Oxygen Isotope Exchange Between Carbon Dioxide and Iron Oxides on Mars' Surface

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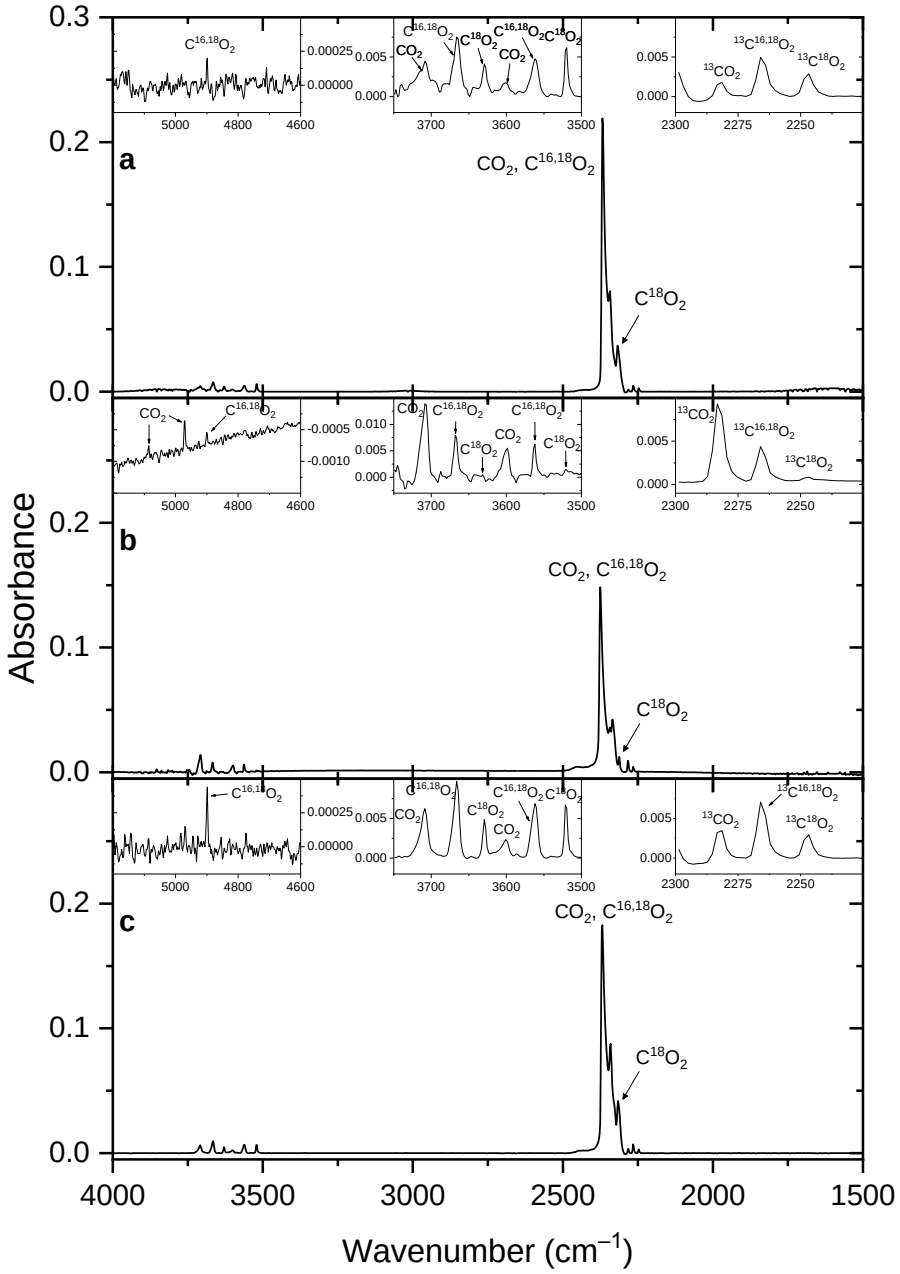
Supporting Information

Previous heterogeneous isotope exchange studies with metal oxides: Sakata et al. (1980) investigated the catalytic effect of iron(III) oxide (γ-Fe_2O_3) on the isotopic exchange of oxygen between carbon dioxide at elevated temperatures up to 573 K.[1] The authors pointed out that the amount of exchangeable oxygen is comparable to one layer of oxygen atoms on the surface of iron(III) oxide. Further, oxygen exchange between carbon dioxide and hydroxylated anatase (TiO_2) in the dark and under illumination with ultraviolet light was a focus of the paper by Sato (1987).[2] The author concluded that oxygen exchange takes place rapidly even in non-illuminated samples at room temperature suggesting that oxygen atoms of the surface hydroxylic groups (-OH) play a critical role. The promotion of the catalytic decomposition by alkali metals was also studied and was found to increase the number of exchangeable oxygens on the surface and also to weaken the bond between these oxygens and the surface.[3] Temperature-programmed desorption (TPD) gas analysis was also conducted to examine the oxygen exchange between adsorbed $C^{18}O_2$ and ZnO and TiO_2 powders.[4] This study revealed that after molecular oxygen ($^{16}O_2$) exposure of the carbon dioxide ($C^{18}O_2$) pre-adsorbed on the surface, the fractional abundances of both of $C^{16}O_2$ and $C^{16}O^{18}O$ isotopologues were increased suggesting that the isotope exchange may occur via a CO_2–O_2 intermediate complex. Another TPD study by Tsuji et al. (2003) examined the $C^{18}O_2$ adsorption on MgO, CaO, and ZrO_2 at room temperature concluding the formation of carbonate-like complexes and complete (statistical) scrambling of their oxygen atoms.[5] The CeO_2–$C^{18}O_2$ system was studied at high temperatures, and a two-step mechanism was proposed for the oxygen exchange;[6] a similar study utilized Al_2O_3 and SiO_2 surfaces.[7] Recently, Civiš et al. presented a series of papers on the photoinduced and spontaneous oxygen exchange between $C^{16}O_2$ and $Ti^{18}O_2$ as well as $C^{18}O_2$ and $Ti^{16}O_2$ nanocrystals and nanopowders.[8–10] A carbonate-like structure at the surface oxygen defect site was proposed to account for the oxygen exchange.[11] It should also be noted that there have been efforts made to unravel the equilibration processes between more than one gas-phase species such as between $C^{16}O_2$ and $^{18}O_2$ in the presence of metal oxide upon UV irradiation or between $C^{16}O_2$ and $H_2{}^{18}O$ in the presence of iron/aluminum oxide.[12,13] The experimental details of the experiments listed above are tabulated in Table S1.

Supplementary Table S1. Experimental results on the isotope exchange between carbon dioxide and oxide surfaces in chronological order.

p (mbar)	T (K)	Method	Admixture / Treatment	Reference
–	273–873	Calculation of fractionation factors	$CaCO_3$	14
0.27–0.48	473–873	FTIR	silica, γ-alumina, silica–alumina, zeolites	15
13	423–573	MS, X-ray powder diffraction	γ-Fe_2O_3	1
4	323–873	MS, FTIR	K_2CO_3/Al_2O_3	3
1	298	FTIR	TiO_2 + UV irrad.	2
N/A	298–800	QMS	ZnO, TiO_2	4
10–20	190–230	MS	kaolinite ($Al_2Si_2O_5(OH)_4$), basalt, fluorite (CaF_2)	16
0.13	308	FTIR	TiO_2 + UV irrad.	12
N/A	298–1000	QMS	MgO, CaO, ZrO_2	5
0.4	296	FTIR	Fe_2O_3 nanoparticles, γ-Al_2O_3 (CO_2 mixed with H_2O)	13
1×10^{-8} (gas pulses)	473–873	MS	CeO_2/Pt	6
52000	673, 773	MS	γ-Al_2O_3/Pd	7
2.6	303	FTIR	TiO_2 + UV irrad.	8
1.5	323–773	FTIR	nanocrystalline TiO_2 + UV irrad.	9
1.5	473–723	FTIR	TiO_2 nanoclusters	10
1.3–2.6	293	FTIR	TiO_2, montmorillonite, $FeCO_3$, $CaCO_3$, basalt	17
1.3–2.6	293	FTIR	TiO_2, montmorillonite, $FeCO_3$, $CaCO_3$, basalt	18



Supplementary Figure S1. FTIR spectra of the $C^{16}O_2$–$C^{18}O_2$ system at 10 K. The samples were deposited from the vial that (**a**) did not contain any solid material, (**b**) contained FeO(OH) (goethite), and (**c**) contained Fe_2O_3 (hematite).

Supplementary Table S2. Full assignment of the FTIR data of the $C^{16}O_2$– $C^{18}O_2$ system.

ν / cm^{-1}	Species	Assignment
5085	$C^{16}O_2$	$2\nu_1 + \nu_3$
5027	$C^{16}O^{18}O$	$2\nu_1 + \nu_3$
4970	$C^{16}O_2$	$\nu_1 + 2\nu_2 + \nu_3$
4899	$C^{16}O^{18}O$	$\nu_1 + 2\nu_2 + \nu_3$
4826	$C^{18}O_2$ (+ $C^{16}O_2$)	$2\nu_1 + \nu_3$ ($4\nu_2 + \nu_3$)
4775	$C^{16}O^{18}O$	$4\nu_2 + \nu_3$
4711	$C^{18}O_2$	$\nu_1 + 2\nu_2 + \nu_3$
3712	$C^{16}O_2$	$\nu_1 + \nu_3$
3668	$C^{16}O^{18}O$	$\nu_1 + \nu_3$
3629	$C^{18}O_2$	$\nu_1 + \nu_3$
3605	$C^{16}O_2$	$2\nu_2 + \nu_3$
3563	$C^{16}O^{18}O$	$2\nu_2 + \nu_3$
3519	$C^{18}O_2$	$2\nu_2 + \nu_3$
2343	$C^{16}O_2$	ν_3
2327	$C^{16}O^{18}O$	ν_3
2307	$C^{18}O_2$	ν_3
2281	$^{13}C^{16}O_2$	ν_3
2266	$^{13}C^{16}O^{18}O$	ν_3
2247	$^{13}C^{18}O_2$	ν_3
671	$C^{16}O_2$	ν_2
655	$C^{16}O^{18}O$	ν_2
652	$C^{18}O_2$	ν_2

Supplementary Table S3. Ion microprobe results of the reference and processed samples.

Sample	Measurement #	$^{18}O/^{16}O$-raw	2-standard error of the mean
FeO(OH)	1	0.0019751	0.0000003
(reference)	2	0.0019738	0.0000003
	3	0.0019699	0.0000003
	4	0.0019767	0.0000003
	5	0.0019650	0.0000004
	6	0.0019749	0.0000003
	7	0.0019755	0.0000004
	8	0.0019687	0.0000003
	9	0.0019742	0.0000008
	10	0.0019761	0.0000007
	11	0.0019673	0.0000003
	12	0.0019713	0.0000006
	13	0.0019739	0.0000012
	14	0.0019749	0.0000013
	15	0.0019754	0.0000016
	16	0.0019748	0.0000011
	17	0.0019739	0.0000012
	18	0.0019742	0.0000015
	19	0.0019625	0.0000004
	20	0.0019740	0.0000003
	21	0.0019731	0.0000009
	22	0.0019732	0.0000008
	23	0.0019705	0.0000004
	24	0.0019720	0.0000008
	25	0.0019699	0.0000006
	26	0.0019691	0.0000003
	27	0.0019541	0.0000003
	28	0.0019534	0.0000004
	29	0.0019708	0.0000003
	30	0.0019732	0.0000015
	31	0.0019730	0.0000020
	32	0.0019583	0.0000003

	mean value	**0.00197**	**0.00001**
FeO(OH)	33	0.0040543	0.0000031
(processed)	34	0.0044623	0.0000063
	35	0.0043165	0.0000036
	36	0.0040905	0.0000030
	37	0.0041963	0.0000028
	38	0.0045399	0.0000019
	39	0.0046281	0.0000015
	40	0.0048553	0.0000044
	41	0.0050759	0.0000007
	mean value	**0.0045**	**0.0007**
Fe_2O_3	42	0.0020101	0.0000002
(reference)	43	0.0020100	0.0000002
	44	0.0020090	0.0000002
	45	0.0020117	0.0000003
	46	0.0020131	0.0000003
	47	0.0020124	0.0000003
	48	0.0020126	0.0000003
	49	0.0020082	0.0000002
	50	0.0020077	0.0000002
	51	0.0020088	0.0000003
	52	0.0020103	0.0000003
	53	0.0020097	0.0000003
	54	0.0020073	0.0000003
	55	0.0020084	0.0000002
	56	0.0020098	0.0000002
	mean value	**0.002010**	**0.000004**
Fe_2O_3	57	0.0038685	0.0000126
(processed)	58	0.0038154	0.0000021
	59	0.0037544	0.0000020
	60	0.0035937	0.0000101
	61	0.0035410	0.0000039
	62	0.0038999	0.0000121
	mean value	**0.0037**	**0.0003**

Calculation of the Gibbs free energy change in an isotopic exchange reaction: In our calculation, the total Gibbs free energy change (ΔG_{tot}) for an isotopic exchange reaction is equal to the total Helmholtz free energy change (ΔF_{tot})

$$\Delta G_{\mathrm{tot}} = \Delta F_{\mathrm{tot}} + \Delta(k_{\mathrm{B}}T) = \Delta F_{\mathrm{tot}}$$

when the Boltzmann constant (k_{B}) and the experimental temperature ($T = 293$ K) are both invariants under an ideal gas assumption. ΔF_{tot} includes the contributions from vibrations (vib), torsions (tor), and rotations (rot)

$$\Delta F_{\mathrm{tot}} = \Delta F_{\mathrm{vib}} + \Delta F_{\mathrm{tor}} + \Delta F_{\mathrm{rot}}$$

Electronic and translational free energies are not included because reactants and products share identical electronic structures and total masses. For other degrees of freedom (say x), the Helmholtz free energy (F_x) is calculated using the corresponding canonical partition function (Q_x)

$$F_x = -k_{\mathrm{B}}T\ln Q_x$$

$$Q_x = \sum_n \exp\left(-\frac{E_{x,n}}{k_{\mathrm{B}}T}\right)$$

where $E_{x,n}$ is the energy of the n^{th} energy level.

Following the quasi-rigid-rotor–harmonic-oscillator (QRRHO)[19] model, high frequency vibrational degrees of freedom are approximated using harmonic oscillators while low frequency modes are treated as one-dimensional free rigid rotors so that their partition functions are

$$Q'_{\mathrm{vib}} = \prod_i \frac{1}{2\sinh\left(\frac{ch\omega_i}{2k_{\mathrm{B}}T}\right)}$$

$$Q'_{\mathrm{tor}} = \prod_j \left(\frac{\pi k_{\mathrm{B}}T}{ch\omega_j}\right)^{\frac{1}{2}}$$

where c is the speed of light in vacuum, ω_i is the frequency (or wave number) of the i^{th} vibrational mode, ω_j is the frequency (or wave number) of the j^{th} torsional mode. The final vibrational-torsional partition function is reconstructed to smoothly switch between the high-frequency (harmonic oscillator) and low-frequency (free rigid rotor) regimes using a damping function

$$Q_{\mathrm{vib}} = \prod_i \left[\frac{1}{2\sinh\left(\frac{ch\omega_i}{2k_{\mathrm{B}}T}\right)} \right]^{w_i}$$

$$Q_{\mathrm{tor}} = \prod_i \left(\frac{\pi k_{\mathrm{B}} T}{ch\omega_j} \right)^{\frac{1-w_i}{2}}$$

Here w_i is the revised Chai–Head-Gordon damping function[20] associated with the i^{th} mode

$$w_i = \frac{1}{1 + \left(\frac{\omega_0}{\omega_i}\right)^4}$$

and $\omega_0 = 100\ \mathrm{cm}^{-1}$ is the cut-off value associated with the transition between the two regimes.

The rotational partition function is modeled using the rigid rotor model, and two cases are considered. For a linear molecule like CO_2,

$$Q_{\mathrm{rot}} = \frac{k_{\mathrm{B}}T}{\sigma chB}$$

where σ is the symmetry number of the molecule, and B is the rotational constant. $\sigma = 2$ is used for $C^{16}O_2$ and $C^{18}O_2$, and $\sigma = 1$ for $C^{16}O^{18}O$. For a non-linear molecule like any other species

$$Q_{\mathrm{rot}} = \frac{(k_{\mathrm{B}}T)^{\frac{3}{2}}}{\sigma} \left(\frac{\pi}{ABC}\right)^{\frac{1}{2}}$$

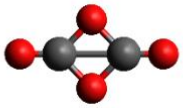
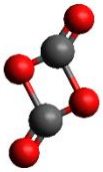
where A, B, C are the rotational constants about the principal axes a, b, and c.

The atomic coordinates (in Å), vibrational frequencies (in cm^{-1}), and vibrational–torsional and rotational Helmholtz free energies (in kJ mol^{-1}) associated with each species evaluated in the present study are presented in Supplementary Tables S3 through S8, and the temperature-dependent equilibrium constant for

$$C^{16}O_2 + C^{18}O_2 \rightarrow 2C^{16}O^{18}O,\ \Delta_r G = -3.3764\ \mathrm{kJ\ mol}^{-1}$$

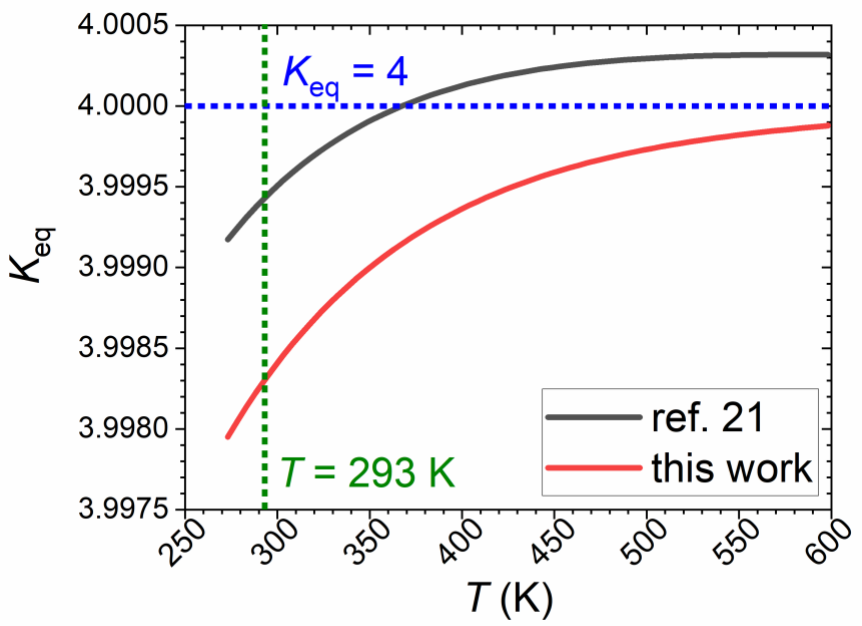
are provided in Figure S2.

Supplementary Table S3. Coordinates (in Å) of the monomer of CO_2, as well as the van der Waals complex (reactant and product), intermediate, and transition state of C_2O_4 relevant to the non-catalytic isotopic exchange reaction of CO_2 ($C^{16}O_2 + C^{18}O_2 \rightarrow 2C^{16}O^{18}O$) were calculated at the ωB97X-V/def2-TZVPPD level of theory.

CO_2 monomer (D_{2h})				van der Waals complex			
							
C	0.000000	0.000000	0.000000	C	–2.115173	0.579142	–0.000007
O	0.000000	0.000000	–1.158330	C	0.876926	0.829891	–0.000002
O	0.000000	0.000000	1.158330	O	0.291207	1.833431	0.000003
				O	–1.529453	–0.424399	–0.000008
				O	1.459242	–0.167122	–0.000006
				O	–2.697489	1.576155	–0.000006
intermediate				transition state			
							
C	–1.503310	1.047622	0.000154	C	–1.641220	0.879964	0.000000
C	0.265057	0.361406	0.000154	C	0.402970	0.529066	0.000000
O	–0.252495	1.649052	–0.000266	O	–0.125700	1.668238	0.000000
O	–0.985759	–0.240024	–0.000257	O	–1.112550	–0.259208	0.000000
O	1.350792	–0.060034	0.000120	O	1.365980	–0.107932	0.000000
O	–2.589045	1.469061	0.000120	O	–2.604230	1.516962	0.000000

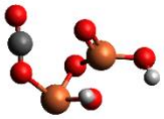
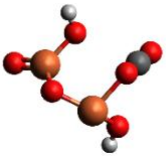
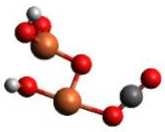
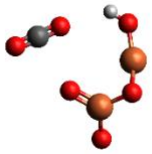
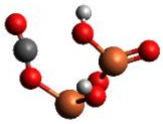
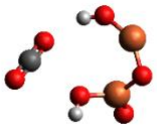
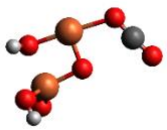
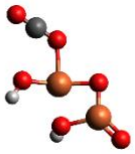
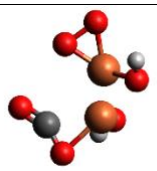
Supplementary Table S4. Frequencies (in cm^{-1}, top 12 rows below structures) and vibrational–torsional and rotational Helmholtz free energies (in kJ/mol, bottow two rows below structures) of different isotologues of the monomer of CO_2, as well as the van der Waals complex (reactant and product), intermediate, and transition state of C_2O_4 relevant to the non-catalytic isotopic exchange reaction of CO_2 ($C^{16}O_2 + C^{18}O_2 \rightarrow 2C^{16}O^{18}O$) were calculated using the quasi-rigid-rotor–harmonic-oscillator (QRRHO) model at the ωB97X-V/def2-TZVPPD level of theory.

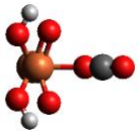
CO_2 monomer			C_2O_4 van der Waals complex		C_2O_4 intermediate	C_2O_4 transition state	
$C^{16}O_2$ 	$C^{18}O_2$ 	$C^{16}O^{18}O$ 	$(C^{16}O_2)(C^{18}O_2)$ reactant 	$(C^{16}O^{18}O)_2$ product 	$C_2{}^{16}O_2{}^{18}O_2$ 	$(C^{16}O_2)(C^{18}O_2)$ early 	$(C^{16}O^{18}O)_2$ late 
664.84	654.67	659.77	23.48	23.48	179.26	136.12	136.09
664.85	654.67	659.78	29.70	29.69	401.86	311.80	311.59
1331.16	1254.86	1292.74	45.05	45.06	637.97	486.55	486.36
2412.66	2375.98	2394.84	96.41	96.38	694.11	668.48	668.65
			671.14	675.35	695.78	683.41	685.32
			672.94	676.52	735.78	748.29	746.84
			681.88	677.71	826.62	748.46	748.14
			684.17	680.64	913.50	1131.99	1136.23
			1309.67	1348.84	1066.41	1288.83	1284.32
			1389.30	1349.51	1311.39	2095.61	2097.36
			2379.52	2395.80	1947.20	2190.12	2188.91
			2416.90	2401.77	2122.68	678.49*i*	678.47*i*
30.149	29.340	29.746	47.576	47.579	66.749	59.596	59.596
–13.576	–13.863	–15.406	–29.734	–29.734	–27.604	–27.914	–27.914



Supplementary Figure S2. Theoretical temperature-dependent equilibrium constant (K_{eq}) of $C^{16}O_2 + C^{18}O_2 \rightarrow 2C^{16}O^{18}O$ reaction. Here D_{2h} structure is assumed for all CO_2 species, and vibrational frequencies are obtained from Urey and Greiff[21] (black) and this work (red). K_{eq} depends majorly on rotational symmetries and minorly on vibrational frequencies.

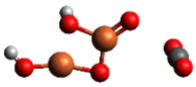
Supplementary Table S5. Coordinates (in Å) of twenty-four $[FeO(OH)]_2$–CO_2 clusters studied in the catalytic isotopic exchange reaction of CO_2 ($Fe_2{}^{16}O_4H_2 + C^{18}O_2 \rightarrow Fe_2{}^{16}O_3{}^{18}OH_2 + C^{16}O^{18}O$ and $Fe_2{}^{16}O_4H_2 + C^{16}O^{18}O \rightarrow Fe_2{}^{16}O_3{}^{18}OH_2 + C^{16}O_2$) were calculated at the ωB97X-V/def2-TZVPPD level of theory.

1				2				3			
											
Fe	0.523855	–1.501644	0.158097	Fe	0.867989	–1.214571	0.227127	Fe	0.731477	–1.060732	–0.095727
Fe	–1.041035	0.588092	0.130882	Fe	–1.612585	0.141019	–0.031717	Fe	–1.466339	0.409172	–0.097739
C	2.279854	0.705732	–0.132314	C	1.881439	1.358450	0.151165	C	2.916170	0.652390	0.117565
O	–0.109782	–0.324660	1.319491	O	–0.865282	–1.151349	0.725017	O	0.326279	0.613084	–0.006251
O	–0.844318	–0.953801	–1.019264	O	1.827256	–0.930856	–1.244126	O	–1.100414	–1.473826	–0.304171
O	2.084589	–0.409255	–0.475991	O	1.701268	0.487760	0.923880	O	2.727325	–0.502591	–0.017406
O	2.600113	1.753811	0.181009	O	2.103091	2.237106	–0.544044	O	3.190029	1.753670	0.252817
O	–2.784740	0.699723	0.167353	O	–0.892574	1.692763	0.314490	O	–2.300273	0.152625	1.437452
O	–0.222767	1.742348	–0.564865	O	–2.908796	0.112459	–0.822180	O	–2.210254	1.222031	–1.167900
H	–3.177374	0.137535	–0.507856	H	–1.323327	2.144209	1.047299	H	–2.385477	0.951714	1.963773
H	–0.598417	–0.628408	–1.889617	H	1.670797	–1.467190	–2.023787	H	–1.582533	–1.910709	0.404849
4				5				6			
											
Fe	–0.803523	–1.525879	–0.05364	Fe	0.413564	–1.482273	0.037553	Fe	1.755492	–0.926044	–0.268065
Fe	–1.020088	1.077435	0.177918	Fe	–1.255872	0.467411	0.045024	Fe	0.402427	1.356261	0.061319
C	3.177288	0.405415	–0.071795	C	2.390621	0.694592	0.079894	C	–2.916716	–1.094788	0.180939
O	–1.776464	–0.285583	0.799521	O	–0.706657	–0.806908	1.184905	O	1.747209	0.720731	–0.778679
O	0.458726	–2.675579	–0.185254	O	–0.578887	–0.665484	–1.352909	O	0.794600	–2.146313	0.359696
O	3.644659	1.419115	0.226023	O	–2.696379	0.997559	0.092650	O	0.438749	2.435248	1.124670
O	2.728696	–0.620425	–0.378807	O	0.087919	1.648529	–0.199627	O	–1.168175	0.903847	–0.528561
O	–1.925178	2.024016	–0.935859	O	2.102300	–0.413172	–0.198667	O	–2.107930	–1.669928	0.784558
O	0.458542	1.389933	0.388829	O	2.851247	1.705469	0.354288	O	–3.756199	–0.560230	–0.404868
H	–1.783362	1.797262	–1.860915	H	–0.095781	–0.121687	–1.981486	H	–0.124102	–2.239902	0.627968
H	1.409873	–2.576691	–0.24532	H	0.090308	2.343200	0.464155	H	–1.542306	1.549392	–1.137694
7				8				9			
											
Fe	0.731103	–1.060680	0.102881	Fe	0.435899	0.230592	–0.194463	Fe	0.846077	0.762104	0.374598
Fe	–1.466139	0.410631	0.096877	Fe	–1.965659	–0.218918	0.068535	Fe	–1.132347	0.054431	–0.396274
C	2.914686	0.651895	–0.122916	C	3.154862	–0.615237	0.064846	C	1.787838	–1.008424	0.091678
O	0.326200	0.612113	–0.005756	O	–0.705826	–1.256501	–0.114292	O	0.208745	0.997696	–1.371990
O	–1.099838	–1.469743	0.325059	O	1.641367	1.461772	0.210723	O	–0.850209	1.473355	0.809718
O	–2.204306	1.236910	1.160757	O	–3.451065	–0.360440	0.356561	O	–1.341255	–1.578140	0.120561
O	–2.309635	0.134799	–1.429760	O	–1.155889	1.398096	–0.139938	O	–2.460974	–0.815092	0.444397
O	2.726715	–0.502984	0.014435	O	2.099461	–1.028682	–0.237434	O	1.541603	–2.150242	0.078644
O	3.188036	1.753069	–0.260004	O	4.215455	–0.286450	0.347391	O	2.563408	–0.060839	–0.023832
H	–1.586107	–1.915233	–0.375763	H	1.327878	2.343099	0.423142	H	–1.259516	1.284003	1.658297
H	–2.399107	0.927730	–1.964651	H	–1.334197	1.808455	–0.992488	H	0.684955	0.602714	–2.104763
10				11				12			



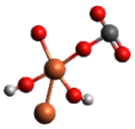
Fe	1.726218	0.122204	–0.002057
Fe	–1.031800	0.744241	0.002544
C	–0.157053	–2.102955	–0.007712
O	0.744256	1.020067	–1.229130
O	0.746142	1.011122	1.233569
O	–1.750320	0.513896	–1.356019
O	–1.749520	0.509643	1.360718
O	0.968951	–1.736001	–0.005656
O	–1.183599	–2.599203	–0.009561
H	0.437625	0.610717	2.050009
H	0.434486	0.626506	–2.048419

13



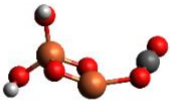
Fe	1.890912	–0.544517	–0.031137
Fe	–0.237467	0.642744	–0.028341
C	–3.595638	–0.651452	0.153828
O	3.617547	–0.514356	–0.161730
O	1.400187	1.276212	0.461723
O	0.092329	–0.944485	–0.313088
O	–1.477972	1.518351	–0.101816
O	–3.833166	–0.634625	–0.979249
O	–3.363596	–0.676703	1.289073
H	1.492214	1.433705	1.407500
H	4.184709	0.255121	–0.091622

14



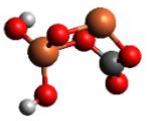
Fe	–1.213220	0.979920	0.000000
Fe	1.318770	1.112500	0.000000
C	3.827700	3.813100	0.164800
O	0.042560	2.431660	0.000000
O	0.187310	–0.332740	0.000000
O	2.730690	2.515520	–0.241650
O	3.135790	–0.125010	0.480700
O	2.793800	4.722400	–0.100800
O	4.795100	2.964600	0.419600
H	–0.283080	–1.177730	–0.102280
H	–0.071970	3.235690	0.523920

15



Fe	0.662890	–1.143254	0.041416
Fe	–1.340319	0.436207	–0.081570
C	2.807248	0.635196	–0.078091
O	–0.946280	–1.166097	0.679071
O	0.230380	0.503664	–0.695653
O	–2.629324	–0.000823	–1.128084
O	–1.719200	1.396162	1.290983
O	2.631237	–0.514700	0.120298
O	3.062457	1.734995	–0.247306
H	–1.687475	0.848731	2.084182
H	–2.842414	–0.932665	–0.999070

16

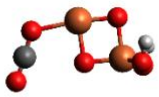


Fe	1.111091	–1.178171	0.057805
Fe	–1.227070	–0.007383	–0.139772
C	1.362669	1.150298	0.223930
O	0.328031	0.374771	0.844448
O	–0.528253	–1.393832	–0.739145
O	–2.294621	–0.137383	1.189561
O	–1.251787	1.361887	–1.169495
O	1.445121	2.324455	0.347661
O	2.126987	0.279695	–0.397643
H	–1.962657	1.335110	–1.823495
H	–1.878134	0.169347	2.004717

17

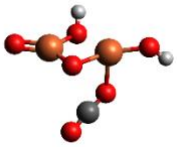
Fe	0.480084	–1.119158	–0.177515
Fe	–1.336350	0.608289	0.288610
O	2.475145	–0.594346	–0.368131
O	–1.186407	–0.963673	–0.612578
O	0.268321	0.451292	0.787087
O	–1.688004	1.657185	–1.024920
O	–2.596064	0.276074	1.404782
C	2.728777	0.529456	–0.112641
O	3.060129	1.601738	0.097414
H	–2.931493	–0.617173	1.266064
H	–1.782412	1.123530	–1.823392

18



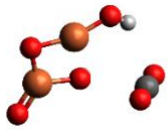
Fe	0.639624	–1.116059	–0.001225
Fe	–1.354033	0.482299	0.000997
C	2.924094	0.542659	0.001865
O	–1.071256	–1.313274	–0.006591
O	0.315942	0.709008	0.004674
O	–2.220231	0.695876	–1.463988
O	–2.224772	0.679346	1.465701
O	3.260647	1.633573	0.003902
O	2.666508	–0.608821	–0.000181
H	–2.377648	–0.183537	1.868479
H	–2.372331	–0.161993	–1.877529

19



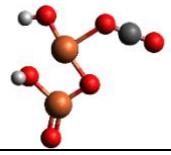
Fe	1.479018	0.405872	–0.068819
Fe	–1.089261	0.662773	–0.054341
C	–0.673989	–2.177030	0.220335
O	0.402105	0.000525	–1.209749
O	0.378945	1.006050	1.257254
O	2.982177	0.272241	0.140562
O	–2.767597	1.205296	–0.154035
O	–0.101897	–3.105051	–0.130366
O	–1.298398	–1.267820	0.620102
H	0.482505	1.939291	1.464994
H	–3.567881	0.784655	0.159987

20

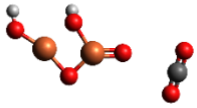


Fe	1.712685	–0.382241	0.066313
Fe	–0.094383	1.253846	–0.074426
C	–2.678554	–1.261962	–0.216593
O	1.714773	1.168114	–0.493256
O	–0.023064	–0.565148	0.619490
O	2.724724	–1.508425	0.161969
O	–1.681393	1.807272	0.356305
O	–3.019519	–0.968690	0.854593
O	–2.357375	–1.559588	–1.285804
H	–0.125215	–0.566449	1.577739
H	–2.335590	1.342756	0.882152

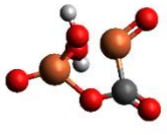
21



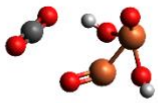
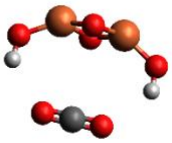
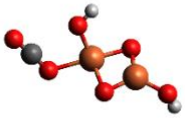
Fe	1.621873	–0.560871	0.022042
Fe	–0.418461	0.790465	–0.137757
C	–2.763709	–0.958753	–0.002309
O	0.050401	–1.034449	–0.124871



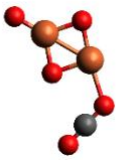
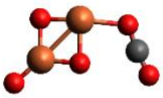
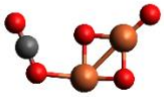
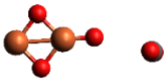
Fe	–0.096525	–0.019261	0.180185
Fe	2.306456	–0.280387	–0.166876
C	–4.434917	0.007628	–0.148914
O	0.813723	–1.378181	0.003352



Fe	1.074837	0.542167	–0.013632
Fe	–1.410693	–0.031054	0.000628
C	1.075252	–1.368712	0.023648
O	–0.385649	0.881965	–1.245254

O	1.506776	1.246569	–0.133686	O	1.168195	1.287845	0.027585	O	–0.365792	0.821517	1.278455
O	2.947960	–1.261397	0.261899	O	–1.572455	0.297313	0.369991	O	2.418520	1.271050	0.012970
O	–0.979000	2.333846	0.479214	O	3.931146	0.290331	0.047106	O	–2.914914	–0.208073	0.025270
O	–3.155426	–2.023322	0.169428	O	–4.532290	1.151338	–0.305372	O	1.888981	–2.222035	0.042221
O	–2.414816	0.143250	–0.182335	O	–4.357397	–1.138119	0.003079	O	–0.250740	–1.454434	0.002870
H	–0.282432	2.953416	0.712349	H	4.242720	1.162129	0.292553	H	–0.293758	0.451608	–2.101172
H	1.806122	1.579724	–0.986022	H	1.348776	1.743062	0.856825	H	–0.556528	1.765047	1.343559
	22				23				24		
											
Fe	–0.290749	–1.199153	0.154250	Fe	1.257232	0.886665	–0.050558	Fe	0.478484	–0.237952	–0.397305
Fe	–1.431007	0.757852	–0.003638	Fe	–1.221129	0.927321	–0.041754	Fe	–1.763895	0.267205	–0.238475
C	2.999076	0.589704	–0.040568	C	–0.048328	–2.644150	0.037491	C	3.195812	0.478976	0.083811
O	–1.991694	–0.908661	–0.539488	O	0.006395	0.544218	–1.188618	O	–0.532221	1.347137	–0.318206
O	–0.361668	0.185484	1.368883	O	0.022924	1.020004	1.146591	O	–1.163563	–1.223892	–0.416277
O	1.124921	–1.508430	–0.434116	O	2.701850	–0.018876	0.095581	O	1.375512	–1.113713	0.851536
O	–1.234732	2.064230	–0.805808	O	–2.697275	0.076045	0.109505	O	–3.428198	0.714280	–0.286161
O	2.333505	0.984159	0.829974	O	–1.206253	–2.632401	0.032350	O	4.106510	0.272573	0.746067
O	3.695866	0.240374	–0.888818	O	1.109194	–2.673966	0.047295	O	2.310253	0.747627	–0.639558
H	0.493208	0.628035	1.472674	H	–2.748185	–0.875045	0.234544	H	–3.781192	0.825450	–1.175785
H	–2.273683	–1.132120	–1.428055	H	2.715504	–0.969720	0.231105	H	0.875552	–1.744726	1.373598

Supplementary Table S6. Coordinates (in Å) of four Fe_2O_3–CO_2 clusters studied in the catalytic isotopic exchange reaction of CO_2 ($Fe_2{}^{16}O_3 + C^{18}O_2 \rightarrow Fe_2{}^{16}O_2{}^{18}O + C^{16}O^{18}O$ and $Fe_2{}^{16}O_3 + C^{16}O^{18}O \rightarrow Fe_2{}^{16}O_2{}^{18}O + C^{16}O_2$) were calculated at the ωB97X-V/def2-TZVPPD level of theory.

1				2			
							
Fe	0.352906	–0.931988	0.003481	Fe	1.481419	–0.383903	0.005861
Fe	–1.547297	0.342539	0.002564	Fe	–0.405871	1.066255	–0.087299
C	2.801810	0.498520	0.001027	C	–2.659696	–0.575407	0.088123
O	0.131660	0.806996	0.002119	O	–0.152547	–0.752660	–0.307244
O	–1.333999	–1.371613	0.002629	O	1.276375	1.331526	0.252623
O	–2.805096	1.200050	0.005332	O	–3.009018	–1.661141	0.117343
O	2.408706	–0.610460	0.002692	O	–2.404740	0.578426	0.072812
O	3.246304	1.551505	–0.000567	O	2.745478	–1.226746	0.072280
3				4			
							
Fe	0.404013	–1.058647	0.087136	Fe	2.562620	–0.154966	–0.054567
Fe	–1.487400	0.387025	–0.003425	Fe	0.310585	0.155890	0.063531
C	2.656536	0.584432	–0.086211	C	–4.034301	–0.123338	–0.067764
O	0.146396	0.759860	0.305698	O	1.266085	–1.293244	–0.065406
O	–1.277428	–1.327379	–0.252701	O	1.627190	1.292937	0.059644
O	–2.755774	1.223536	–0.065995	O	–1.194615	0.360705	0.158717
O	2.401267	–0.569328	–0.076014	O	–4.146150	–0.216750	1.081399
O	3.005588	1.670344	–0.111156	O	–3.946151	–0.035081	–1.219518

Supplementary Table S7. Frequencies (in cm^{-1}, top 27 rows below structures) and vibrational–torsional and rotational Helmholtz free energies (in kJ/mol, bottow two rows below structures) of different isotologues of $[FeO(OH)]_2$–CO_2 clusters studied in the catalytic isotopic exchange reaction of CO_2 ($Fe_2{}^{16}O_4H_2 + C^{18}O_2 \rightarrow Fe_2{}^{16}O_3{}^{18}OH_2 + C^{16}O^{18}O$ and $Fe_2{}^{16}O_4H_2 + C^{16}O^{18}O \rightarrow Fe_2{}^{16}O_3{}^{18}OH_2 + C^{16}O_2$) were calculated using the quasi-rigid-rotor–harmonic-oscillator (QRRHO) model at the ωB97X-V/def2-TZVPPD level of theory.

1									
									
48.68	47.21	48.53	47.47	48.39	47.33	48.91	48.77	48.62	47.57
59.95	59.21	59.88	59.17	59.97	59.27	60.13	60.24	60.15	59.44
105.39	103.37	103.57	105.29	103.42	105.17	105.68	105.55	103.72	105.47
126.62	125.65	127.04	125.83	126.47	125.22	127.36	126.75	127.20	126.00
156.57	158.11	157.21	157.72	157.02	157.51	157.80	157.58	158.19	158.71
170.92	173.95	172.32	172.74	171.88	172.33	172.82	172.41	174.04	174.47
218.92	222.04	220.07	219.89	221.21	221.11	220.64	221.83	222.79	222.66
262.50	267.21	264.12	263.88	266.04	265.71	264.23	266.16	267.70	267.35
301.92	303.66	302.32	302.55	303.04	303.29	302.60	303.32	303.69	303.94
360.77	353.32	358.02	355.52	358.29	355.83	361.23	361.48	358.78	356.34
431.03	443.24	442.92	446.26	430.15	431.05	446.31	431.07	443.35	446.40
459.86	456.39	456.07	462.11	451.91	460.20	462.73	460.85	456.75	463.01
525.21	529.38	525.62	525.57	528.98	528.95	525.67	529.02	529.47	529.43
561.22	556.33	559.77	557.70	560.10	557.94	561.45	561.86	560.27	558.10
582.27	604.90	588.65	588.49	584.93	585.14	588.75	585.23	604.99	604.92
596.04	621.73	614.77	615.20	616.02	616.29	615.22	616.36	621.77	622.26
705.72	683.97	690.82	698.93	691.18	699.45	705.79	706.35	691.27	699.50
739.09	747.28	739.18	739.28	746.97	746.97	739.31	746.98	747.28	747.29
758.26	783.54	758.51	758.61	781.30	781.33	758.68	781.36	783.57	783.61
782.99	787.64	787.11	787.16	785.43	785.51	787.17	785.51	787.64	787.71
911.64	914.83	914.73	914.75	911.80	911.82	915.11	912.18	915.26	915.29
974.47	974.72	974.61	974.61	974.59	974.59	974.61	974.59	974.72	974.72
1059.86	1059.45	1059.74	1059.74	1059.72	1059.72	1059.88	1059.87	1059.74	1059.75
1158.20	1103.86	1123.31	1138.25	1123.26	1138.21	1158.26	1158.22	1123.33	1138.27
2048.44	2012.84	2043.80	2018.08	2043.80	2018.08	2048.44	2048.44	2043.80	2018.08
3677.91	3677.91	3677.91	3677.91	3677.91	3677.91	3677.91	3677.91	3677.91	3677.91
3697.67	3709.85	3709.85	3709.85	3697.67	3697.67	3709.85	3697.67	3709.85	3709.85
109.403	109.439	109.421	109.433	109.411	109.422	109.983	109.972	109.990	110.003
–33.305	–33.378	–33.314	–33.363	–33.321	–33.371	–33.277	–33.284	–33.293	–33.342
2									
									
44.44	44.31	44.63	44.29	44.47	44.15	44.69	44.53	44.71	44.37
58.45	59.69	59.62	59.47	58.64	58.48	59.72	58.73	59.93	59.79
73.64	72.31	73.88	72.27	73.68	72.10	73.93	73.73	73.97	72.37
97.42	96.89	98.45	97.38	97.05	95.88	99.10	97.67	98.69	97.60
115.40	115.63	114.88	115.02	115.86	116.13	115.56	116.59	116.04	116.27
128.15	123.64	123.96	127.62	124.18	127.75	128.23	128.40	124.26	127.84
145.57	147.98	147.42	147.32	146.28	146.18	147.54	146.39	148.18	148.08
216.67	216.85	216.87	216.90	216.57	216.63	216.97	216.71	216.91	216.95
241.98	243.94	243.59	245.03	240.02	241.89	245.56	242.66	244.56	246.22
253.75	257.18	254.25	255.11	256.53	256.97	255.46	257.10	257.32	257.91
270.47	275.57	270.49	270.54	275.47	275.60	270.55	275.61	275.58	275.73
332.94	322.97	323.81	331.76	324.03	331.93	332.96	333.13	324.05	331.94
468.15	471.76	471.67	471.72	468.20	468.24	471.75	468.28	471.79	471.84
474.84	474.98	474.97	474.95	474.87	474.85	474.97	474.87	475.01	474.99
556.88	584.62	560.52	560.54	580.10	580.12	560.59	580.18	584.75	584.77
630.76	622.73	627.27	627.13	626.25	626.14	632.05	630.88	627.65	627.50
671.87	674.57	678.60	682.35	671.51	672.81	685.85	673.87	678.70	682.48
691.92	698.96	698.84	699.20	685.76	688.52	700.34	692.26	699.58	699.92
719.38	724.93	720.16	720.16	723.52	723.53	720.20	723.59	724.97	724.97
760.79	792.78	761.47	761.48	792.26	792.27	761.52	792.30	792.80	792.81

808.58	814.33	814.23	814.24	808.81	808.82	814.25	808.83	814.34	814.34
881.82	883.31	881.82	881.82	883.31	883.31	881.83	883.32	883.32	883.32
1096.91	1096.99	1096.92	1096.92	1096.98	1096.98	1096.92	1096.98	1096.99	1096.99
1370.93	1292.93	1327.76	1335.65	1327.76	1335.65	1370.93	1370.93	1327.77	1335.65
2419.64	2382.64	2408.24	2395.05	2408.24	2395.05	2419.64	2419.64	2408.25	2395.06
3838.20	3838.20	3838.20	3838.20	3838.20	3838.20	3838.20	3838.20	3838.20	3838.20
3869.37	3882.10	3882.10	3882.10	3869.37	3869.37	3882.10	3869.37	3882.10	3882.10
102.899	102.752	102.744	102.849	102.803	102.909	103.418	103.478	103.322	103.427
–33.776	–33.817	–33.760	–33.810	–33.784	–33.833	–33.729	–33.754	–33.736	–33.787

3

									
32.31	30.73	32.06	30.80	32.27	31.03	32.18	32.40	32.14	30.88
55.33	55.26	54.80	55.52	55.06	55.78	55.60	55.84	55.32	56.04
68.61	66.20	68.61	66.05	68.76	66.20	68.60	68.75	68.76	66.19
129.27	128.94	128.22	129.35	128.95	130.09	129.66	130.40	129.24	130.45
164.20	164.10	163.34	165.01	163.46	165.14	165.29	165.48	164.63	166.18
172.54	171.23	171.39	170.99	172.18	171.84	172.96	173.78	172.87	172.56
190.61	190.52	190.35	191.68	189.60	190.83	191.85	190.94	190.64	191.96
226.03	229.48	228.54	229.04	226.53	226.95	229.21	227.15	229.63	230.07
258.41	258.81	257.61	259.86	257.62	260.17	260.11	260.44	259.16	261.78
289.08	286.68	285.11	289.35	285.94	290.23	289.89	290.80	287.11	291.17
315.51	316.85	315.32	316.45	315.96	316.87	316.72	317.09	317.00	317.97
419.64	433.89	432.82	432.81	420.37	420.36	432.82	420.37	433.89	433.89
456.73	459.29	458.71	458.70	457.57	457.57	458.71	457.57	459.29	459.29
540.32	564.07	563.84	563.83	540.50	540.48	563.85	540.50	564.09	564.07
614.03	628.29	613.38	613.90	630.25	631.73	614.63	633.48	630.59	632.09
664.31	655.22	658.38	659.75	660.23	660.22	664.37	665.20	660.24	660.23
666.65	666.21	661.06	663.04	667.80	669.88	666.81	671.94	668.26	670.41
680.41	684.66	682.55	682.64	682.44	682.88	682.75	683.56	684.93	685.30
703.94	721.96	704.67	704.66	720.18	720.20	704.93	720.20	721.97	721.98
735.07	751.81	736.71	736.81	751.21	751.24	736.93	751.41	751.95	751.99
888.71	892.71	892.70	892.70	888.73	888.73	892.70	888.73	892.71	892.71
904.24	905.33	905.15	905.15	904.40	904.40	905.15	904.40	905.33	905.34
1062.90	1062.94	1062.91	1062.91	1062.93	1062.93	1062.91	1062.93	1062.94	1062.94
1369.47	1291.58	1326.40	1334.18	1326.41	1334.19	1369.47	1369.48	1326.41	1334.19
2415.36	2378.31	2403.84	2390.83	2403.85	2390.84	2415.36	2415.36	2403.85	2390.84
3823.03	3835.43	3835.43	3835.43	3823.03	3823.03	3835.43	3823.03	3835.43	3835.43
3863.13	3863.13	3863.13	3863.13	3863.13	3863.13	3863.13	3863.13	3863.13	3863.13
108.487	108.365	108.389	108.450	108.405	108.467	109.041	109.057	108.959	109.020
–33.771	–33.869	–33.782	–33.831	–33.810	–33.859	–33.738	–33.765	–33.777	–33.826

4

									
15.28	15.67	15.54	15.40	15.51	15.39	15.52	15.50	15.78	15.64
27.73	28.21	28.46	28.19	27.79	27.52	28.49	27.81	28.55	28.27
35.81	34.40	34.92	35.34	34.83	35.25	35.83	35.75	34.85	35.28
57.32	57.05	56.76	56.95	57.37	57.77	57.50	58.25	57.50	57.89
61.47	62.12	61.32	61.41	62.39	62.23	61.60	62.54	62.50	62.30
69.73	70.47	70.36	69.71	70.28	69.65	70.43	70.35	71.08	70.53
91.21	92.74	93.18	92.49	91.42	90.76	93.23	91.48	93.47	92.78
106.10	105.10	105.42	105.85	105.35	105.76	106.19	106.11	105.44	105.87
124.38	122.88	124.17	123.09	124.17	123.09	124.39	124.39	124.18	123.10
226.28	221.05	223.62	223.73	223.62	223.73	226.28	226.28	223.62	223.73
266.16	260.44	262.66	264.08	262.66	264.08	266.16	266.16	262.66	264.08
291.04	283.33	289.77	284.55	289.77	284.55	291.04	291.04	289.77	284.55
457.73	454.65	455.09	457.26	455.09	457.26	457.74	457.73	455.09	457.26
469.16	468.54	468.60	469.12	468.59	469.11	469.16	469.16	468.60	469.12
552.16	551.97	552.07	552.07	552.05	552.06	552.17	552.16	552.07	552.07
614.08	613.99	614.02	614.06	614.02	614.06	614.09	614.08	614.02	614.06
661.80	672.15	666.99	667.00	667.00	667.01	667.01	667.01	672.16	672.17
672.47	682.86	677.67	677.67	677.70	677.70	677.67	677.70	682.86	682.86
750.98	729.18	730.53	750.22	730.53	750.22	751.00	751.01	730.53	750.25
760.67	751.16	751.40	759.68	751.41	759.68	760.67	760.67	751.43	759.68
807.97	805.35	805.76	807.72	805.76	807.72	807.97	807.97	805.76	807.72
874.97	870.56	870.71	874.79	870.71	874.79	874.97	874.97	870.71	874.79
1088.40	1041.62	1088.35	1041.72	1088.35	1041.72	1088.41	1088.41	1088.36	1041.73
1312.32	1392.08	1352.53	1352.53	1351.26	1351.26	1352.53	1351.26	1392.08	1392.08

2382.64	2419.54	2400.69	2400.69	2402.64	2402.64	2400.69	2402.64	2419.54	2419.54
3834.85	3822.39	3822.39	3834.85	3822.39	3834.85	3834.85	3834.85	3822.39	3834.85
3902.63	3902.63	3902.63	3902.63	3902.63	3902.63	3902.63	3902.63	3902.63	3902.63
89.566	89.569	89.616	89.560	89.578	89.523	90.108	90.071	90.119	90.063
–34.732	–34.672	–34.744	–34.704	–34.702	–34.662	–34.688	–34.646	–34.656	–34.617

5

									
31.12	29.94	31.12	30.07	30.97	29.93	31.25	31.10	31.10	30.05
49.70	48.65	49.20	48.90	49.44	49.13	49.71	49.96	49.45	49.15
85.32	83.85	83.65	85.45	83.72	85.52	85.45	85.53	83.86	85.65
105.39	105.15	105.85	104.77	105.73	104.67	105.96	105.86	106.34	105.27
142.62	146.91	144.13	144.38	145.07	145.30	144.40	145.32	146.93	147.17
216.89	217.37	217.20	217.58	216.74	217.08	217.89	217.37	217.67	218.07
229.96	233.58	232.57	232.60	231.03	231.13	232.83	231.32	233.81	233.86
267.81	268.46	267.35	267.94	268.53	269.14	268.85	270.17	269.57	270.14
322.75	321.36	322.35	320.45	324.31	322.12	324.03	326.05	325.43	323.13
336.47	335.48	335.17	335.21	335.82	336.12	336.77	337.27	336.28	336.73
420.75	414.81	413.78	421.37	414.09	421.53	422.13	422.23	415.41	422.95
444.25	460.22	459.92	459.88	444.42	444.47	459.93	444.60	460.28	460.24
501.39	504.14	502.32	502.51	503.08	503.28	502.58	503.32	504.17	504.35
546.28	542.68	546.25	543.99	545.84	543.56	547.84	547.26	546.77	544.44
559.01	577.78	564.08	563.91	562.14	562.16	564.52	562.74	578.11	578.06
577.69	603.55	595.41	595.64	595.62	595.76	595.68	596.03	603.75	604.02
699.21	679.50	685.37	692.91	686.19	693.68	699.44	700.16	686.45	693.92
735.80	737.39	736.82	737.00	735.90	736.14	737.37	736.50	737.60	737.81
780.59	786.70	784.83	784.92	782.15	782.21	784.93	782.23	786.72	786.79
801.49	835.69	801.98	802.04	835.49	835.52	802.04	835.53	835.70	835.72
933.87	934.05	933.98	933.98	933.95	933.95	933.98	933.95	934.06	934.06
995.48	999.82	1000.18	1000.28	995.21	995.30	1000.61	995.61	1000.31	1000.42
1069.13	1068.81	1069.03	1069.07	1069.00	1069.03	1069.17	1069.14	1069.04	1069.08
1167.79	1112.77	1132.95	1147.02	1132.84	1146.93	1167.88	1167.81	1132.97	1147.04
2048.24	2012.66	2043.13	2018.40	2043.14	2018.40	2048.24	2048.24	2043.14	2018.40
3680.51	3692.53	3692.53	3692.53	3680.51	3680.51	3692.53	3680.51	3692.53	3692.53
3727.04	3727.05	3727.05	3727.05	3727.04	3727.04	3727.05	3727.04	3727.05	3727.05
108.268	108.334	108.305	108.305	108.299	108.299	108.852	108.847	108.884	108.883
–33.266	–33.352	–33.296	–33.323	–33.293	–33.320	–33.242	–33.239	–33.271	–33.298

6

									
20.76	23.39	21.99	22.15	22.02	22.37	20.92	20.97	22.14	22.54
19.86	21.64	20.81	20.84	20.89	20.71	20.31	20.37	21.35	21.13
49.08	49.94	49.70	49.58	49.43	49.32	49.75	49.47	50.11	49.99
59.88	58.71	59.20	59.51	59.03	59.32	60.12	59.94	59.26	59.57
86.87	88.27	88.12	89.17	86.01	87.06	89.19	87.06	88.33	89.38
124.66	120.69	122.94	123.10	123.20	123.37	124.86	125.18	123.28	123.46
136.10	133.33	134.07	134.24	134.19	134.31	136.38	136.41	134.62	134.76
153.57	146.15	151.23	148.82	150.84	148.47	153.97	153.65	151.32	148.91
182.62	185.18	184.83	184.82	182.96	182.96	184.85	182.97	185.20	185.19
219.83	229.08	224.77	224.76	224.21	224.21	224.77	224.21	229.08	229.08
250.04	251.62	250.35	250.34	251.32	251.31	250.34	251.31	251.63	251.62
291.91	297.02	294.60	294.60	294.38	294.38	294.60	294.38	297.02	297.02
565.50	584.90	566.43	566.44	583.98	583.98	566.44	583.99	584.90	584.91
620.18	625.83	620.25	620.26	625.58	625.60	620.26	625.60	625.84	625.85
650.41	654.55	653.57	653.79	651.18	651.38	653.94	651.50	654.75	654.96
701.40	695.03	699.34	699.28	700.37	700.31	703.70	705.60	700.43	700.36
706.93	700.50	705.73	705.55	704.42	704.34	710.73	708.41	705.76	705.59
710.62	730.48	711.16	711.15	715.02	714.93	712.11	716.14	730.49	730.48
726.67	740.17	735.12	735.13	739.16	739.16	735.21	739.25	740.25	740.26
738.64	753.10	751.56	751.52	742.19	742.18	751.64	742.28	753.19	753.16
860.72	870.74	861.15	861.16	870.37	870.38	861.16	870.38	870.74	870.75
979.05	984.42	984.30	984.30	979.17	979.17	984.30	979.17	984.43	984.42
1032.94	1033.14	1032.99	1032.99	1033.09	1033.09	1032.99	1033.09	1033.14	1033.14
1339.45	1262.69	1300.91	1300.63	1300.91	1300.63	1339.45	1339.45	1300.91	1300.63
2316.67	2281.41	2299.33	2299.87	2299.33	2299.87	2316.67	2316.67	2299.33	2299.87
3666.18	3678.04	3678.04	3678.04	3666.18	3666.18	3678.04	3666.18	3678.04	3678.04
3752.80	3752.80	3752.80	3752.80	3752.80	3752.80	3752.80	3752.80	3752.80	3752.80
96.515	96.634	96.588	96.588	96.591	96.589	97.095	97.097	97.166	97.165

–34.533	–34.624	–34.565	–34.600	–34.560	–34.593	–34.515	–34.510	–34.542	–34.576
7									
									
29.28	26.95	28.79	27.32	28.97	27.52	29.04	29.22	28.72	27.24
56.28	56.45	55.85	56.37	56.35	56.86	56.43	56.92	56.50	57.02
69.04	66.66	69.04	66.53	69.18	66.67	69.03	69.17	69.17	66.66
130.82	130.34	129.66	130.86	130.40	131.60	131.16	131.91	130.65	131.92
163.83	164.05	163.14	164.73	163.32	164.91	164.97	165.21	164.55	166.01
172.26	170.81	171.04	170.63	171.86	171.50	172.62	173.45	172.47	172.13
190.26	190.21	190.07	191.42	189.19	190.43	191.59	190.55	190.33	191.66
224.24	227.52	226.60	227.08	224.72	225.14	227.27	225.36	227.69	228.13
257.89	258.41	257.15	259.33	257.22	259.70	259.58	259.96	258.75	261.30
288.69	286.20	284.67	288.91	285.52	289.82	289.46	290.40	286.64	290.72
315.40	316.68	315.17	316.36	315.77	316.73	316.63	316.96	316.83	317.85
419.12	433.39	432.31	432.30	419.85	419.85	432.31	419.85	433.40	433.39
456.21	458.76	458.16	458.16	457.07	457.07	458.16	457.08	458.76	458.76
539.64	563.34	563.11	563.10	539.81	539.80	563.12	539.82	563.35	563.34
613.52	627.82	612.83	613.37	629.76	631.26	614.09	632.98	630.10	631.62
664.37	655.22	658.33	659.82	660.25	660.22	664.43	665.21	660.25	660.23
666.29	665.95	660.88	662.71	667.52	669.57	666.47	671.57	667.99	670.11
679.93	684.09	682.03	682.14	681.89	682.38	682.27	683.11	684.38	684.78
704.17	722.23	704.85	704.85	720.48	720.50	705.12	720.50	722.23	722.24
734.71	751.32	736.33	736.43	750.73	750.77	736.55	750.94	751.47	751.50
889.67	893.57	893.56	893.56	889.69	889.69	893.56	889.69	893.58	893.58
904.99	906.19	906.01	906.01	905.15	905.15	906.01	905.15	906.19	906.19
1062.90	1062.94	1062.91	1062.91	1062.92	1062.93	1062.91	1062.93	1062.94	1062.94
1369.37	1291.50	1326.30	1334.10	1326.31	1334.11	1369.38	1369.39	1326.32	1334.11
2415.25	2378.20	2403.74	2390.72	2403.75	2390.72	2415.25	2415.26	2403.75	2390.73
3822.73	3835.13	3835.13	3835.13	3822.73	3822.73	3835.13	3822.73	3835.13	3835.13
3862.82	3862.82	3862.82	3862.82	3862.82	3862.82	3862.82	3862.82	3862.82	3862.82
108.368	108.211	108.260	108.302	108.282	108.325	108.912	108.934	108.826	108.867
–33.770	–33.869	–33.782	–33.830	–33.809	–33.858	–33.736	–33.765	–33.776	–33.826
8									
									
27.07	26.00	26.70	26.33	26.74	26.39	27.09	27.14	26.76	26.40
67.02	69.53	69.74	69.55	67.01	66.81	69.73	67.00	69.72	69.52
80.10	80.98	79.52	79.80	81.34	81.27	80.23	81.97	81.48	81.54
88.62	87.07	88.65	87.25	88.41	87.30	89.13	88.95	88.89	87.70
147.81	144.54	146.01	146.06	146.21	146.26	148.19	148.33	146.55	146.60
169.33	167.64	167.88	169.24	167.75	169.09	169.54	169.40	167.93	169.30
175.09	177.87	177.43	177.75	175.19	175.46	177.92	175.64	178.04	178.34
242.03	245.12	242.29	242.35	244.00	244.69	242.40	244.73	245.16	245.32
246.66	246.86	246.74	248.01	246.09	246.97	248.15	247.15	247.06	248.24
268.05	262.56	263.02	270.01	261.42	267.47	270.76	268.18	263.17	270.13
277.01	278.14	277.81	278.15	276.13	277.30	278.55	277.74	278.48	278.85
422.13	423.07	422.14	422.15	423.05	423.06	422.16	423.07	423.08	423.08
498.16	522.60	499.23	499.24	521.39	521.39	499.25	521.40	522.61	522.61
579.24	582.50	582.54	582.53	579.21	579.20	582.58	579.25	582.55	582.54
638.85	643.77	643.80	644.00	638.36	638.75	644.04	638.86	643.91	644.11
664.74	658.13	662.42	664.14	660.49	662.62	668.77	665.35	662.50	664.17
670.26	661.11	665.91	667.46	665.42	665.63	671.72	670.32	665.93	667.53
683.76	699.03	697.94	698.02	681.79	682.57	698.75	684.71	699.53	699.59
745.84	746.36	746.34	746.35	745.89	745.90	746.35	745.90	746.36	746.37
789.51	798.51	795.82	795.85	792.06	792.12	795.87	792.15	798.53	798.57
843.50	853.39	844.37	844.40	852.98	852.98	844.41	852.99	853.40	853.40
854.00	880.96	854.16	854.16	880.68	880.69	854.16	880.70	880.97	880.98
1101.39	1101.94	1101.41	1101.41	1101.92	1101.92	1101.41	1101.92	1101.94	1101.94
1379.12	1300.46	1336.27	1342.82	1336.27	1342.82	1379.13	1379.13	1336.28	1342.82
2416.72	2379.96	2404.05	2393.70	2404.04	2393.69	2416.73	2416.72	2404.05	2393.70
3828.08	3828.08	3828.08	3828.08	3828.08	3828.08	3828.08	3828.08	3828.08	3828.08
3871.69	3884.39	3884.39	3884.39	3871.69	3871.69	3884.39	3871.69	3884.39	3884.39
107.882	107.718	107.750	107.828	107.774	107.853	108.403	108.428	108.295	108.373
–33.517	–33.556	–33.504	–33.549	–33.527	–33.571	–33.462	–33.485	–33.472	–33.516
9									
									

50.75	49.14	49.67	50.29	49.58	50.20	50.97	50.87	49.81	50.42
95.02	93.36	93.57	94.77	93.58	94.76	95.16	95.16	93.70	94.91
123.72	122.24	123.62	122.36	123.45	122.28	124.01	123.85	123.75	122.53
132.00	131.11	131.11	131.93	131.29	132.09	132.21	132.41	131.54	132.32
158.22	160.33	159.63	158.79	159.61	158.79	159.91	159.90	161.42	160.64
209.14	209.18	208.20	208.24	210.14	210.10	209.33	211.18	210.24	210.21
225.24	226.39	225.58	225.53	226.14	226.05	225.71	226.32	226.62	226.53
266.95	273.92	272.11	271.68	269.62	269.28	272.45	269.92	274.77	274.40
310.37	306.98	308.77	308.65	308.51	308.36	311.75	311.56	310.07	309.96
394.00	396.14	394.10	394.81	394.47	395.55	396.52	396.97	397.67	398.63
415.70	429.04	417.81	418.10	426.11	425.43	418.26	426.14	429.21	429.17
434.88	445.53	446.42	445.43	435.96	435.53	446.77	436.62	446.70	445.79
545.35	566.08	550.61	549.66	558.37	556.91	550.73	558.60	568.37	566.61
584.88	597.93	599.08	599.40	589.44	589.60	600.69	590.37	599.39	599.82
606.62	608.12	609.13	604.53	609.72	607.68	610.53	611.59	614.31	610.13
618.55	614.79	616.92	616.86	617.06	616.41	618.57	618.58	617.27	616.88
633.45	623.49	632.26	623.45	631.55	621.25	634.27	633.84	632.70	624.31
674.34	676.79	673.69	672.27	678.48	677.22	674.43	679.18	678.55	677.29
717.15	719.32	717.73	717.52	718.89	718.71	717.76	718.91	719.52	719.34
759.49	764.03	764.04	764.00	759.53	759.49	764.10	759.59	764.13	764.09
821.84	827.99	822.59	822.52	826.32	826.29	822.70	826.37	828.13	828.08
836.52	842.73	841.55	841.51	838.75	838.68	841.61	838.88	842.88	842.83
1039.19	1037.92	1038.69	1038.83	1038.59	1038.73	1039.34	1039.23	1038.73	1038.87
1200.35	1138.22	1173.35	1164.45	1173.39	1164.49	1200.37	1200.41	1173.41	1164.51
2104.73	2069.62	2077.86	2097.30	2077.86	2097.30	2104.74	2104.73	2077.87	2097.30
3845.95	3858.52	3858.51	3858.51	3845.95	3845.95	3858.51	3845.95	3858.52	3858.52
3869.96	3882.70	3869.96	3869.96	3882.70	3882.70	3869.96	3882.70	3882.70	3882.70
112.016	112.024	112.037	112.008	112.033	112.004	112.598	112.594	112.615	112.587
–32.956	–33.008	–32.990	–32.970	–32.994	–32.975	–32.915	–32.919	–32.954	–32.933

10

									
72.79	72.19	72.64	71.82	73.17	72.38	73.04	73.59	73.42	72.62
151.70	152.80	152.76	154.20	150.42	151.40	154.76	152.12	153.16	154.64
163.89	164.35	164.30	163.91	164.70	164.20	164.61	164.97	165.23	164.83
174.83	173.13	173.80	175.09	172.32	173.97	176.62	175.38	174.66	175.91
209.15	211.07	208.55	210.39	209.63	211.54	210.40	211.55	211.07	212.86
226.74	222.74	227.47	222.83	226.49	221.95	228.13	227.13	227.83	223.19
304.60	294.78	299.05	299.69	299.50	300.54	304.75	305.13	299.74	300.58
304.74	308.75	306.77	306.49	307.47	306.61	306.78	307.69	309.39	308.79
317.31	321.43	319.16	318.67	320.79	320.38	319.16	320.81	321.90	321.44
322.63	330.48	325.38	325.31	327.50	327.48	325.44	327.51	330.48	330.49
368.29	374.80	371.20	371.29	370.80	370.71	371.96	371.27	375.45	375.49
409.62	412.81	412.07	413.38	410.40	412.05	413.65	412.53	413.66	415.31
436.71	428.30	430.97	431.68	432.21	432.75	436.80	437.69	432.47	432.90
590.71	608.01	590.98	590.99	608.99	608.99	590.99	608.99	609.20	609.20
614.16	609.21	611.18	611.11	611.09	611.02	614.27	614.18	611.20	611.14
637.76	645.41	637.56	637.73	645.47	645.69	637.81	645.78	645.55	645.77
734.65	737.32	734.48	734.91	737.40	737.75	734.94	737.77	737.68	738.06
760.75	742.62	747.52	759.79	747.52	760.96	760.85	762.45	747.61	761.04
771.63	765.04	763.30	767.81	765.18	768.55	771.69	771.99	765.25	768.62
882.18	885.81	883.41	883.47	884.70	884.76	883.47	884.76	885.81	885.87
898.72	901.64	898.65	898.86	901.22	901.45	899.03	901.63	901.84	902.07
977.15	1007.52	1007.50	1007.51	977.25	977.27	1007.52	977.27	1007.52	1007.53
1055.42	1069.33	1069.19	1069.19	1055.57	1055.57	1069.19	1055.57	1069.33	1069.33
1168.48	1121.25	1134.45	1154.79	1134.53	1154.86	1168.50	1168.56	1134.54	1154.87
1944.80	1907.26	1942.48	1910.03	1942.47	1910.03	1944.81	1944.80	1942.48	1910.03
3736.75	3748.94	3736.75	3736.75	3748.94	3748.94	3736.75	3748.94	3748.94	3748.94
3753.39	3753.41	3753.39	3753.39	3753.41	3753.41	3753.39	3753.41	3753.41	3753.41
117.244	117.142	117.160	117.204	117.183	117.225	117.796	117.818	117.734	117.778
–32.881	–32.907	–32.865	–32.904	–32.884	–32.924	–32.829	–32.849	–32.832	–32.872

11

									
16.07	15.56	14.82	15.54	16.08	16.72	15.49	16.65	15.40	16.09
6.75	7.27	6.80	5.47	7.98	6.82	6.01	7.23	7.50	6.16
12.85	9.64	10.84	11.04	11.50	11.59	12.26	12.71	10.80	10.91
43.42	43.66	43.47	43.44	43.65	43.61	43.41	43.58	43.64	43.61

52.71	51.13	51.07	52.86	50.98	52.76	52.92	52.81	51.19	52.97
70.67	68.75	70.90	68.88	70.48	68.45	71.17	70.77	71.00	69.00
114.26	115.73	115.77	115.73	114.25	114.22	115.78	114.26	115.78	115.74
162.10	165.24	164.98	164.98	162.34	162.33	164.98	162.33	165.25	165.24
216.49	218.16	217.35	217.34	217.32	217.32	217.34	217.32	218.16	218.16
226.02	232.20	230.84	230.84	227.40	227.40	230.84	227.40	232.20	232.20
246.45	249.78	248.15	248.15	248.11	248.11	248.15	248.11	249.79	249.79
426.59	443.26	426.76	426.76	443.11	443.11	426.76	443.11	443.26	443.26
515.15	517.48	515.99	515.99	516.57	516.57	515.99	516.57	517.49	517.49
532.24	532.63	532.26	532.26	532.61	532.61	532.26	532.61	532.63	532.63
606.53	626.86	606.96	606.96	626.62	626.62	606.98	626.65	626.89	626.89
678.08	667.77	672.96	672.93	672.96	672.93	678.11	678.11	672.99	672.96
683.26	672.93	678.11	678.10	678.14	678.13	683.27	683.31	678.15	678.13
687.25	695.15	687.49	687.49	694.80	694.80	687.51	694.80	695.15	695.15
725.05	727.82	725.15	725.15	727.72	727.72	725.15	727.72	727.82	727.82
746.50	747.78	746.52	746.52	747.75	747.75	746.53	747.76	747.79	747.79
845.25	850.06	845.29	845.29	850.02	850.02	845.29	850.02	850.06	850.06
864.24	867.24	867.13	867.13	864.32	864.32	867.13	864.32	867.24	867.24
1053.12	1098.59	1098.53	1098.53	1053.21	1053.21	1098.54	1053.21	1098.59	1098.59
1389.67	1310.02	1349.65	1349.41	1349.65	1349.41	1389.67	1389.67	1349.65	1349.41
2416.01	2379.08	2397.91	2398.34	2397.91	2398.34	2416.01	2416.01	2397.91	2398.34
3811.19	3823.61	3811.19	3811.19	3823.61	3823.61	3811.19	3823.61	3823.61	3823.61
3894.44	3894.44	3894.44	3894.44	3894.44	3894.44	3894.44	3894.44	3894.44	3894.44
92.514	92.293	92.254	92.066	92.631	92.494	92.770	93.138	92.926	92.750
–34.180	–34.257	–34.218	–34.212	–34.226	–34.219	–34.137	–34.146	–34.184	–34.178

12

									
23.21	24.66	23.14	23.16	24.72	24.73	23.17	24.73	24.66	24.67
87.08	84.04	87.37	84.02	87.11	83.81	87.35	87.08	87.37	84.02
93.52	93.26	95.10	93.82	93.12	91.83	95.34	93.31	94.89	93.61
121.54	118.81	120.44	120.06	120.23	119.85	122.04	121.94	120.78	120.44
171.04	169.07	170.13	170.05	169.96	169.88	171.42	171.24	170.34	170.27
198.65	194.04	194.35	197.92	194.68	198.15	198.85	199.05	194.88	198.36
220.45	223.37	220.55	220.71	222.95	223.13	221.09	223.53	223.69	223.87
259.61	258.29	257.92	261.80	257.26	260.66	262.33	261.13	259.12	263.11
271.17	274.22	271.29	271.44	273.17	273.74	271.48	273.80	274.25	274.44
285.44	281.68	281.63	286.00	280.92	285.45	286.80	286.32	282.23	286.60
320.93	322.74	320.18	321.73	321.74	323.21	322.10	323.54	322.95	324.35
481.84	482.40	482.40	482.40	481.84	481.85	482.41	481.85	482.41	482.41
536.42	561.40	560.43	560.45	537.22	537.26	560.49	537.30	561.43	561.45
660.63	661.50	660.83	660.83	661.18	661.18	660.83	661.19	661.50	661.50
693.55	683.08	688.65	688.22	688.50	688.09	693.72	693.57	688.65	688.22
711.78	700.62	705.73	707.84	705.30	707.36	712.83	712.33	705.81	707.96
712.99	738.22	718.39	718.42	731.42	731.45	718.48	731.56	738.24	738.24
744.71	753.40	744.66	744.72	751.57	751.59	744.74	751.59	753.41	753.44
803.45	836.81	833.63	833.76	809.16	809.35	833.82	809.43	836.86	836.99
849.42	850.37	850.35	850.36	849.49	849.50	850.37	849.49	850.38	850.39
926.67	926.97	926.77	926.77	926.90	926.90	926.77	926.90	926.97	926.97
936.44	942.99	937.03	937.04	942.46	942.47	937.04	942.48	943.00	943.00
1031.47	1032.14	1032.08	1032.09	1031.53	1031.53	1032.09	1031.53	1032.14	1032.15
1338.08	1261.62	1296.75	1302.43	1296.76	1302.44	1338.08	1338.09	1296.76	1302.44
2324.05	2288.75	2310.97	2302.89	2310.97	2302.89	2324.05	2324.05	2310.97	2302.89
3672.72	3672.72	3672.72	3672.72	3672.72	3672.72	3672.72	3672.72	3672.72	3672.72
3695.23	3707.26	3695.23	3695.23	3707.26	3707.26	3695.23	3707.26	3707.26	3707.26
112.989	112.773	112.873	112.912	112.854	112.893	113.540	113.520	113.404	113.442
–33.928	–33.987	–33.951	–34.016	–33.898	–33.963	–33.917	–33.864	–33.887	–33.952

13

									
30.86	30.27	31.03	30.31	30.82	30.10	31.06	30.84	31.02	30.30
60.47	59.13	60.19	59.26	60.33	59.37	60.55	60.69	60.41	59.46
88.40	86.64	87.61	87.74	87.33	87.48	88.90	88.62	87.80	87.98
121.75	119.19	119.50	121.56	119.34	121.40	122.03	121.87	119.65	121.69
155.86	154.70	155.29	155.23	155.34	155.28	156.09	156.15	155.60	155.54
172.61	171.25	171.20	171.96	171.83	172.63	172.75	173.45	171.95	172.75
193.39	199.51	194.02	194.13	198.52	198.62	194.25	198.71	199.58	199.67
233.29	234.01	233.88	234.01	233.32	233.44	234.16	233.59	234.15	234.28

271.95	268.29	268.86	274.48	267.01	271.78	275.06	272.20	268.90	274.51
281.43	288.87	287.59	288.00	281.32	282.45	288.15	282.75	288.97	289.36
334.76	334.50	333.12	335.30	333.75	336.04	335.69	336.45	334.79	336.96
413.22	413.40	413.22	413.23	413.38	413.39	413.24	413.39	413.40	413.41
506.04	509.85	509.30	509.30	506.76	506.76	509.31	506.77	509.85	509.85
550.00	572.82	562.43	562.41	553.61	553.63	562.45	553.63	572.83	572.82
577.95	602.50	587.80	587.99	598.14	598.44	588.10	598.72	602.89	603.24
662.12	653.26	654.84	658.54	657.31	661.00	662.58	665.11	657.42	661.11
668.38	658.28	663.29	663.43	663.32	663.51	668.41	668.48	663.33	663.53
688.64	715.78	689.95	690.24	713.91	713.98	690.55	714.03	715.84	715.92
717.63	728.91	724.69	724.69	722.48	722.52	724.69	722.57	728.92	728.93
792.92	797.79	797.72	797.72	794.77	794.87	797.72	794.98	797.79	797.79
797.61	821.17	819.42	819.50	797.70	797.70	819.61	797.70	821.26	821.34
909.59	909.86	909.59	909.59	909.85	909.85	909.59	909.85	909.86	909.86
928.41	929.95	928.51	928.52	929.86	929.86	928.52	929.86	929.95	929.96
1364.37	1286.85	1321.27	1329.51	1321.27	1329.50	1364.38	1364.37	1321.28	1329.51
2412.55	2375.40	2401.59	2387.36	2401.59	2387.36	2412.56	2412.56	2401.60	2387.37
3813.79	3813.79	3813.79	3813.79	3813.79	3813.79	3813.79	3813.79	3813.79	3813.79
3818.39	3818.39	3818.39	3818.39	3818.39	3818.39	3818.39	3818.39	3818.39	3818.39
107.967	107.873	107.884	107.977	107.864	107.957	108.539	108.519	108.436	108.530
–33.624	–33.723	–33.659	–33.706	–33.641	–33.687	–33.614	–33.595	–33.631	–33.679

14

									
60.35	59.85	60.18	60.43	59.77	60.05	60.83	60.43	60.25	60.52
107.41	105.47	105.75	106.83	105.89	106.90	107.52	107.63	105.99	107.03
135.53	130.16	133.17	132.45	133.35	132.64	135.58	135.78	133.40	132.70
166.82	165.86	166.37	166.54	166.15	166.35	167.22	167.03	166.55	166.76
189.86	190.05	189.81	189.87	190.04	190.14	190.17	190.43	190.34	190.44
228.48	230.08	229.30	229.31	229.23	229.23	229.43	229.35	230.20	230.21
272.62	276.39	275.61	275.62	272.90	273.04	275.85	273.14	276.61	276.63
278.28	285.30	285.20	285.30	278.81	278.80	285.44	279.07	285.47	285.55
415.72	413.79	411.24	412.24	418.18	418.26	416.38	423.37	418.79	418.92
425.59	429.24	423.30	424.12	430.52	432.20	425.60	433.63	430.61	432.35
465.10	465.12	465.05	465.14	465.12	465.24	465.20	465.35	465.22	465.34
494.15	498.14	493.20	494.86	496.52	497.73	497.92	499.83	500.69	501.82
517.93	519.45	518.10	517.99	520.02	519.82	518.50	521.11	520.26	520.06
558.49	579.14	578.92	579.09	558.53	558.59	579.45	559.12	579.50	579.57
640.00	654.21	634.69	636.46	658.21	659.15	640.88	664.08	659.04	659.93
729.03	733.47	735.98	719.42	730.31	730.22	736.54	730.38	737.04	735.85
737.68	738.00	737.10	736.86	752.80	736.74	737.90	754.93	754.33	738.85
804.64	805.61	805.61	805.13	805.03	804.85	807.06	805.92	807.43	807.07
815.72	830.94	829.42	829.29	815.45	813.21	831.09	816.28	832.67	832.48
832.45	831.97	836.73	831.73	834.50	833.59	840.38	837.03	838.98	835.56
852.90	857.10	851.85	850.74	857.37	854.72	856.35	863.14	861.80	860.31
933.80	934.39	933.28	933.11	935.20	934.98	933.92	935.96	935.35	935.12
941.99	942.14	942.02	942.01	942.12	942.11	942.02	942.13	942.16	942.15
1153.14	1118.77	1145.67	1125.52	1146.19	1126.10	1153.26	1153.87	1146.32	1126.25
1908.47	1871.93	1872.95	1907.61	1872.99	1907.65	1908.48	1908.51	1872.99	1907.66
3789.85	3789.85	3789.85	3789.85	3789.85	3789.85	3789.85	3789.85	3789.85	3789.85
3805.82	3805.82	3805.82	3805.82	3805.82	3805.82	3805.82	3805.82	3805.82	3805.82
118.043	118.005	117.989	117.986	118.064	118.059	118.605	118.679	118.625	118.622
–33.002	–33.081	–33.051	–33.013	–33.070	–33.032	–32.971	–32.990	–33.040	–33.002

15

									
27.49	26.59	27.55	26.67	27.43	26.55	27.56	27.44	27.49	26.60
60.01	58.80	59.51	59.07	59.73	59.27	60.10	60.31	59.82	59.36
89.38	87.11	88.55	88.25	88.26	87.96	89.81	89.52	88.66	88.39
114.82	112.63	113.05	114.55	112.89	114.39	115.12	114.96	113.22	114.69
155.99	155.19	155.53	155.41	155.79	155.66	156.16	156.43	155.98	155.86
174.25	172.35	172.79	173.46	173.04	173.72	174.41	174.68	173.18	173.88
193.29	199.91	194.06	194.16	198.84	198.94	194.23	199.00	199.97	200.07
231.47	232.13	231.97	232.20	231.44	231.67	232.33	231.80	232.27	232.51
275.03	268.77	269.33	275.52	268.33	274.39	276.23	275.06	269.44	275.60
279.26	289.07	287.91	287.94	280.61	280.62	287.97	280.68	289.11	289.12
334.10	334.14	332.63	334.73	333.26	335.48	335.13	335.89	334.43	336.51
423.45	423.64	423.48	423.49	423.60	423.60	423.49	423.60	423.64	423.64

513.90	518.71	518.03	518.03	514.81	514.81	518.03	514.81	518.71	518.71
552.98	574.98	563.58	563.57	556.61	556.62	563.64	556.62	575.01	574.99
576.86	600.94	587.75	587.96	596.55	596.90	588.05	597.23	601.38	601.78
658.16	649.51	650.89	654.50	653.52	656.99	658.62	661.08	653.62	657.10
669.27	659.12	664.05	664.38	664.13	664.55	669.30	669.47	664.14	664.57
690.25	717.10	691.55	691.79	715.14	715.19	692.04	715.24	717.15	717.22
718.87	730.84	726.15	726.15	724.31	724.37	726.15	724.42	730.85	730.86
793.34	798.92	798.85	798.86	794.91	795.02	798.86	795.13	798.93	798.93
799.35	821.88	820.20	820.30	799.64	799.65	820.42	799.67	821.98	822.08
905.96	906.48	906.00	906.00	906.45	906.45	906.00	906.45	906.48	906.48
932.85	934.26	932.92	932.93	934.19	934.19	932.93	934.19	934.26	934.26
1363.46	1286.01	1320.48	1328.55	1320.47	1328.54	1363.47	1363.46	1320.48	1328.55
2412.23	2375.11	2401.26	2387.08	2401.26	2387.08	2412.23	2412.23	2401.26	2387.08
3806.97	3806.97	3806.97	3806.97	3806.97	3806.97	3806.97	3806.97	3806.97	3806.97
3820.10	3820.10	3820.10	3820.10	3820.10	3820.10	3820.10	3820.10	3820.10	3820.10
107.817	107.709	107.736	107.807	107.722	107.792	108.385	108.371	108.290	108.360
–33.595	–33.695	–33.631	–33.678	–33.613	–33.659	–33.587	–33.569	–33.604	–33.651

16

									
10.00	10.35	11.79	6.87	13.37	10.00	10.00	7.61	13.31	10.00
60.55	60.77	61.05	60.98	60.40	59.96	61.52	60.49	61.00	60.93
64.34	61.59	61.93	64.45	61.42	64.31	64.45	64.31	61.89	64.41
134.85	134.84	134.73	134.85	134.84	134.97	134.92	135.04	134.92	135.04
144.98	141.18	144.83	141.38	144.75	141.30	145.03	144.95	144.79	141.35
163.43	159.24	161.49	161.15	161.37	161.02	163.82	163.71	161.78	161.42
181.71	188.10	183.16	182.93	186.67	186.44	183.16	186.67	188.33	188.10
219.85	219.91	220.26	219.90	219.89	219.52	220.44	220.06	220.47	220.10
270.01	266.24	272.48	266.76	271.17	265.57	273.07	271.42	272.52	266.81
271.70	279.49	278.33	278.29	271.43	271.37	278.33	271.76	279.54	279.49
336.77	336.08	337.10	334.37	338.34	335.52	337.55	338.80	339.12	336.42
444.91	445.31	444.92	444.92	445.30	445.30	444.92	445.30	445.31	445.31
524.69	528.34	528.17	528.17	524.97	524.97	528.17	524.98	528.34	528.34
539.33	564.77	540.93	540.82	562.02	561.90	540.98	562.09	565.04	564.88
579.91	602.40	601.82	601.75	581.03	580.91	601.84	581.08	602.54	602.45
665.44	654.32	661.72	657.32	662.68	658.34	665.85	666.76	662.89	658.52
670.92	660.69	666.29	665.38	666.28	665.36	670.93	670.92	666.29	665.38
717.25	725.24	723.84	723.84	719.28	719.28	723.84	719.30	725.24	725.24
758.18	789.65	760.54	760.48	783.08	782.98	760.59	783.18	789.74	789.70
795.40	795.64	795.54	795.54	795.49	795.49	795.54	795.49	795.64	795.64
800.52	830.00	826.57	826.49	808.22	808.18	826.66	808.26	830.14	830.08
894.39	894.68	894.39	894.39	894.68	894.68	894.39	894.68	894.68	894.68
918.20	921.59	918.38	918.37	921.45	921.44	918.38	921.45	921.60	921.59
1366.75	1289.11	1332.00	1323.41	1332.00	1323.40	1366.76	1366.76	1332.01	1323.42
2414.30	2377.02	2389.06	2403.27	2389.07	2403.27	2414.30	2414.31	2389.07	2403.28
3813.30	3813.30	3813.30	3813.30	3813.30	3813.30	3813.30	3813.30	3813.30	3813.30
3816.32	3816.32	3816.32	3816.32	3816.32	3816.32	3816.32	3816.32	3816.32	3816.32
106.212	106.163	106.447	105.672	106.559	106.087	106.792	106.418	107.133	106.667
–33.686	–33.789	–33.774	–33.724	–33.752	–33.703	–33.680	–33.658	–33.746	–33.696

17

									
41.41	40.74	41.03	41.07	41.07	41.10	41.44	41.48	41.10	41.14
55.82	54.97	55.12	55.63	55.20	55.73	55.89	55.99	55.27	55.79
63.88	64.43	65.21	64.41	63.90	63.18	65.28	63.96	65.29	64.50
88.51	89.29	87.47	88.21	89.65	90.35	88.56	90.76	89.71	90.41
134.14	132.10	133.65	132.61	133.57	132.35	134.42	134.26	133.81	132.74
151.00	152.05	152.92	151.55	151.27	149.96	153.65	152.03	154.09	152.74
193.21	190.93	193.15	190.63	193.45	191.02	193.39	193.69	193.59	191.16
202.79	203.66	203.06	202.83	203.62	203.38	203.08	203.63	203.91	203.67
232.40	234.88	233.70	233.53	233.76	233.64	233.73	233.78	235.03	234.91
247.23	250.86	248.54	247.86	250.52	249.70	248.61	250.61	251.86	250.97
295.42	288.96	294.61	289.41	294.68	289.54	295.60	295.67	294.89	289.81
391.33	407.90	403.31	403.30	394.18	394.17	403.31	394.18	407.91	407.90
458.97	482.55	465.01	464.97	478.25	478.21	465.02	478.25	482.59	482.55
510.05	510.43	510.43	510.42	510.07	510.05	510.44	510.08	510.45	510.43
611.49	616.54	616.46	616.52	611.79	611.79	616.53	611.80	616.56	616.62
621.64	642.35	642.44	642.36	621.72	621.78	642.62	621.86	642.77	642.69

657.90	648.01	652.82	653.12	652.80	653.09	657.92	657.91	652.83	653.13
674.27	663.56	670.49	667.72	670.05	667.24	674.75	674.39	670.65	667.89
696.42	696.80	696.99	696.80	696.36	696.15	697.19	696.58	697.11	696.91
722.96	726.60	726.61	726.56	722.98	722.92	726.65	723.02	726.67	726.62
832.30	839.02	835.61	835.61	835.10	835.10	835.62	835.10	839.02	839.02
867.67	904.75	868.55	868.54	904.50	904.48	868.57	904.51	904.77	904.76
1104.09	1105.05	1104.15	1104.15	1104.99	1104.99	1104.15	1104.99	1105.06	1105.05
1380.39	1301.60	1343.99	1337.50	1343.99	1337.50	1380.39	1380.39	1343.99	1337.50
2420.23	2383.26	2397.12	2407.44	2397.13	2407.44	2420.23	2420.23	2397.13	2407.44
3833.50	3846.06	3846.06	3846.06	3833.50	3833.50	3846.06	3833.50	3846.06	3846.06
3909.79	3909.79	3909.79	3909.79	3909.79	3909.79	3909.79	3909.79	3909.79	3909.79
104.710	104.689	104.767	104.633	104.768	104.632	105.289	105.290	105.347	105.213
–33.646	–33.723	–33.711	–33.652	–33.719	–33.660	–33.620	–33.629	–33.694	–33.635

18

									
16.01	15.75	16.01	15.78	16.00	15.77	16.06	16.05	16.05	15.82
30.79	30.19	30.81	30.02	31.00	30.17	30.81	31.00	31.02	30.20
62.60	61.42	61.57	62.89	61.18	62.36	63.17	62.69	61.70	62.99
69.81	71.41	71.40	71.49	69.66	69.89	71.71	70.10	71.65	71.76
89.53	88.08	87.43	89.19	88.25	90.27	89.56	90.58	88.29	90.30
107.10	105.49	105.82	106.82	105.85	106.68	107.54	107.32	106.29	107.13
121.64	122.17	121.33	121.25	122.52	122.41	122.01	123.25	122.89	122.77
164.16	168.17	168.07	168.14	164.23	164.30	168.14	164.31	168.18	168.25
219.79	222.97	222.08	222.09	220.64	220.65	222.09	220.65	222.97	222.98
238.15	240.86	239.37	239.38	239.63	239.64	239.38	239.64	240.86	240.88
256.65	259.13	256.76	256.73	259.06	259.03	256.77	259.07	259.17	259.14
433.55	450.69	433.57	433.57	450.68	450.68	433.57	450.68	450.69	450.69
521.80	524.25	522.63	522.63	523.42	523.42	522.63	523.42	524.26	524.25
563.07	566.25	566.00	565.84	563.43	563.27	566.07	563.49	566.49	566.33
610.59	633.54	611.01	611.00	632.75	632.74	611.04	632.79	633.61	633.61
669.13	661.12	666.01	665.97	664.96	664.90	670.77	669.37	666.04	666.00
683.40	674.76	679.63	679.85	678.78	678.97	684.73	683.48	679.67	679.90
692.13	708.47	704.00	704.13	693.80	693.93	704.49	694.92	708.72	708.84
718.35	736.50	735.93	735.97	720.83	720.93	736.02	721.02	736.54	736.59
756.65	760.31	757.27	757.28	759.72	759.73	757.29	759.75	760.32	760.34
857.47	862.55	857.97	857.99	862.25	862.27	857.99	862.27	862.55	862.56
866.02	867.42	867.02	867.02	866.21	866.22	867.03	866.22	867.42	867.44
1106.57	1106.67	1106.61	1106.62	1106.63	1106.63	1106.62	1106.63	1106.67	1106.67
1387.91	1308.38	1347.19	1348.49	1347.19	1348.49	1387.91	1387.91	1347.19	1348.49
2414.24	2377.48	2397.62	2395.24	2397.62	2395.24	2414.24	2414.24	2397.62	2395.24
3805.39	3817.80	3805.39	3805.39	3817.80	3817.80	3805.39	3817.80	3817.80	3817.80
3867.78	3880.50	3880.50	3880.50	3867.78	3867.78	3880.50	3867.78	3880.50	3880.50
99.607	99.633	99.565	99.606	99.638	99.679	100.130	100.204	100.161	100.203
–34.132	–34.216	–34.152	–34.156	–34.194	–34.197	–34.085	–34.125	–34.146	–34.148

19

									
41.01	41.07	41.56	40.84	41.26	40.51	41.68	41.36	41.91	41.18
50.66	49.46	49.33	50.67	49.46	50.80	50.77	50.91	49.61	50.92
65.54	67.03	67.22	67.16	65.42	65.35	67.35	65.57	67.23	67.16
87.27	88.85	87.35	86.57	89.51	88.76	87.48	89.63	89.70	88.97
158.21	155.83	157.03	156.70	157.22	156.87	158.58	158.79	157.64	157.30
177.32	175.91	177.50	175.92	177.31	175.70	177.56	177.37	177.55	175.96
190.71	193.34	193.66	192.74	191.13	190.54	193.86	191.35	194.38	193.49
219.42	217.13	221.42	217.44	219.33	215.06	221.98	219.85	221.80	217.74
247.09	249.88	247.07	246.65	250.14	249.24	247.10	250.16	250.27	249.97
251.54	250.41	252.60	250.30	251.75	250.09	252.80	251.94	252.86	250.47
284.03	285.77	286.82	285.25	284.44	282.70	286.99	284.64	287.41	285.88
416.17	416.91	416.22	416.21	416.89	416.88	416.22	416.89	416.93	416.92
495.75	520.29	496.63	496.60	519.34	519.31	496.63	519.34	520.32	520.29
601.71	604.83	604.83	604.82	601.72	601.70	604.84	601.72	604.85	604.84
649.48	651.03	650.76	650.76	649.64	649.64	650.76	649.65	651.04	651.03
665.13	655.04	659.98	660.23	659.99	660.23	665.14	665.15	660.00	660.25
680.24	669.76	676.64	674.52	675.91	674.01	681.42	680.34	676.77	674.64
692.25	716.66	714.88	714.82	693.56	693.23	714.91	693.95	716.76	716.67
739.99	741.79	741.76	741.75	740.02	740.01	741.77	740.02	741.81	741.79
810.83	827.89	814.91	814.77	822.24	822.16	814.95	822.26	827.99	827.90

844.76	853.18	847.61	847.62	852.44	852.44	847.62	852.44	853.18	853.18
852.50	871.65	853.19	853.19	870.94	870.91	853.19	870.96	871.68	871.66
1102.37	1102.89	1102.40	1102.39	1102.87	1102.86	1102.40	1102.87	1102.90	1102.89
1386.95	1307.67	1349.80	1344.29	1349.80	1344.29	1386.96	1386.95	1349.80	1344.30
2422.46	2385.61	2400.39	2408.77	2400.39	2408.77	2422.46	2422.46	2400.39	2408.77
3828.02	3828.02	3828.02	3828.02	3828.02	3828.02	3828.02	3828.02	3828.02	3828.02
3846.80	3859.37	3859.37	3859.37	3846.80	3846.80	3859.37	3846.80	3859.37	3859.37
108.162	108.086	108.178	108.029	108.220	108.069	108.686	108.728	108.745	108.595
–33.929	–33.987	–33.963	–33.898	–34.017	–33.952	–33.864	–33.918	–33.952	–33.888

20

									
37.77	38.19	37.80	37.69	38.26	38.16	37.70	38.17	38.20	38.09
11.78	12.14	11.78	11.96	11.96	12.15	11.76	11.95	11.94	12.12
12.92	13.06	13.07	12.98	13.01	12.91	12.99	12.92	13.08	12.98
29.42	33.18	31.84	31.67	30.91	30.75	31.23	30.28	32.74	32.58
48.15	46.90	47.77	47.26	47.70	47.18	48.26	48.19	47.82	47.31
67.87	66.11	67.16	67.12	67.14	67.12	67.94	67.92	67.20	67.17
73.35	71.93	72.12	72.87	72.17	72.93	73.38	73.45	72.21	72.97
152.90	153.52	153.24	153.21	153.20	153.17	153.26	153.22	153.57	153.53
207.07	209.13	208.39	208.38	207.80	207.79	208.39	207.81	209.14	209.13
268.38	276.12	270.74	270.75	273.98	273.98	270.74	273.98	276.12	276.12
283.97	286.65	285.38	285.38	285.10	285.11	285.38	285.11	286.65	286.65
462.11	468.65	468.54	468.54	462.89	462.89	468.54	462.89	468.65	468.65
478.21	492.39	487.86	487.86	480.81	480.81	487.86	480.81	492.39	492.39
550.41	573.37	553.31	553.31	571.73	571.73	553.31	571.73	573.37	573.37
619.02	621.59	626.39	626.33	618.95	618.95	630.48	619.09	626.40	626.34
631.92	632.67	633.05	633.04	627.18	627.11	633.85	631.93	633.07	633.06
642.56	633.05	637.73	637.71	637.73	637.70	642.56	642.56	637.74	637.71
677.94	696.35	694.80	694.80	679.27	679.27	694.80	679.27	696.35	696.35
776.60	784.48	776.88	776.88	784.26	784.26	776.88	784.26	784.48	784.48
797.92	802.48	801.54	801.54	798.72	798.72	801.54	798.72	802.48	802.48
840.10	857.84	841.77	841.77	854.87	854.87	841.77	854.87	857.84	857.84
877.22	894.75	879.97	879.97	893.55	893.55	879.97	893.55	894.75	894.75
1083.72	1084.69	1083.84	1083.84	1084.57	1084.57	1083.84	1084.58	1084.70	1084.70
1372.40	1293.77	1332.86	1332.74	1332.86	1332.74	1372.40	1372.40	1332.86	1332.74
2435.90	2398.70	2417.75	2417.95	2417.75	2417.95	2435.90	2435.90	2417.75	2417.95
3671.02	3683.01	3683.01	3683.01	3671.02	3671.02	3683.01	3671.02	3683.01	3683.01
3779.45	3779.45	3779.45	3779.45	3779.45	3779.45	3779.45	3779.45	3779.45	3779.45
92.195	92.514	92.365	92.367	92.350	92.352	92.796	92.780	92.948	92.949
–34.251	–34.346	–34.299	–34.297	–34.302	–34.299	–34.208	–34.211	–34.259	–34.256

21

									
81.81	80.50	81.08	81.21	81.15	81.27	82.53	82.59	81.91	81.96
126.04	124.25	125.48	125.01	125.29	124.82	126.29	126.09	125.53	125.06
141.14	142.05	141.39	141.19	141.84	141.64	141.57	142.04	142.39	142.21
174.81	177.54	176.74	176.14	176.29	175.71	176.85	176.40	178.28	177.63
208.15	205.59	205.52	206.92	205.96	207.16	208.77	209.39	206.13	208.16
210.73	209.02	210.49	210.73	209.79	210.25	211.75	210.89	211.20	210.92
278.67	279.47	279.84	276.67	281.47	278.00	280.09	281.77	283.01	279.65
287.14	291.05	290.36	289.20	288.89	287.79	291.01	289.40	292.46	291.65
300.31	297.51	300.08	298.01	300.02	298.13	301.03	301.01	300.78	298.59
357.32	356.77	354.18	357.59	356.24	359.79	358.26	360.56	357.56	361.02
394.19	409.24	402.46	402.58	399.54	399.50	402.76	399.58	409.29	409.34
443.56	449.11	448.40	445.71	449.00	446.35	449.26	449.82	452.98	450.15
519.06	511.18	514.96	514.94	514.29	514.35	520.88	520.18	516.28	516.49
527.08	522.11	523.40	525.54	523.65	525.73	527.30	527.63	523.87	525.97
606.91	635.58	611.07	611.10	610.55	610.56	611.14	610.61	635.65	635.59
615.50	640.38	637.92	637.92	638.76	638.77	637.96	638.81	640.40	640.44
739.26	744.36	742.93	742.86	739.79	739.73	742.95	739.80	744.43	744.36
749.25	754.07	751.28	751.06	753.87	753.59	751.53	754.15	755.18	754.86
795.56	773.15	790.02	779.18	789.93	779.15	795.73	795.62	790.11	779.35
866.10	869.46	869.42	869.25	866.30	866.14	869.46	866.33	869.68	869.51
913.47	917.67	913.55	913.24	918.11	917.69	913.68	918.28	918.30	917.90
1017.59	984.33	1011.83	989.56	1011.95	989.76	1017.88	1017.97	1012.25	990.07
1092.60	1089.81	1092.34	1089.91	1092.34	1089.91	1092.60	1092.60	1092.34	1089.91
1107.30	1107.22	1107.23	1107.29	1107.23	1107.29	1107.31	1107.31	1107.24	1107.30

1886.16	1845.86	1846.26	1885.85	1846.26	1885.86	1886.16	1886.16	1846.26	1885.86
3797.98	3810.35	3810.34	3810.34	3797.99	3797.99	3810.34	3797.99	3810.35	3810.35
3829.66	3842.24	3829.67	3829.67	3842.24	3842.24	3829.67	3842.24	3842.24	3842.24
117.081	117.113	117.108	117.084	117.110	117.086	117.675	117.676	117.704	117.680
–32.968	–33.019	–33.025	–32.963	–33.024	–32.962	–32.936	–32.935	–32.994	–32.931

22

									
19.82	19.63	19.60	19.83	19.63	19.86	19.86	19.89	19.66	19.90
49.65	48.15	48.31	49.52	48.26	49.47	49.79	49.74	48.41	49.62
67.47	67.59	67.51	66.91	68.13	67.53	67.64	68.26	68.30	67.68
89.06	87.65	88.84	87.85	88.83	87.88	89.16	89.15	88.93	87.95
99.17	98.34	99.13	99.35	98.26	98.40	100.23	99.34	99.29	99.54
109.80	110.14	109.65	109.93	110.11	110.37	110.26	110.69	110.47	110.80
127.86	128.48	128.32	128.33	127.96	128.01	128.45	128.13	128.59	128.60
145.00	142.37	141.71	145.13	141.90	145.38	145.64	145.90	142.80	146.14
160.54	160.65	160.54	160.57	160.61	160.64	160.58	160.65	160.66	160.70
228.02	235.02	232.69	232.86	230.36	230.49	232.91	230.53	235.05	235.20
344.81	346.23	345.86	345.86	345.18	345.18	345.86	345.18	346.23	346.24
415.01	428.22	417.67	417.67	425.10	425.11	417.67	425.11	428.22	428.22
430.82	444.64	435.63	435.64	438.38	438.38	435.64	438.38	444.65	444.65
505.83	524.20	518.07	518.07	513.75	513.75	518.07	513.75	524.20	524.20
616.82	643.17	640.18	640.18	618.90	618.90	640.18	618.90	643.24	643.24
646.29	652.16	647.55	647.60	657.02	657.70	647.72	662.56	657.18	657.84
663.20	668.98	657.68	658.28	668.62	668.57	663.25	668.83	669.56	669.52
679.92	670.24	674.87	674.78	674.91	674.84	679.94	679.96	674.92	674.86
722.27	733.28	731.48	731.53	724.74	724.78	731.53	724.78	733.28	733.32
770.62	774.95	770.69	770.69	774.88	774.88	770.70	774.89	774.95	774.96
865.72	868.34	868.32	868.32	865.74	865.74	868.33	865.75	868.35	868.35
1012.10	1013.03	1012.59	1012.59	1012.55	1012.55	1012.60	1012.56	1013.04	1013.04
1044.58	1044.69	1044.62	1044.62	1044.65	1044.65	1044.63	1044.65	1044.69	1044.69
1390.21	1310.66	1348.80	1351.49	1348.80	1351.48	1390.21	1390.21	1348.80	1351.49
2420.42	2383.68	2404.89	2400.34	2404.89	2400.34	2420.42	2420.42	2404.89	2400.34
3729.01	3741.06	3741.07	3741.07	3729.00	3729.00	3741.08	3729.01	3741.07	3741.07
3887.12	3900.04	3887.12	3887.12	3900.04	3900.04	3887.12	3900.04	3900.04	3900.04
99.758	99.823	99.759	99.845	99.740	99.825	100.361	100.341	100.343	100.428
–33.931	–34.015	–33.962	–34.001	–33.947	–33.988	–33.911	–33.897	–33.926	–33.967

23

									
25.33	23.62	24.46	24.50	24.49	24.53	25.28	25.30	24.42	24.46
36.20	34.76	35.54	35.52	35.46	35.42	36.31	36.20	35.53	35.50
38.21	38.69	38.37	38.37	38.48	38.48	38.45	38.58	38.76	38.75
63.03	61.41	62.16	62.26	62.19	62.23	63.13	63.13	62.27	62.34
97.78	95.26	96.51	96.15	96.62	96.57	98.05	98.33	97.05	96.87
118.12	122.45	120.07	120.41	120.19	120.33	120.53	120.54	122.64	122.86
127.64	130.67	128.67	128.62	128.96	128.99	128.69	129.01	130.72	130.70
133.84	136.69	135.82	135.87	135.39	135.35	135.91	135.44	136.76	136.76
168.81	172.23	170.83	170.83	170.34	170.34	170.87	170.38	172.26	172.26
277.22	278.58	277.91	277.90	277.88	277.87	277.95	277.92	278.63	278.62
301.39	305.24	303.32	303.32	303.35	303.35	303.32	303.35	305.24	305.24
375.57	375.87	375.73	375.73	375.71	375.71	375.73	375.71	375.87	375.87
507.49	511.53	508.03	508.03	509.96	509.96	508.04	509.97	511.54	511.54
513.55	517.85	517.15	517.15	515.27	515.26	517.15	515.27	517.85	517.85
576.22	576.81	576.54	576.54	576.50	576.50	576.54	576.50	576.81	576.81
674.15	663.73	668.98	668.96	668.97	668.96	674.18	674.18	669.00	668.98
678.35	667.94	673.16	673.17	673.16	673.17	678.35	678.35	673.17	673.17
721.05	743.59	723.89	723.89	725.41	725.41	723.90	725.42	743.60	743.60
731.22	761.79	754.85	754.85	752.98	752.98	754.85	752.98	761.79	761.79
777.72	778.73	778.24	778.24	778.21	778.21	778.25	778.22	778.74	778.74
795.24	801.35	795.75	795.74	799.04	799.04	795.75	799.05	801.36	801.35
803.37	809.48	808.79	808.80	806.01	806.01	808.80	806.01	809.48	809.49
823.67	830.69	827.44	827.44	827.28	827.28	827.44	827.28	830.69	830.69
1392.78	1312.96	1352.55	1352.57	1352.55	1352.57	1392.78	1392.78	1352.55	1352.57
2417.33	2380.56	2399.53	2399.51	2399.53	2399.51	2417.34	2417.34	2399.53	2399.51
3852.60	3865.07	3854.99	3854.99	3854.00	3854.00	3855.00	3854.00	3865.07	3865.07
3857.19	3869.78	3867.32	3867.32	3868.33	3868.33	3867.32	3868.33	3869.78	3869.78
96.772	96.739	96.758	96.761	96.755	96.758	97.313	97.310	97.297	97.299

–33.955	–33.977	–33.967	–33.966	–33.966	–33.967	–33.901	–33.901	–33.913	–33.913
				24					
									
36.04	35.41	35.87	35.90	35.56	35.60	36.45	36.14	35.97	35.99
69.22	70.93	70.61	71.02	69.17	69.54	71.07	69.59	70.97	71.38
98.68	97.85	98.52	98.57	97.81	97.97	99.39	98.77	98.60	98.72
107.53	108.71	107.24	107.41	108.90	109.08	107.66	109.29	108.99	109.20
123.74	124.58	125.74	124.35	124.08	122.71	126.03	124.43	126.40	124.95
138.79	136.91	136.79	137.92	137.67	138.77	138.90	139.67	137.74	138.84
173.00	173.92	174.29	173.57	173.30	172.51	174.82	173.85	175.11	174.40
201.02	200.96	201.32	200.67	201.25	200.60	201.58	201.50	201.82	201.18
257.85	258.21	258.18	257.47	260.60	258.75	258.24	260.68	260.97	258.78
268.27	261.50	267.51	260.09	267.59	261.34	268.35	268.43	267.67	261.74
298.11	298.49	298.31	298.01	298.52	298.21	298.64	298.85	299.08	298.77
418.16	433.63	418.64	418.64	433.53	433.53	418.65	433.54	433.63	433.63
440.80	444.28	442.09	442.07	442.60	442.58	442.09	442.60	444.31	444.29
509.51	515.57	511.80	511.80	513.29	513.29	511.80	513.29	515.57	515.57
545.87	546.21	546.12	546.13	545.92	545.92	546.15	545.95	546.23	546.24
665.72	654.09	661.94	658.26	661.81	658.14	665.92	665.75	661.96	658.28
669.73	659.61	664.78	664.69	664.77	664.69	669.73	669.74	664.79	664.69
697.61	697.50	697.37	697.42	697.32	697.34	698.09	698.07	697.99	698.05
723.14	754.18	748.98	748.97	726.42	726.40	748.99	726.42	754.19	754.18
782.52	804.46	785.31	785.31	803.84	803.84	785.32	803.84	804.46	804.46
838.63	845.34	839.53	839.47	843.78	843.74	839.54	843.80	845.40	845.35
866.96	875.24	871.49	871.48	871.28	871.26	871.49	871.28	875.25	875.24
912.90	918.83	913.84	913.83	918.06	918.05	913.85	918.06	918.84	918.83
1375.49	1297.11	1339.46	1332.66	1339.46	1332.66	1375.49	1375.49	1339.46	1332.66
2416.58	2379.76	2393.06	2404.32	2393.06	2404.32	2416.58	2416.58	2393.06	2404.32
3812.46	3824.83	3824.83	3824.83	3812.46	3812.46	3824.83	3812.46	3824.83	3824.83
3881.29	3881.29	3881.29	3881.29	3881.29	3881.29	3881.29	3881.29	3881.29	3881.29
105.040	104.887	104.991	104.887	105.042	104.939	105.547	105.598	105.548	105.445
–33.404	–33.439	–33.429	–33.385	–33.459	–33.416	–33.340	–33.371	–33.396	–33.352

Supplementary Table S8. Frequencies (in cm^{-1}, top 18 rows below structures) and vibrational-torsional and rotational free energies (in kJ/mol, bottow two rows below structures) of different isotologues of Fe_2O_3–CO_2 clusters studied in the catalytic isotopic exchange reaction of CO_2 ($Fe_2{}^{16}O_3 + C^{18}O_2 \rightarrow Fe_2{}^{16}O_2{}^{18}O + C^{16}O^{18}O$ and $Fe_2{}^{16}O_3 + C^{16}O^{18}O \rightarrow Fe_2{}^{16}O_2{}^{18}O + C^{16}O_2$) were calculated using the rigid-rotor–harmonic-oscillator (RRHO) model at the ωB97X-V/def2-TZVPPD level of theory.

1									
									
42.55	41.39	42.37	41.47	42.4	41.51	42.64	42.68	42.51	41.59
83.31	81.75	83.05	81.41	83.61	81.93	83.40	83.94	83.70	82.05
136.33	137.84	137.84	137.38	136.86	136.42	137.8	136.83	138.27	137.83
151.92	141.57	145.25	148.19	145.34	148.26	151.48	151.56	144.85	147.82
226.80	228.16	227.32	227.35	227.59	227.61	227.35	227.61	228.16	228.18
257.67	254.76	255.97	256.32	256.01	256.42	258.20	258.26	256.53	256.87
304.06	302.01	304.68	302.77	304.43	302.47	306.57	306.26	306.32	304.33
332.69	338.18	335.33	335.06	334.90	334.64	336.39	336.03	339.14	338.98
417.67	410.36	411.53	416.66	411.04	416.20	418.63	418.15	412.01	417.12
482.78	501.15	490.97	490.66	490.50	490.16	491.22	490.72	501.71	501.38
569.57	596.03	583.67	583.88	584.43	584.58	583.90	584.61	596.04	596.25
646.83	639.70	644.19	642.49	644.16	642.48	647.32	647.29	644.55	642.87
721.01	697.78	703.48	715.76	703.56	715.83	721.31	721.49	703.85	716.13
801.69	839.90	801.78	801.62	814.82	814.95	802.11	814.96	840.33	840.17
815.02	854.82	854.34	854.40	840.50	840.30	854.41	840.73	854.83	854.86
1034.43	1033.86	1034.41	1034.42	1034.26	1034.27	1034.76	1034.59	1034.60	1034.60
1126.29	1071.06	1091.50	1104.82	1091.73	1105.06	1126.29	1126.49	1091.73	1105.06
1965.03	1931.03	1959.99	1936.72	1959.99	1936.73	1965.03	1965.03	1959.99	1936.73
46.241	46.013	46.129	46.145	46.116	46.131	46.757	46.743	46.629	46.645
–32.247	–32.333	–32.260	–32.308	–32.271	–32.318	–32.200	–32.210	–32.225	–32.271
2									
									
41.46	40.90	40.47	41.32	41.06	41.92	41.42	42.03	41.01	41.89
78.00	76.41	75.91	78.21	76.17	78.37	78.33	78.53	76.53	78.76
99.71	98.81	100.52	98.72	99.85	98.23	100.81	100.15	100.88	99.12
154.87	153.27	155.76	153.48	154.62	152.24	156.03	154.90	155.79	153.51
173.07	170.62	171.72	172.00	171.66	171.93	173.53	173.44	172.12	172.39
214.19	213.22	213.69	213.73	213.56	213.62	214.66	214.55	214.04	214.08
246.40	243.57	246.36	242.88	247.24	243.75	246.65	247.54	247.47	243.92
276.30	282.90	280.25	279.66	279.83	279.25	280.31	279.90	283.73	283.01
306.02	301.76	306.44	301.61	305.66	300.83	307.44	306.67	307.15	302.53
461.98	482.86	469.24	469.32	473.31	473.41	469.34	473.41	482.86	482.96
586.69	613.71	601.85	601.42	600.86	600.68	602.01	600.88	614.43	613.98
650.06	640.41	647.84	643.39	647.74	642.89	651.63	651.81	649.01	644.41
669.72	659.56	664.77	664.56	664.77	664.56	669.73	669.73	664.79	664.57
733.55	769.94	741.51	741.16	734.12	734.12	741.96	734.13	769.95	769.96
741.33	773.41	769.96	769.97	772.80	772.60	769.97	773.11	773.87	773.66
1088.39	1088.60	1088.43	1088.43	1088.56	1088.55	1088.44	1088.56	1088.61	1088.60
1361.95	1284.69	1327.53	1318.67	1327.55	1318.69	1361.96	1361.97	1327.55	1318.69
2410.33	2373.15	2384.73	2399.73	2384.74	2399.73	2410.33	2410.34	2384.74	2399.73
45.048	44.835	45.004	44.907	44.980	44.883	45.576	45.551	45.505	45.408
–32.869	–32.969	–32.935	–32.875	–32.964	–32.903	–32.828	–32.856	–32.925	–32.862
3									
									
43.61	42.91	43.53	42.56	44.00	43.02	43.64	44.13	44.04	43.04
77.06	75.28	77.25	74.82	77.42	75.06	77.32	77.52	77.74	75.36
103.00	102.01	101.80	103.78	101.44	103.27	104.04	103.53	102.28	104.23
155.17	153.74	153.94	156.14	152.63	154.93	156.40	155.21	153.97	156.17
173.06	170.53	171.94	171.67	171.88	171.62	173.51	173.42	172.33	172.07

214.27	213.40	213.87	213.81	213.75	213.68	214.75	214.63	214.22	214.17
246.09	243.36	242.64	246.06	243.52	246.95	246.34	247.23	243.69	247.18
276.71	283.21	280.00	280.64	279.59	280.22	280.71	280.30	283.33	284.11
307.23	302.99	302.83	307.67	302.01	306.86	308.68	307.88	303.76	308.39
463.73	484.74	471.05	470.98	475.28	475.19	471.06	475.29	484.84	484.74
587.10	614.12	601.92	602.35	601.03	601.20	602.51	601.23	614.40	614.84
650.18	640.51	643.48	647.93	643.01	647.86	651.73	651.93	644.51	649.11
669.82	659.65	664.64	664.87	664.65	664.88	669.83	669.84	664.66	664.89
733.83	770.34	741.16	741.51	734.48	734.48	741.96	734.49	770.36	770.35
741.41	773.40	770.36	770.35	772.60	772.80	770.36	773.11	773.65	773.86
1088.73	1088.94	1088.77	1088.78	1088.90	1088.90	1088.78	1088.91	1088.95	1088.95
1362.20	1284.91	1318.90	1327.76	1318.92	1327.78	1362.20	1362.21	1318.92	1327.78
2410.96	2373.76	2400.34	2385.36	2400.34	2385.37	2410.96	2410.96	2400.34	2385.37
45.212	44.993	45.070	45.166	45.044	45.139	45.740	45.714	45.570	45.665
–32.867	–32.969	–32.873	–32.935	–32.903	–32.964	–32.828	–32.856	–32.862	–32.925

4

									
31.76	33.88	32.81	33.10	32.50	32.78	32.64	32.33	33.42	33.71
12.46	12.38	12.41	12.44	12.41	12.44	12.50	12.49	12.44	12.47
22.16	22.97	22.72	22.55	22.57	22.41	22.58	22.45	23.00	22.84
40.23	40.11	40.23	39.64	40.69	40.09	40.25	40.71	40.72	40.11
51.51	50.15	50.30	51.39	50.26	51.35	51.65	51.60	50.39	51.50
87.24	85.53	86.62	86.31	86.45	86.15	87.49	87.32	86.71	86.40
117.54	118.17	117.82	117.73	117.97	117.89	117.95	118.11	118.38	118.29
285.10	294.10	289.73	289.73	289.71	289.71	289.73	289.71	294.11	294.10
355.06	360.86	357.06	357.06	358.75	358.75	357.06	358.75	360.86	360.86
477.85	499.23	482.17	482.17	492.41	492.41	482.17	492.41	499.23	499.23
542.61	564.89	560.94	560.94	548.99	548.99	560.94	548.99	564.89	564.89
629.99	620.14	625.11	625.07	625.11	625.07	630.00	630.00	625.11	625.07
642.43	632.70	637.59	637.58	637.59	637.58	642.43	642.43	637.59	637.58
769.91	810.18	808.16	808.16	771.16	771.16	808.16	771.16	810.17	810.17
832.20	872.96	833.10	833.10	872.92	872.92	833.10	872.92	872.96	872.96
1079.12	1079.28	1079.23	1079.22	1079.18	1079.18	1079.23	1079.18	1079.29	1079.29
1372.46	1293.83	1332.90	1332.81	1332.90	1332.81	1372.46	1372.46	1332.90	1332.81
2436.18	2398.98	2418.05	2418.22	2418.05	2418.22	2436.18	2436.18	2418.05	2418.22
31.501	31.681	31.585	31.589	31.599	31.603	32.046	32.060	32.141	32.146
–33.620	–33.712	–33.670	–33.660	–33.670	–33.662	–33.567	–33.567	–33.619	–33.609

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