-4.19002918194340
H	3.38430626489261	1.57414745102003	-2.13649659663182
H	3.41428645047135	4.07034454043444	-1.11306432851058
H	1.89990904159951	5.62920161467274	-2.68692281875064
H	0.82504019023408	4.06703265774655	-4.60636484903944
Mo	-3.06610812443255	0.60751081728160	1.77802889906767
C	-4.25132041730625	-0.95224741325439	1.93927604588475
O	-4.97154225568144	-1.84017109986304	2.06981300492622
C	-1.63301803778368	-0.65624402608527	2.32098429890720
O	-0.86346423337085	-1.32047709077265	2.87315511782543
C	-3.63365261303483	0.59597433196807	-0.12877022794080
O	-4.14746739614531	0.70074718769374	-1.16179935257899
C	-2.41670033062623	1.93139698697822	3.59691696920553
C	-3.73967828839094	1.47329750978819	3.80771551459040
C	-4.56621927601264	2.04184760241331	2.79319346174783
C	-3.74443401013461	2.84416840558290	1.96693885107807
C	-2.41162237710431	2.79076453500106	2.46595123411673
H	-1.55127247630928	1.68152717534165	4.18926881082643
H	-4.06735998022068	0.82677988192183	4.60573546947534
H	-5.62955272643429	1.90079515641832	2.68581271675768
H	-4.07073880396240	3.41467080082751	1.11142201901318
H	-1.57452774926075	3.38502716197270	2.13469760235180

3a

Au	1.38637772596172	1.28370287356816	0.04734827428275
Au	-1.53002244167777	0.53364211663667	0.02260720130052
Au	0.33287182118422	-1.67616025471604	0.00891892632822
Mo	-0.65349630969824	3.20057254083981	0.00289477314306
C	-0.63686450859512	2.16651737970082	1.72712367238794
O	-0.70377334076810	1.80501149389797	2.82073702510614
C	-0.72150362947281	2.17217164505306	-1.71863773560801
O	-0.82569655338509	1.80465959131522	-2.80680700724728
C	1.27579355603926	3.64039458871078	-0.10882543692245
O	2.28231978209984	4.21576749810936	-0.19235900260402
C	-1.92112240287806	4.71966835455637	1.24829581582607
C	-2.78499818351349	4.14497506926047	0.27675181071800
C	-0.90150260076549	5.43022475156992	0.57443201079687
C	-2.28772501533010	4.49804282483864	-1.00302849482966
C	-1.12585550030529	5.29739727324507	-0.82779943065647
H	-3.65738417843800	3.54554001499014	0.47875751204234
H	-0.10040979469113	5.98211295441420	1.03870846683917
H	-2.72345154204320	4.21460124334798	-1.94803464173889

H	-0.53299286356461	5.73985278334685	-1.61153709418426
H	-2.02353002883708	4.62450402488361	2.31780724804596
Mo	-2.46195879625300	-2.09308291234573	0.03108681047163
C	-1.54369442186599	-1.75584906578168	1.78434131331392
O	-1.20817485333240	-1.62894587585424	2.87747382138536
C	-1.73684367005373	-3.93300319264636	0.13863558479770
O	-1.41368046384106	-5.03170363028651	0.20301277629015
C	-1.45599573713597	-1.89639650081395	-1.69154173177848
O	-1.10617613461782	-1.84366383236758	-2.78842300337191
C	-4.52670013781468	-2.88019313629180	0.66811664060270
C	-4.46575671911604	-1.52684057873644	1.08310843140299
C	-4.46534345827920	-2.90210079500696	-0.75666242354511
C	-4.36667256942515	-1.56089711073192	-1.20529781107721
C	-4.38325543363572	-0.70452981156305	-0.07275535992890
H	-4.62202546409944	-3.73795157105106	1.31399557224470
H	-4.50660017108759	-3.77880788171199	-1.38243633347620
H	-4.38383764522202	0.37246174393199	-0.08987834778492
H	-4.29604526581026	-1.24138364318921	-2.23295467010564
H	-4.48430771785969	-1.17723551500185	2.10320080580970
Mo	3.01639049657931	-0.95577350086218	-0.01129041145746
C	2.16778214401947	-0.46942651437545	1.74308018065142
O	1.89555705441937	-0.25423840037215	2.84136546695076
C	2.41834152667669	-2.85225830182727	-0.02693545158091
O	2.38596842118015	-4.00995616848907	-0.04245375740826
C	2.12091548693203	-0.43202690027264	-1.73211023032732
O	1.81267957693986	-0.18363082536944	-2.81281777050832
C	5.06618768254932	-1.78421895071488	0.63498824557547
C	4.98344401304616	-0.45696516949463	1.12485239336624
C	5.04110376731151	-1.72451096497006	-0.79086683174647
C	4.91186804470833	0.42873492176492	0.01746727226083
C	4.94233480566789	-0.35895275048541	-1.16259547051410
H	5.10458465600159	-2.56389730629983	-1.46395591722268
H	4.83582182041188	1.50279391249902	0.06397832654491
H	4.89840822949737	0.01962252975171	-2.17158200535273
H	5.14906709840916	-2.67759660186471	1.23230497118337
H	4.97535384377820	-0.16692646673865	2.16361102130879

3b

Au	-0.33976234546833	-1.62300888720970	0.01323787330030
Au	1.61575080799212	0.53572518917914	-0.06775565183543
Au	-1.26702245808765	1.13114063737443	0.06731955048295
Mo	2.45239843805348	-2.10134438918963	-0.13101050932200
C	1.44126559813779	-1.72893443458386	-1.82641932423189
O	1.04720703945171	-1.58894130863084	-2.89914723993730
C	1.54346166084623	-1.81088184132785	1.63420545242732
O	1.24522304082711	-1.71569734405053	2.74394341157388
C	1.61899933365367	-3.89630197312371	-0.15337394237099
O	1.21228892406910	-4.97199140887035	-0.16944502114382
C	4.46245444926321	-3.00577131644193	0.52063711670118

C	4.45357008146007	-1.66615756224140	0.98302662243518
C	4.43549991097420	-0.79974170021661	-0.14303375835096
C	4.40456093928906	-1.61529872004127	-1.30675467466539
C	4.43224104265400	-2.97418427050809	-0.90508053558927
H	4.50465074523343	-3.88889413068807	1.13736845634623
H	4.46618840318534	-1.35311901893024	2.01499600180853
H	4.49610507652588	0.27565012219668	-0.12004247735209
H	4.37334429801010	-1.25627418963537	-2.32323338430167
H	4.44781403273659	-3.82944410117992	-1.56104823633429
Mo	0.60265364191645	3.17488975555225	0.04903692695751
C	2.57686476736552	3.33342173035171	0.01815973359997
O	3.71128406614871	3.52314356063988	0.00359172138549
C	0.80301539375686	2.13575395188376	1.75655213877022
O	0.89147166191825	1.74065929208629	2.83439404456336
C	0.73330394110432	2.21902988734213	-1.71108514841464
O	0.76194688623356	1.89121448431514	-2.81542949410424
C	0.43044827446823	5.34528889533734	0.78536509367961
C	-0.72266040278870	4.66635323912594	1.25240569820761
C	-1.49787513261248	4.26843193843998	0.12990217672040
C	-0.80083939337323	4.68227609694323	-1.03699509248267
C	0.38191226239850	5.35615810483976	-0.64026820004287
H	1.19656058270037	5.79031191571211	1.39944522786056
H	-0.97660719651263	4.48650968699907	2.28503455880077
H	-2.46231724690422	3.78957346816488	0.15934210072155
H	-1.12490106080191	4.51605148932852	-2.05213933447792
H	1.10401173196085	5.81106826128357	-1.29875612599101
Mo	-3.05401065415466	-1.07569783267624	0.07610694059062
C	-4.27775031604462	0.47834110497900	0.11790981276829
O	-5.05879557919079	1.32139299648481	0.14373656581912
C	-2.29103614910955	-0.38132588345766	1.79822324684509
O	-2.01158597939893	-0.13388580510247	2.88831423316447
C	-2.36072767714997	-0.34370544829241	-1.66025179029928
O	-2.12350163619975	-0.07005797969080	-2.75389946075133
C	-2.81161648408807	-3.43667973997607	0.05756261666694
C	-3.57116079686042	-3.03485918002956	-1.07497483950529
C	-4.77104931151251	-2.43220455876691	-0.62188103135409
C	-4.75084075486617	-2.44151509868715	0.80463887781473
C	-3.53908320482233	-3.04992899314039	1.21608492016005
H	-1.89143975364426	-3.99693158250353	0.04093843175370
H	-3.28239737781455	-3.17486351742444	-2.10458944280974
H	-5.56466245405827	-2.05283594147531	-1.24503413785536
H	-5.52648971396883	-2.07037454985257	1.45478533786463
H	-3.22180495290189	-3.20309410061476	2.23538396373327

3c

Au	-1.92665398536911	-0.99666264127899	-0.66728246348223
Au	0.72391700260842	-1.63370528351412	-0.15752456239921
Au	1.52970988261673	0.99898635440358	0.17470544925221
Au	-1.14840253825098	1.70407931069456	-0.33026303567707

Mo	-0.87901882012159	-3.49068596273544	-1.55938837165262
C	-2.71420789325446	-4.16572233444120	-1.55236118940960
O	-3.78104472222089	-4.60068167757680	-1.56178149834002
C	-1.66581538527695	-2.01324457355672	-2.66400950120852
O	-2.04280206981289	-1.42103110296251	-3.58645201315455
C	-1.20866901732926	-3.43525252913259	0.41814070108179
O	-1.42813417147163	-3.57308648433488	1.54335510022444
C	0.95557803349624	-4.95513421709942	-1.44527905763520
C	1.40825688298883	-3.82706783881163	-2.18377127525550
C	0.61646014618253	-3.73314968851049	-3.35277017747000
C	-0.30851985727989	-4.81026038496110	-3.35428101352481
C	-0.09272187423113	-5.57155963730217	-2.16809613945806
H	1.35534592839791	-5.29608883154755	-0.50358833710010
H	2.23000403889954	-3.17892612931488	-1.92990454586205
H	0.70724195804083	-2.97155752786870	-4.11079077603838
H	-1.02814804536314	-5.02633116727440	-4.12729529507666
H	-0.62038325677836	-6.46717997031722	-1.88243444213659
Mo	3.14037871116471	-1.09653211646396	1.21110810532940
C	4.54636948424487	0.26433827209435	1.30259843939567
O	5.40110150565917	1.03382516970262	1.37140398246837
C	3.30548819237045	-0.78361605146544	-0.75946334449425
O	3.55142004113622	-0.68534348017995	-1.88395649703336
C	2.08264229048487	0.23566223617614	2.27371540175916
O	1.63743488835075	0.82857209386700	3.16186657731722
C	2.65079249115271	-2.59000615410122	2.95376752820995
C	4.02604297152230	-2.24403365072640	2.99852884127624
C	4.63976198119315	-2.74068504358282	1.81124059040251
C	3.63800469484585	-3.38372242272261	1.04516569091403
C	2.40957345287992	-3.30803290417604	1.75730429772754
H	1.91047095480166	-2.35389120744327	3.70149231978936
H	4.52161243265652	-1.71861438032078	3.79876885538537
H	5.68332380215138	-2.66035318424599	1.55341372510454
H	3.78677302003317	-3.86442109214631	0.09117900480748
H	1.47099823365780	-3.75054307319593	1.46921433317131
Mo	0.97851763386109	3.16830974941737	-1.46433632503468
C	-0.57988954478639	4.01105848424423	-2.34332413599117
O	-1.41890330651855	4.56263605123668	-2.89759818956336
C	0.13940634810109	3.67076228346597	0.29340987004378
O	-0.15437561850188	4.17197675215394	1.29089184481799
C	0.46573837724419	1.48601070280162	-2.43040143724943
O	0.31288106860823	0.57632052064584	-3.11625856707592
C	3.06519682382248	2.96548180599430	-2.48084601810150
C	3.33163408385344	3.20196431367178	-1.10690806773065
C	2.79700986757386	4.47438204261090	-0.77975314167670
C	2.22661799897457	5.03695886409200	-1.94931866190797
C	2.39544388624711	4.09918285135687	-3.01027543168886
H	3.33755760653303	2.07487386275530	-3.02498335511715
H	3.88527045939295	2.55709713671269	-0.44511646332537
H	2.82781604179646	4.93636397623418	0.19434652136812
H	1.76747092250299	6.00922193567261	-2.02641371486370

H	2.08807476711386	4.23491334691368	-4.03455459131570
Mo	-3.58771870843253	0.75006742365742	0.70040646135157
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O	-3.52288726143365	3.59702503774872	1.98322344465541
C	-1.98279156224327	0.30529877854657	1.81947458277471
O	-1.19715283132853	-0.02508948803123	2.59020021751110
C	-3.41674840289867	1.62509256254938	-1.10180421661446
O	-3.61552574240064	2.07724088690847	-2.14589635425488
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C	-4.64869638951201	-1.05922503463562	1.71268701379072
C	-4.87629017485937	-1.21319084339622	0.31946834039725
C	-5.61490240225969	-0.08496285800123	-0.11999816262835
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H	-5.29765496934664	0.52086471257491	3.14905894713935
H	-4.10334877174505	-1.75008014349596	2.33622999519797
H	-4.58658499483606	-2.05775792760567	-0.28366262960341
H	-5.93324507453292	0.10075418378871	-1.13364637609037
H	-6.43005964053133	1.67043669976047	0.98525355755550

3d

Au	-1.82443156147698	-0.00008368256968	0.00018584132425
Au	-0.00039340460232	-2.11169351702591	-0.00061506510264
Au	1.82428599364461	-0.00042347408279	0.00065061626253
Au	0.00044495170626	2.11102794991993	-0.00126823851993
Mo	-2.25021758191404	-2.21508279596411	1.69930874914102
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O	0.50285469358182	-1.47675414421906	2.99308601230688
C	-1.70451564256821	-4.08876016059629	1.98196729084222
O	-1.44820324701138	-5.18589535024533	2.20245610147350
C	-2.50672508189570	-2.76480867062594	-0.21398360618337
O	-2.86131568175802	-3.13734021253694	-1.24704058654836
C	-3.03061447336399	-0.84726579312727	3.42908564372920
C	-3.35755441759257	-2.19838164168789	3.71133791054456
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H	-2.99690787607279	-2.77754913896703	4.54595935805027
H	-3.75999677812323	0.55131325516733	1.86061652242088
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H	-5.13851827978688	-1.58463941236737	0.95594335905259
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C	3.03049994866664	-0.84233310266834	-3.42540206429798

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H	3.76545206381346	0.54965230135193	-1.85385186850158
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O	-0.50319990134763	1.47478588986322	2.99289757071262
C	1.70264222951537	4.08788968531375	1.98283562346487
O	1.44560765307716	5.18479694282124	2.20360970045823
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O	2.86054176195424	3.13798741886967	-1.24651838135350
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H	2.99680141754746	2.77607080988464	4.54642965600369
H	3.76207753954214	-0.55028242022294	1.85863219177960
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Mo	-2.25075822588136	2.21419997812753	-1.69903674603003
C	-0.42521440675508	1.75163934477924	-2.36132007687839
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C	-1.70477408317682	4.08780018830074	-1.98188475547318
O	-1.44823913355763	5.18487440471585	-2.20237531737647
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3e

Au	-1.71611100763554	-0.96947462389576	-0.12728461178218
Au	0.96990032983567	-1.71576137030359	0.12698319447972
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Mo	-0.90919332939801	-3.45044370812534	-1.09732252784200
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C	0.07424546379806	-2.11047759467407	-2.22741395043595
O	0.54984543567569	-1.45545599957029	-3.04383206500428
C	-0.58067251112672	-3.49793489285966	0.87851300921947
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Mo	3.45078456348193	-0.90924617595636	1.09776079392271
C	4.52173487881895	0.73722147733324	1.21873986404640
O	5.19672838806501	1.66616523878559	1.30696873883885
C	3.49837637291670	-0.58025845721067	-0.87800425270921
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C	2.11133835638883	0.07465397010373	2.22804952307339
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C	5.30318795121322	-2.23925613913565	1.38976169665638
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C	3.23752706086557	-3.24242582068423	1.55016567075637
H	2.82091121785197	-2.51007420607466	3.60940306111945
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H	6.26937576210585	-1.93781545811718	1.01887943805216
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Mo	0.90898865198837	3.45035816279493	-1.09845071213636
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O	-1.66820079042140	5.19339415159179	-1.31051688635650
C	0.57989428846110	3.49977051299628	0.87725070538292
O	0.53042124750802	3.73661470012165	2.00739808927744
C	-0.07288521489097	2.10809478232796	-2.22716933530009
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C	3.03167219333882	4.35481057070997	-0.69892488407976
C	2.23722723877185	5.30374632012489	-1.39228168531775
C	1.94029185420468	4.76427688904007	-2.67853177586221
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H	3.86434427189611	2.38578770173977	-1.33769036625869
H	3.42428799138340	4.46098405297314	0.29994131665028
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H	1.36900900818411	5.24709768361133	-3.45482726797267
Mo	-3.45019168838045	0.90941852493757	1.09849555630582
C	-4.51903861093550	-0.73835449502290	1.22079228016358
O	-5.19272802634875	-1.66817225159958	1.30981158053570
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O	-1.45177809573109	-0.54686344613883	3.04368110096339
C	-3.49856595930507	0.58020232132047	-0.87714525348952
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C	-3.49096776812381	2.55282356558786	2.76474263453897
C	-4.76628239119967	1.94084204240634	2.67672610923366
C	-5.30361908491208	2.23819090639135	1.38969027002623
C	-4.35331727342711	3.03242713925257	0.69794162208282
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